

Second Edition

HANDBOOK OF

Physical-Chemical Properties and Environmental Fate for Organic Chemicals

Volume I

Introduction and Hydrocarbons

Volume II

Halogenated Hydrocarbons

Volume III

Oxygen Containing Compounds

Volume IV

Nitrogen and Sulfur Containing Compounds
and Pesticides

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Preface

This handbook is a compilation of environmentally relevant physical-chemical data for similarly structured groups of chemical substances. These data control the fate of chemicals as they are transported and transformed in the multimedia environment of air, water, soils, sediments, and their resident biota. These fate processes determine the exposure experienced by humans and other organisms and ultimately the risk of adverse effects. The task of assessing chemical fate locally, regionally, and globally is complicated by the large (and increasing) number of chemicals of potential concern; by uncertainties in their physical-chemical properties; and by lack of knowledge of prevailing environmental conditions such as temperature, pH, and deposition rates of solid matter from the atmosphere to water, or from water to bottom sediments. Further, reported values of properties such as solubility are often in conflict. Some are measured accurately, some approximately, and some are estimated by various correlation schemes from molecular structures. In some cases, units or chemical identity are wrongly reported. The user of such data thus has the difficult task of selecting the “best” or “right” values. There is justifiable concern that the resulting deductions of environmental fate may be in substantial error. For example, the potential for evaporation may be greatly underestimated if an erroneously low vapor pressure is selected.

To assist the environmental scientist and engineer in such assessments, this handbook contains compilations of physical-chemical property data for over 1000 chemicals. It has long been recognized that within homologous series, properties vary systematically with molecular size, thus providing guidance about the properties of one substance from those of its homologs. Where practical, plots of these systematic property variations can be used to check the reported data and provide an opportunity for interpolation and even modest extrapolation to estimate unmeasured properties of other substances. Most handbooks treat chemicals only on an individual basis and do not contain this feature of chemical-to-chemical comparison, which can be valuable for identifying errors and estimating properties. This most recent edition includes about 1250 compounds and contains about 30 percent additional physical-chemical property data. There is a more complete coverage of PCBs, PCDDs, PCDFs, and other halogenated hydrocarbons, especially brominated and fluorinated substances that are of more recent environmental concern. Values of the physical-chemical properties are generally reported in the literature at a standard temperature of 20 or 25°C. However, environmental temperatures vary considerably, and thus reliable data are required on the temperature dependence of these properties for fate calculations. A valuable enhancement to this edition is the inclusion of extensive measured temperature-dependent data for the first time. The data focus on water solubility, vapor pressure, and Henry’s law constant but include octanol/water and octanol/air partition coefficients where available. They are provided in the form of data tables and correlation equations as well as graphs.

We also demonstrate in [Chapter 1](#) how the data may be taken a stage further and used to estimate likely environmental partitioning tendencies, i.e., how the chemical is likely to become distributed between the various media that comprise our biosphere. The results are presented numerically and pictorially to provide a visual impression of likely environmental behavior. This will be of interest to those assessing environmental fate by confirming the general fate characteristics or behavior profile. It is, of course, only possible here to assess fate in a “typical” or “generic” or “evaluative” environment. No claim is made that a chemical will behave in this manner in all situations, but this assessment should reveal the broad characteristics of behavior. These evaluative fate assessments are generated using simple fugacity models that flow naturally from the compilations of data on physical-chemical properties of relevant chemicals. Illustrations of estimated environmental fate are given in Chapter 1 using Levels I, II, and III mass balance models. These and other models are available for downloading gratis from the website of the Canadian Environmental Modelling Centre at Trent University (www.trent.ca/cemc).

It is hoped that this new edition of the handbook will be of value to environmental scientists and engineers and to students and teachers of environmental science. Its aim is to contribute to better assessments of chemical fate in our multimedia environment by serving as a reference source for environmentally relevant physical-chemical property data of classes of chemicals and by illustrating the likely behavior of these chemicals as they migrate throughout our biosphere.

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Much credit goes to the team of professionals at CRC Press/Taylor & Francis Group who worked on this second edition. Especially important were Dr. Fiona Macdonald, Publisher, Chemistry; Dr. Janice Shackleton, Input Supervisor; Patrica Roberson, Project Coordinator; Elise Oranges and Jay Margolis, Project Editors; and Marcela Peres, Production Assistant.

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Biographies

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His awards include the SETAC Founders Award, the Honda Prize for Eco-Technology, the Order of Ontario, and the Order of Canada. He has served on the editorial boards of several journals and is a member of SETAC, the American Chemical Society, and the International Association of Great Lakes Research.

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1.1 THE INCENTIVE

It is believed that there are some 50,000 to 100,000 chemicals currently being produced commercially in a range of quantities with approximately 1000 being added each year. Most are organic chemicals, and many are pesticides and biocides designed to modify the biotic environment. Of these, perhaps 1000 substances are of significant environmental concern because of their presence in detectable quantities in various components of the environment, their toxicity, their tendency to bioaccumulate, their persistence and their potential to be transported long distances. Some of these chemicals, including pesticides, are of such extreme environmental concern that international actions have been taken to ensure that all production and use should cease, i.e., as a global society we should elect not to synthesize or use these chemicals. They should be “sunsetting.” PCBs, “dioxins” and DDT are examples. A second group consists of less toxic and persistent chemicals which are of concern because they are used or discharged in large quantities. They are, however, of sufficient value to society that their continued use is justified, but only under conditions in which we fully understand and control their sources, fate and the associated risk of adverse effects. This understanding is essential if society is to be assured that there is negligible risk of adverse ecological or human health effects. Other groups of more benign chemicals can presumably be treated with less rigor.

A key feature of this “cradle-to-grave” approach to chemical management is that society must improve its skills in assessing chemical fate in the environment. We must better understand where chemicals originate, how they migrate in, and between, the various media of air, water, soils, sediments and their biota which comprise our biosphere. We must understand how these chemicals are transformed by chemical and biochemical processes and, thus, how long they will persist in the environment. We must seek a fuller understanding of the effects that they will have on the multitude of interacting organisms that occupy these media, including ourselves.

It is now clear that the fate of chemicals in the environment is controlled by a combination of three groups of factors. First are the prevailing environmental conditions such as temperatures, flows and accumulations of air, water and solid matter and the composition of these media. Second are the properties of the chemicals which influence partitioning and reaction tendencies, i.e., the extent to which the chemical evaporates or associates with sediments, and how fast the chemical is eventually destroyed by conversion to other chemical species. Third are the patterns of use, into which compartments the substance is introduced, whether introduction is episodic or continuous and in the case of pesticides how and with which additives the active ingredient is applied.

In recent decades there has emerged a discipline within environmental science concerned with increasing our understanding of how chemicals behave in our multimedia environment. It has been termed environmental chemistry or “chemodynamics.” Practitioners of this discipline include scientists and engineers, students and teachers who attempt to measure, assess and predict how this large number of chemicals will behave in laboratory, local, regional and global environments. These individuals need data on physical-chemical and reactivity properties, as well as information on how these properties translate into environmental fate. This handbook provides a compilation of such data and outlines how to use them to estimate the broad features of environmental fate. It does so for classes or groups of chemicals, instead of the usual approach of treating chemicals on an individual basis. This has the advantage that systematic variations in properties with molecular structure can be revealed and exploited to check reported values, interpolate and even extrapolate to other chemicals of similar structure.

With the advent of inexpensive and rapid computation there has been a remarkable growth of interest in this general area of quantitative structure-property relationships (QSPRs). The ultimate goal is to use information about chemical structure to deduce physical-chemical properties, environmental partitioning and reaction tendencies, and even uptake and effects on biota. The goal is far from being fully realized, but considerable progress has been made. In this series of handbooks we have adopted a simple and well-tried approach of using molecular structure to deduce a molar volume, which in turn is related to physical-chemical properties. In the case of pesticides, the application of QSPR approaches is complicated by the large number of chemical classes, the frequent complexity of molecules and the lack of experimental data. Where there is a sufficient number of substances in each class or homologous series QSPRs are presented, but in some cases there is a lack of data to justify them. QSPRs based on other more complex molecular descriptors are, of course, widely available, especially in the proceedings of the biennial QSAR conferences.

Regrettably, the scientific literature contains a great deal of conflicting data, with reported values often varying over several orders of magnitude. There are some good, but more not-so-good reasons for this lack of accuracy. Many of these properties are difficult to measure because they involve analyzing very low concentrations of 1 part in 10^9 or 10^{12} . For many purposes an approximate value is adequate. There may be a mistaken impression that if a vapor pressure is low, as is the case with DDT, it is not important. DDT evaporates appreciably from solution in water, despite its low vapor pressure, because of its low solubility in water. In some cases the units are reported incorrectly. There may be uncertainties about temperature or pH. In other cases the chemical is wrongly identified. Errors tend to be perpetuated

by repeated citation. The aim of this handbook is to assist the user to identify such problems, provide guidance when selecting appropriate values and where possible determine their temperature dependence.

The final aspect of chemical fate treated in this handbook is the depiction or illustration of likely chemical fate. This is done using multimedia “fugacity” models as described later in this chapter. The aim is to convey an impression of likely environmental partitioning and transformation characteristics, i.e., a “behavior profile.” A fascinating feature of chemodynamics is that chemicals differ so greatly in their behavior. Some, such as chloroform, evaporate rapidly and are dissipated in the atmosphere. Others, such as DDT, partition into the organic matter of soils and sediments and the lipids of fish, birds and mammals. Phenols and carboxylic acids tend to remain in water where they may be subject to fairly rapid transformation processes such as hydrolysis, biodegradation and photolysis. By entering the physical-chemical data into a model of chemical fate in a generic or evaluative environment, it is possible to estimate the likely general features of the chemical’s behavior and fate. The output of these calculations can be presented numerically and pictorially.

In summary, the aim of this series of handbooks is to provide a useful reference work for those concerned with the assessment of the fate of existing and new chemicals in the environment.

1.2 PHYSICAL-CHEMICAL PROPERTIES

1.2.1 THE KEY PHYSICAL-CHEMICAL PROPERTIES

In this section we describe the key physical-chemical properties and discuss how they may be used to calculate partition coefficients for inclusion in mass balance models. Situations in which data require careful evaluation and use are discussed.

The major differences between behavior profiles of organic chemicals in the environment are attributable to their physical-chemical properties. The key properties are recognized as solubility in water, vapor pressure, the three partition coefficients between air, water and octanol, dissociation constant in water (when relevant) and susceptibility to degradation or transformation reactions. Other essential molecular descriptors are molar mass and molar volume, with properties such as critical temperature and pressure and molecular area being occasionally useful for specific purposes. A useful source of information and estimation methods on these properties is the handbook by Boethling and Mackay (2000).

Chemical identity may appear to present a trivial problem, but most chemicals have several names, and subtle differences between isomers (e.g., *cis* and *trans*) may be ignored. The most commonly accepted identifiers are the IUPAC name and the Chemical Abstracts System (CAS) number. More recently, methods have been sought of expressing the structure in line notation form so that computer entry of a series of symbols can be used to define a three-dimensional structure. For environmental purposes the SMILES (Simplified Molecular Identification and Line Entry System, Anderson et al. 1987) is favored, but the Wisniewski Line Notation is also quite widely used.

Molar mass or molecular weight is readily obtained from structure. Also of interest for certain purposes are molecular volume and area, which may be estimated by a variety of methods.

When selecting physical-chemical properties or reactivity classes the authors have been guided by:

1. The acknowledgment of previous supporting or conflicting values,
2. The method of determination,
3. The perception of the objectives of the authors, not necessarily as an indication of competence, but often as an indication of the need of the authors to obtain accurate values, and
4. The reported values for structurally similar, or homologous compounds.

The literature contains a considerable volume of “calculated” data as distinct from experimental data. We have generally not included such data because they may be of questionable reliability. In some cases an exception has been made when no experimental data exist and the calculation is believed to provide a useful and reliable estimate.

1.2.2 PARTITIONING PROPERTIES

Solubility in water and vapor pressure are both “saturation” properties, i.e., they are measurements of the maximum capacity that a solvent phase has for dissolved chemical. Vapor pressure P (Pa) can be viewed as a “solubility in air,” the corresponding concentration C (mol/m³) being P/RT where R is the ideal gas constant (8.314 J/mol.K) and T is absolute temperature (K). Although most chemicals are present in the environment at concentrations well below saturation, these concentrations are useful for estimating air-water partition coefficients as ratios of saturation values. It is usually assumed

that the same partition coefficient applies at lower sub-saturation concentrations. Vapor pressure and solubility thus provide estimates of the air-water partition coefficient K_{AW} , the dimensionless ratio of concentration in air (mass/volume) to that in water. The related Henry's law constant H (Pa.m³/mol) is the ratio of partial pressure in air (Pa) to the concentration in water (mol/m³). Both express the relative air-water partitioning tendency.

When solubility and vapor pressure are both low in magnitude and thus difficult to measure, it is preferable to measure the air-water partition coefficient or Henry's law constant directly. It is noteworthy that atmospheric chemists frequently use K_{WA} , the ratio of water-to-air concentrations. This may also be referred to as the Henry's law constant.

The octanol-water partition coefficient K_{OW} provides a direct estimate of hydrophobicity or of partitioning tendency from water to organic media such as lipids, waxes and natural organic matter such as humin or humic acid. It is invaluable as a method of estimating K_{OC} , the organic carbon-water partition coefficient, the usual correlation invoked being that of Karickhoff (1981)

$$K_{OC} = 0.41 K_{OW}$$

Seth et al. (1999) have suggested that a better correlation is

$$K_{OC} = 0.35 K_{OW}$$

and that the error limits on K_{OC} resulting from differences in the nature of organic matter are a factor of 2.5 in both directions, i.e. the coefficient 0.35 may vary from 0.14 to 0.88.

K_{OC} is an important parameter which describes the potential for movement or mobility of pesticides in soil, sediment and groundwater. Because of the structural complexity of these agrochemical molecules, the above simple relationship which considers only the chemical's hydrophobicity may fail for polar and ionic compounds. The effects of pH, soil properties, mineral surfaces and other factors influencing sorption become important. Other quantities, K_D (sorption partition coefficient to the whole soil on a dry weight basis) and K_{OM} (organic matter-water partition coefficient) are also commonly used to describe the extent of sorption. K_{OM} is often estimated as $0.56 K_{OC}$, implying that organic matter is 56% carbon.

K_{OW} is also used to estimate equilibrium fish-water bioconcentration factors K_B , or BCF using a correlation similar to that of Mackay (1982)

$$K_B = 0.05 K_{OW}$$

where the term 0.05 corresponds to a lipid content of the fish of 5%. The basis for this correlation is that lipids and octanol display very similar solvent properties, i.e., K_{LW} (lipid-water) and K_{OW} are equal. If the rate of metabolism is appreciable, equilibrium will not apply and the effective K_B will be lower to an extent dictated by the relative rates of uptake and loss by metabolism and other clearance processes. If uptake is primarily from food, the corresponding bioaccumulation factor also depends on the concentration of the chemical in the food.

For dissociating chemicals it is essential to quantify the extent of dissociation as a function of pH using the dissociation constant pK_a . The parent and ionic forms behave and partition quite differently; thus pH and the presence of other ions may profoundly affect chemical fate. This is discussed later in more detail in Section 1.2.4.

The octanol-air partition coefficient K_{OA} was originally introduced by Paterson et al. (1991) for describing the partitioning of chemicals from the atmosphere to foliage. It has proved invaluable for this purpose and for describing partitioning to aerosol particles and to soils. It can be determined experimentally using the technique devised by Harner and Mackay (1995). Although there are fewer data for K_{OA} than for K_{OW} , its use is increasing and when available, data are included in this handbook. K_{OA} has been applied to several situations involving partitioning of organic substances from the atmosphere to solid or liquid phases. Finizio et al. (1997) have shown that K_{OA} is an excellent descriptor of partitioning to aerosol particles, while McLachlan et al. (1995) and Tolls and McLachlan (1994) have used it to describe partitioning to foliage, especially grasses. Hippelein and McLachlan (1998) have used K_{OA} to describe partitioning between air and soil.

An attractive feature of K_{OA} is that it can replace the liquid or supercooled liquid vapor pressure in a correlation. K_{OA} is an experimentally measurable or accessible quantity, whereas the supercooled liquid vapor pressure must be estimated from the solid vapor pressure, the melting point and the entropy of fusion. The use of K_{OA} thus avoids the potentially erroneous estimation of the fugacity ratio, i.e., the ratio of solid and liquid vapor pressures. This is especially important for solutes with high melting points and, thus, low fugacity ratios.

The availability of data on K_{AW} , K_{OW} and K_{OA} raises the possibility of a consistency test. At first sight it appears that K_{OA} should equal K_{OW}/K_{AW} , and indeed this is often approximately correct. The difficulty is that in the case of K_{AW} , the water phase is pure water, and for K_{OA} the octanol phase is pure “dry” octanol. For K_{OW} , the water phase inevitably contains dissolved octanol, and the octanol phase contains dissolved water and is thus not “dry.” Beyer et al. (2002) and Cole and Mackay (2000) have discussed this issue.

If the partition coefficients are regarded as ratios of solubilities S (mol/m³)

$$K_{AW} = S_A/S_W \text{ or } \log K_{AW} = \log S_A - \log S_W$$

$$K_{OA} = S_O/S_A \text{ or } \log K_{OA} = \log S_O - \log S_A$$

$$K_{OW} = S_{OW}/S_{WO} \text{ or } \log K_{OW} = \log S_{OW} - \log S_{WO}$$

where subscript A applies to the gas phase or air, W to pure water, O to dry octanol, OW to “wet” octanol and WO to water saturated with octanol. It follows that the assumption that K_{OA} is K_{OW}/K_{AW} is essentially that

$$(\log S_{OW} - \log S_O) - (\log S_{WO} - \log S_W) = 0$$

$$\text{or } S_{OW} S_W / (S_O \cdot S_{WO}) \text{ is } 1.0$$

This is obviously satisfied when S_{OW} equals S_O and S_{WO} equals S_W , but this is not necessarily valid, especially when K_{OW} is large.

There are apparently two sources of this effect. The molar volume of water changes relatively little as a result of the presence of a small quantity of dissolved octanol, however the quantity of dissolved water in the octanol is considerable, causing a reduction in molar volume of the octanol phase. The result is that even if activity coefficients are unaffected, $\log S_O/S_W$ will be about 0.1 units less than that of $\log K_{OW}$. Effectively, the octanol phase “swells” as a result of the presence of water, and the concentration is reduced. In addition, when $\log K_{OW}$ exceeds 4.0 there is an apparent effect on the activity coefficients which causes $\log (S_O/S_W)$ to increase. This increase can amount to about one log unit when $\log K_{OW}$ is about 8. A relatively simple correlation based on the analysis by Beyer et al. (2002) (but differing from their correlation) is that

$$\log K_{OA} = \log (K_{OW}/K_{AW}) - 0.10 + [0.30 \log K_{OW} - 1.20]$$

when $\log K_{OW}$ is 4 or less the term in square brackets is ignored

when $\log K_{OW}$ is 4 or greater that term is included

1.2.3 TEMPERATURE DEPENDENCE

All partitioning properties change with temperature. The partition coefficients, vapor pressure, K_{AW} and K_{OA} , are more sensitive to temperature variation because of the large enthalpy change associated with transfer to the vapor phase. The simplest general expression theoretically based temperature dependence correlation is derived from the integrated Clausius-Clapeyron equation, or van't Hoff form expressing the effect of temperature on an equilibrium constant K_p ,

$$R \cdot \ln K_p = A_o - B/T$$

which can be rewritten as

$$\ln (\text{Property}) = A - \Delta H/RT$$

where A_o , B and A are constants, ΔH is the enthalpy of the phase change, i.e., evaporation from pure state for vapor pressure, dissolution from pure state into water for solubility, and for air-water transition in the case of Henry's law constant.

The fit is improved by adding further coefficients in additional terms. The variation of these equilibrium constants with temperature can be expressed by (Clarke and Glew 1966),

$$R \cdot \ln K_p(T) = A + B/T + C \cdot \ln T + DT + ET^2 + FT^3 + \dots$$

where A, B, C, D, E, F are constants.

There have been numerous approaches to describing the temperature dependence of the properties. For aqueous solubility, the most common expression is the van't Hoff equation of the form (Hildebrand et al. 1970):

$$d(\ln x)/d(1/T) = -\Delta_{\text{sol}}H/R$$

where x is the mole fraction solubility, T is the temperature in K, R is the ideal gas constant, and $\Delta_{\text{sol}}H$ is the enthalpy of solution of the solute. The enthalpy of solution can be considered as the sum of various contributions such as cavity formation and interactions between solute-solute or solute-solvent as discussed by Bohon and Claussen (1951), Arnold et al. (1958), Owen et al. (1986) and many others. Assuming the enthalpy of solution is constant over a narrow temperature range, integrating gives,

$$\ln x = -\Delta_{\text{sol}}H/RT + C$$

where C is a constant.

The relation between aqueous solubility and temperature is complicated because of the nature of the interactions between the solute and water structure. The enthalpy of solution can vary greatly with temperature, e.g., some liquid aromatic hydrocarbons display a minimum solubility corresponding to zero enthalpy of solution between 285 and 320 K. For instance, benzene has a minimum solubility at 291 K (Bohon and Claussen 1951, Arnold et al. 1958, Shaw 1989a) and alkylbenzenes display similar behavior (Shaw 1989a,b, Owens 1986). As is illustrated later in [chapter 3](#), solid aromatic hydrocarbons show a slight curvature in plots of logarithm of mole fraction solubility versus reciprocal absolute temperature. For narrow ranges in environmental temperatures, the enthalpy of solution may be assumed to be constant, and the linear van't Hoff plot of $\ln x$ versus $1/T$ is often used (Dickhut et al. 1986). Other relationships such as quadratic or cubic equations have been reported (May et al. 1978), and polynomial series (Clarke and Glew 1966, May et al. 1983, Owens et al. 1986) have been used when the data justify such treatment.

Equations relating vapor pressure to temperature are usually based on the two-parameter Clausius-Clapeyron equation,

$$d(\ln P^S)/dT = \Delta_{\text{vap}}H/RT^2$$

where P^S is vapor pressure, $\Delta_{\text{vap}}H$ is the enthalpy of vaporization. Again assuming $\Delta_{\text{vap}}H$ is constant over a narrow range of temperature, this gives,

$$\ln P^S = -\Delta_{\text{vap}}H/RT + C$$

which can be rewritten as the Clapeyron equation

$$\log P^S = A - B/T$$

This can be empirically modified by introducing additional parameters to give the three-parameter Antoine equation by replacing T with $(T + C)$, where C is a constant, which is the most common vapor pressure correlation used to represent experimental data (Zwolinski and Wilhoit 1971, Boublik et al. 1984, Stephenson and Malanowski 1987, and other handbooks).

$$\log P^S = A - B/(t + C)$$

where A, B and C are constants and t often has units of °C.

Other forms of vapor pressure equations, such as Cox equation (Osborn and Douslin 1974, Chao et al. 1983), Chebyshev polynomial (Ambrose 1981), Wagner's equation (Ambrose 1986), have also been widely used. Although

the enthalpy of vaporization varies with temperature, for the narrow environmental temperature range considered in environmental conditions, it is often assumed to be constant, for example, for the more volatile monoaromatic hydrocarbons and the less volatile polynuclear aromatic hydrocarbons.

The van't Hoff equation also has been used to describe the temperature effect on Henry's law constant over a narrow range for volatile chlorinated organic chemicals (Ashworth et al. 1988) and chlorobenzenes, polychlorinated biphenyls, and polynuclear aromatic hydrocarbons (ten Hulscher et al. 1992, Alaei et al. 1996). Henry's law constant can be expressed as the ratio of vapor pressure to solubility, i.e., p/c or p/x for dilute solutions. Note that since H is expressed using a volumetric concentration, it is also affected by the effect of temperature on liquid density whereas k_H using mole fraction is unaffected by liquid density (Tucker and Christian 1979), thus

$$\ln (k_H/\text{Pa}) = \ln [(P^S/\text{Pa})/x];$$

or,
$$\ln (H/\text{Pa}\cdot\text{m}^3\cdot\text{mol}^{-1}) = \ln [(P^S/\text{Pa})/(C_w^S/\text{mol}\cdot\text{m}^{-3})];$$

where C_w^S is the aqueous solubility.

By substituting equations for vapor pressure and solubility, the temperature dependence equation for Henry's law constant can be obtained, as demonstrated by Glew and Robertson (1956), Tsonopoulos and Wilson (1983), Heiman et al. (1985), and ten Hulscher et al. (1991).

Care must be taken to ensure that the correlation equations are applied correctly, especially since the units of the property, the units of temperature and whether the logarithm is base e or base 10. The equations should not be used to extrapolate beyond the stated temperature range.

1.2.4 TREATMENT OF DISSOCIATING COMPOUNDS

In the case of dissociating or ionizing organic chemicals such as organic acids and bases, e.g., phenols, carboxylic acids and amines, it is desirable to calculate the concentrations of ionic and non-ionic species, and correct for this effect. A number of authors have discussed and reviewed the effect of pH and ionic strength on the distribution of these chemicals in the environment, including Westall et al. (1985), Schwarzenbach et al. (1988), Jafvert et al. (1990), Johnson and Westall (1990) and the text by Schwarzenbach, Gschwend and Imboden (1993).

A simple approach is suggested here for estimating the effect of pH on properties and environmental fate using the phenols as an example. A similar approach can be used for bases. The extent of dissociation is characterized by the acid dissociation constant, K_a , expressed as its negative logarithm, $\text{p}K_a$, which for most chloro-phenolic compounds range between 4.75 for pentachlorophenol and 10.2 to phenol, and between 10.0 and 10.6 for the alkylphenols. The dissolved concentration in water is thus the sum of the undissociated, parent or protonated compound and the dissociated phenolate ionic form. When the $\text{p}K_a$ exceeds pH by 2 or more units, dissociation is 1% or less and for most purposes is negligible. The ratio of ionic to non-ionic or dissociated to undissociated species concentrations is given by,

$$\text{ionic/non-ionic} = 10^{(\text{pH}-\text{p}K_a)} = I$$

The fraction ionic x_I is $I/(1 + I)$. The fraction non-ionic x_N is $1/(1 + I)$. For compounds such as pentachlorophenol in which pH generally exceeds $\text{p}K_a$, I and x_I can be appreciable, and there is an apparently enhanced solubility (Horvath and Getzen 1985, NRCC 1982, Yoshida et al. 1987, Arcand et al. 1995, Huang et al. 2000). There are other reports of pH effects on octanol-water partition coefficient (Kaiser and Valdmann 1982, Westall et al. 1985, Lee et al. 1990, Smejtek and Wang 1993), soil sorption behavior (Choi and Amoine 1974, Lee et al. 1990, Schellenberg et al. 1984, Yoshida et al. 1987, Lee et al. 1990), bioconcentration and uptake kinetics to goldfish (Stehly and Hayton 1990) and toxicity to algae (Smith et al. 1987, Shigeoka et al. 1988).

The following treatment has been suggested by Shiu et al. (1994) and is reproduced briefly below. The simplest, "first-order" approach is to take into account the effect of dissociation by deducing the ratio of ionic to non-ionic species I , the fraction ionic x_I and the fraction non-ionic x_N for the chemical at both the pH and temperature of experimental data determination (I_D , x_{ID} , x_{ND}) and at the pH and temperature of the desired environmental simulation (I_E , x_{IE} , x_{NE}). It is assumed that dissociation takes place only in aqueous solution, not in air, organic carbon, octanol or lipid phases. Some ions and ion pairs are known to exist in the latter two phases, but there are insufficient data to justify a general procedure for estimating the quantities. No correction is made for the effect of cations other than H^+ . This approach must be regarded as merely a first correction for the dissociation effect. An accurate evaluation should preferably be based on experimental

determinations. The reported solubility C mol/m³ and K_{OW} presumably refer to the total of ionic and non-ionic forms, i.e., C_T and $K_{OW,T}$, at the pH of experimental determination, i.e.,

$$C_T = C_N + C_I$$

The solubility and K_{OW} of the non-ionic forms can be estimated as

$$C_N = C_T \cdot x_{ND}; \quad K_{OW,N} = K_{OW,T} / x_{ND}$$

Vapor pressure P^S is not affected, but the apparent Henry's law constant H_T , must also be adjusted to H_T/x_N , being P^S/C_N or $P^S/(C_T \cdot x_N)$.

C_N and $K_{OW,N}$ can be applied to environmental conditions with a temperature adjustment if necessary. Values of I_E , x_{Ix} and x_{NE} can be deduced from the environmental pH and the solubility and K_{OW} of the total ionic and non-ionic forms calculated.

In the tabulated data presented in this handbook the aqueous solubilities selected are generally those estimated to be of the non-ionic form unless otherwise stated.

1.2.5 TREATMENT OF WATER-MISCIBLE COMPOUNDS

In the multimedia models used in this series of volumes, an air-water partition coefficient K_{AW} or Henry's law constant (H) is required and is calculated from the ratio of the pure substance vapor pressure and aqueous solubility. This method is widely used for hydrophobic chemicals but is inappropriate for water-miscible chemicals for which no solubility can be measured. Examples are the lower alcohols, acids, amines and ketones. There are reported "calculated" or "pseudo-solubilities" that have been derived from QSPR correlations with molecular descriptors for alcohols, aldehydes and amines (by Leahy 1986; Kamlet et al. 1987, 1988 and Nirmalakhandan and Speece 1988a,b). The obvious option is to input the H or K_{AW} directly. If the chemical's activity coefficient γ in water is known, then H can be estimated as $v_w \gamma P_L^S$, where v_w is the molar volume of water and P_L^S is the liquid vapor pressure. Since H can be regarded as P_L^S/C_L^S , where C_L^S is the solubility, it is apparent that $(1/v_w \gamma)$ is a "pseudo-solubility." Correlations and measurements of γ are available in the physical-chemical literature. For example, if γ is 5.0, the pseudo-solubility is 11100 mol/m³ since the molar volume of water v_w is 18×10^{-6} m³/mol or 18 cm³/mol. Chemicals with γ less than about 20 are usually miscible in water. If the liquid vapor pressure in this case is 1000 Pa, H will be 1000/11100 or 0.090 Pa·m³/mol and K_{AW} will be H/RT or 3.6×10^{-5} at 25°C. Alternatively, if H or K_{AW} is known, C_L^S can be calculated. It is possible to apply existing models to hydrophilic chemicals if this pseudo-solubility is calculated from the activity coefficient or from a known H (i.e., C_L^S , P_L^S/H or P_L^S or $K_{AW} \cdot RT$). This approach is used here. In the fugacity model illustrations all pseudo-solubilities are so designated and should not be regarded as real, experimentally accessible quantities.

1.2.6 TREATMENT OF PARTIALLY MISCIBLE SUBSTANCES

Most hydrophobic substances have low solubilities in water, and in the case of liquids, water is also sparingly soluble in the pure substance. Some substances such as butanols and chlorophenols display relatively high mutual solubilities. As temperature increases, these mutual solubilities increase until a point of total miscibility is reached at a critical solution temperature. Above this temperature, no mutual solubilities exist. A simple plot of solubility versus temperature thus ends at this critical point. At low temperatures near freezing, the phase diagram also become complex. Example of such systems have been reported for *sec*-butyl alcohol (2-butanol) by Ochi et al. (1996) and for chlorophenols by Jaoui et al. (1999).

1.2.7 TREATMENT OF GASES AND VAPORS

A volatile substance may exist in one of three broad classes that can be loosely termed gases, vapors and liquids.

A *gaseous* substance such as oxygen at normal environmental conditions exists at a temperature exceeding its critical temperature of 155 K. No vapor pressure can be defined or measured under this super-critical condition, thus no Henry's law constant can be calculated. Empirical data are required.

A substance such as propane with a critical temperature of 370 K has a measurable vapor pressure of 998000 Pa, or approximately 10 atm at 27°C, which exceeds atmospheric pressure of 101325 Pa, the boiling point being -42°C or 231 K. It is thus a *vapor* at normal temperatures and pressures. A Henry's law constant can be calculated from this vapor pressure and a solubility as described earlier.

Most substances treated in this handbook are liquids or solids at environmental conditions; thus their boiling points exceed 25°C. Benzene, for example, has a critical temperature of 562 K, a boiling point of 80°C and a vapor pressure of 12700 Pa at 25°C.

When a solubility in water is measured and reported for gases and vapors an ambiguity is possible. For gases the solubility and the corresponding partial or total pressure in the gas phase must be reported since the solubility is dependent on this pressure as dictated by Henry's Law. For liquids and solids the solubility is presumably measured under conditions when the partial pressure equals the vapor pressure. For vapors such as propane the solubility can be measured either at a specified pressure (usually 1 atmosphere) or under high-pressure conditions (e.g., 10 atm) when the substance is a liquid. When calculating H or K_{AW} it is essential to use the correct pressure corresponding to the solubility measurement. Care must be exercised when treating substances with boiling points at or below environmental temperatures to ensure that the solubility is interpreted and used correctly.

1.2.8 SOLIDS, LIQUIDS AND THE FUGACITY RATIO

Saturation properties such as solubility in water and vapor pressure can be measured directly for solids and liquids. For certain purposes it is useful to estimate the solubility that a solid substance would have if it were liquid at a temperature below the melting point. For example, naphthalene melts at 80°C and at 25°C the solid has a solubility in water of 33 g/m³ and a vapor pressure of 10.9 Pa. If naphthalene was a liquid at 25°C it is estimated that its solubility would be 115 g/m³ and its vapor pressure 38.1 Pa, both a factor of 3.5 greater. This ratio of solid to liquid solubilities or vapor pressures is referred to as the fugacity ratio. It is 1.0 at the melting point and falls, in this case at lower temperatures to 0.286 at 25°C.

Solubilities and vapor pressures of a solid substance in the liquid state are often reported for the following four reasons.

Measurements of gas chromatographic retention time are often used as a fast and easy method of estimating vapor pressure. These estimated pressures are related to the gas/substrate partition coefficient, which can be regarded as a ratio of solubility of the substance in the gas to that in the substrate, both solubilities being of the substance in the liquid state. As a result the estimated vapor pressures are of the liquid state. To obtain the solid vapor pressure requires multiplication by the fugacity ratio. It is important to establish if the estimated and reported property is of the vapor or liquid.

QSPRs in which solubilities and vapor pressures are correlated against molecular structure are done exclusively using the liquid state property. This avoids the complication introduced by the effect of fugacity ratio or melting point on the solid state property.

When a solid is in liquid solution it behaves according to its liquid state properties because it is in a liquid mixture. When applying Raoult's Law or similar expressions, the pure substance property is that of the liquid. Liquids such as crude oils and PCB mixtures consist largely of solid substances, but they are in the liquid state and generally unable to precipitate as solid crystals because of their low individual concentrations.

When estimating air-aerosol partitioning of gas phase substances such as PAHs, most of which are solids, it is usual to use the liquid state vapor pressure as the correlating parameter. This is because the PAH is effectively in a liquid-like state on or in the aerosol particle. It does not exist in crystalline form.

When calculating partition coefficients such as K_{AW} , K_{OW} or K_{OA} from solubilities it is immaterial if the values used are of solids or liquids, but it is erroneous to mix the two states, e.g., a solid solubility and a liquid vapor pressure.

The fugacity ratio F can be estimated at temperature T (K) from the expression

$$\ln F = -\Delta S (T_M - T)/RT$$

where ΔS is the entropy of fusion, T_M is the melting point, and R is the gas constant. ΔS is related to the measurable enthalpy of fusion ΔH at the melting point as $\Delta H/T_M$. The reader should use experimental data for ΔH , ΔS and melting point whenever possible. The most reliable method is to measure ΔH calorimetrically, calculate ΔS and use this value to estimate F . Only in the absence of ΔH data should a QSPR be used or Walden's Rule applied that ΔS is approximately 56.5 J/mol K. This assumption leads to the equations

$$F = \exp(-6.79(T_M/T - 1))$$

$$\log F = -0.01(T_M - 298)$$

F is thus 1.0 at the melting point, with lower values at lower temperatures. It is not applied at temperatures exceeding T_M . This issue is discussed by Mackay (2001), Tesconi and Yalkowsky (2000), Yalkowsky and Banerjee (1992) and Chickos et al. (1999).

1.2.9 CHEMICAL REACTIVITY AND HALF-LIVES

Characterization of chemical reactivity presents a challenging problem in environmental science in general and especially in handbooks. Whereas radioisotopes have fixed half-lives, the half-life of a chemical in the environment depends not only on the intrinsic properties of the chemical, but also on the nature of the environmental compartments. Factors such as sunlight intensity, hydroxyl radical concentration and the nature of the microbial community, as well as temperature, affect the chemical's half-life so it is impossible (and misleading) to document a single reliable half-life. We suggest that the best approach is to suggest a semi-quantitative classification of half-lives into groups or ranges, assuming average environmental conditions to apply. Obviously, a different class will generally apply between compartments such as in air and bottom sediment. In this compilation we use the following class ranges for chemical reactivity in a single medium such as water.

These times are divided logarithmically with a factor of approximately 3 between adjacent classes. With the present state of knowledge it is probably misleading to divide the classes into finer groupings; indeed, a single chemical is likely to experience half-lives ranging over three classes, depending on season. These half-lives apply to the reaction of the parent substance. Often a degradation product or metabolite is formed that is of environmental concern. Since it has different properties it requires separate assessment. The ultimate degradation to inorganic species may require a much longer time than is indicated by the initial half-life.

class	mean half-life (hours)	range (hours)
1	5 < 10	
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	30,000–100,000
10	> 11 years	> 100,000

When compiling the suggested reactivity classes, the authors have examined the available information on reaction rates of the chemical in each medium by all relevant processes. These were expressed as an overall half-life for transformation. The product of the half-life and the corresponding rate constant is $\ln 2$ or 0.693. For example, a chemical may be subject to biodegradation with a half-life of 20 days or 480 hours (rate constant 0.0014 h^{-1}) and simultaneous photolysis with a rate constant of 0.0011 h^{-1} (half-life 630 hours). The overall rate constant is thus 0.0025 h^{-1} and the half-life is 277 hours or 12 days. Data for homologous chemicals have also been compiled, and insights into the reactivity of various functional groups considered. In most cases a single reaction class is assigned to the series; in the above case, class 4 with a mean half-life of 170 hours would be chosen. These half-lives must be used with caution, and it is wise to test the implications of selecting longer and shorter half-lives.

The most reliable kinetic data are for atmospheric oxidation by hydroxyl radicals. These data are usually reported as second-order rate constants applied to the concentration of the chemical and the concentration of hydroxyl radicals (usually of the order of 10^6 radicals per cm^3). The product of the assumed hydroxyl radical concentration and the second-order rate constant is a first-order rate constant from which a half-life can be deduced.

Extensive research has been conducted into the atmospheric chemistry of organic chemicals because of air quality concerns. Recently, Atkinson and coworkers (1984, 1985, 1987, 1988, 1989, 1990, 1991), Altshuller (1980, 1991) and Sabljic and Güsten (1990) have reviewed the photochemistry of many organic chemicals of environmental interest for their gas phase reactions with hydroxyl radicals (OH), ozone (O_3) and nitrate radicals (NO_3) and have provided detailed information on reaction rate constants and experimental conditions, which allowed the estimation of atmospheric lifetimes. Klöpffer (1991) has estimated the atmospheric lifetimes for the reaction with OH radicals to range from 1 hour to 130 years, based on these reaction rate constants and an assumed constant concentration of OH

radicals in air. As Atkinson (1985) has pointed out, the gas phase reactions with OH radicals are the major tropospheric loss process for the alkanes, haloalkanes, the lower alkenes, the aromatic hydrocarbons, and a majority of the oxygen-containing organics. In addition, photooxidation reactions with O_3 and NO_3 radicals can result in transformation of these compounds. The night-time reaction with NO_3 radicals may also be important (Atkinson and Carter 1984, Sabljic and Güsten 1990).

There are fewer studies on direct or indirect photochemical degradation in the water phase; however, Klöpffer (1991) had pointed out that the rate constant or lifetimes derived from these studies “is valid only for the top layer or surface waters.” Mill (1982, 1989, 1993) and Mill and Mabey (1985) have estimated half-lives of various chemicals in aqueous solutions from their reaction rate constants with singlet oxygen, as well as photooxidation with hydroxyl and peroxy radicals. Buxton et al. (1988) gave a critical review of rate constants for reactions with hydrated electrons, hydrogen atoms and hydroxyl radicals in aqueous solutions. Mabey and Mill (1978) also reviewed the hydrolysis of organic chemicals in water under environmental conditions. Recently, Ellington and coworkers (1987a,b, 1988, 1989) also reported the hydrolysis rate constants in aqueous solutions for a variety of organic chemicals.

In most cases, a review of the literature suggested that reaction rates in water by chemical processes are 1 to 2 orders of magnitude slower than in air, but with biodegradation often being significant, especially for hydrocarbons and oxygen-containing chemicals. Generally, the water half-life class is three more than that in air, i.e., a factor of about 30 slower. Chemicals in soils tend to be shielded from photolytic processes, and they are less bioavailable, thus the authors have frequently assigned a reactivity class to soil of one more than that for water. Bottom sediments are assigned an additional class to that of soils largely on the basis that there is little or no photolysis, there may be lack of oxygen, and the intimate sorption to sediments renders the chemicals less bioavailable.

Because of the requirements of regulations for certain chemicals such as pesticides, extensive data usually exist on partitioning properties and reactivity or half-lives of active ingredients. In some cases these data have been peer-reviewed and published in the scientific literature, but often they are not generally available. A reader with interest in a specific pesticide can often obtain additional data from manufacturers or from registration literature, including accounts of chemical fate under field application conditions. Frequently these data are used as input to pesticide fate models, and the results of these modeling exercises may be available or published in the scientific literature.

The chemical reactivity of these substances is a topic which continues to be the subject of extensive research; thus there is often detailed, more recent information about the fate of chemical species which are of particular relevance to air or water quality. The reader is thus urged to consult the original and recent references because when considering the entire multimedia picture, it is impossible in a volume such as this to treat this subject in the detail it deserves.

1.3 EXPERIMENTAL METHODS

1.3.1 SOLUBILITY IN WATER AND pK_a

Most conventional organic contaminants are fairly hydrophobic and thus exhibit a low but measurable solubility in water. Solubility is often used to estimate the air-water partition coefficient or Henry's law constant, but this is not possible for miscible chemicals; indeed the method is suspect for chemicals of appreciable solubility in water, i.e., exceeding 1 g/100 g. Direct measurement of the Henry's law constant is thus required.

The conventional method of preparing saturated solutions for the determination of solubility is batch equilibration. An excess amount of solute chemical is added to water and equilibrium is achieved by shaking gently (generally referred as the “shake flask method”) or slow stirring with a magnetic stirrer. The aim is to prevent formation of emulsions or suspensions and thus avoid extra experimental procedures such as filtration or centrifuging which may be required to ensure that a true solution is obtained. Experimental difficulties can still occur with sparingly soluble chemicals such as longer chain alkanes and polycyclic aromatic hydrocarbons (PAHs) because of the formation of emulsion or micro-crystal suspensions. An alternative approach is to coat a thin layer of the chemical on the surface of the equilibration flask before water is added. An accurate “generator column” method is also used (Weil et al. 1974, May et al. 1978a,b) in which a column is packed with an inert solid support, such as glass beads and then coated with the solute chemical. Water is pumped through the column at a controlled, known flow rate to achieve saturation.

The method of concentration measurement of the saturated solution depends on the solute solubility and its chemical properties. Some common methods used for solubility measurement are listed below.

1. Gravimetric or volumetric methods (Booth and Everson 1948)

An excess amount of solid compound is added to a flask containing water to achieve saturation solution by shaking, stirring, centrifuging until the water is saturated with solute and undissolved solid or liquid

residue appears, often as a cloudy phase. For liquids, successive known amounts of solute may be added to water and allowed to reach equilibrium, and the volume of excess undissolved solute is measured.

2. Instrumental methods

- a. UV spectrometry (Andrews and Keefer 1950, Bohon and Claussen 1951, Yalkowsky and Valvani 1976);
- b. Gas chromatographic analysis with FID, ECD or other detectors (McAuliffe 1966, Mackay et al. 1975, Chiou et al. 1982, Bowman and Sans 1983);
- c. Fluorescence spectrophotometry (Mackay and Shiu 1977);
- d. Interferometry (Gross and Saylor 1931);
- e. High-pressure liquid chromatography (HPLC) with I.R., UV or fluorescence detection (May et al. 1978a,b, Wasik et al. 1983, Shiu et al. 1988, Doucette and Andren 1988a);
- f. Liquid phase elution chromatography (Schwarz 1980, Schwarz and Miller 1980);
- g. Nephelometric methods (Davis and Parke 1942, Davis et al. 1942, Hollifield 1979);
- h. Radiotracer or liquid scintillation counting (LSC) method (Banerjee et al. 1980, Lo et al. 1986).

For most organic chemicals the solubility is reported at a defined temperature in distilled water. For substances which dissociate (e.g., phenols, carboxylic acids and amines) it is essential to report the pH of the determination because the extent of dissociation affects the solubility. It is common to maintain the desired pH by buffering with an appropriate electrolyte mixture. This raises the complication that the presence of electrolytes modifies the water structure and changes the solubility. The effect is usually "salting-out." For example, many hydrocarbons have solubilities in seawater about 75% of their solubilities in distilled water. Care must thus be taken to interpret and use reported data properly when electrolytes are present.

The dissociation constant K_a or its commonly reported negative logarithmic form pK_a is determined in principle by simultaneous measurement or deduction of the ionic and non-ionic concentrations and the pH of the solution.

The most common problem encountered with reported data is inaccuracy associated with very low solubilities, i.e., those less than 1.0 mg/L. Such solutions are difficult to prepare, handle and analyze, and reported data often contain appreciable errors.

As was discussed earlier, care must be taken when interpreting solubility data for gases, i.e., substances for which the temperature exceeds the boiling point. Solubility then depends on the pressure which may be atmospheric or the higher vapor pressure.

1.3.2 VAPOR PRESSURE

In principle, the determination of vapor pressure involves the measurement of the saturation concentration or pressure of the solute in a gas phase. The most reliable methods involve direct determination of these concentrations, but convenient indirect methods are also available based on evaporation rate measurements or chromatographic retention times. Some methods and approaches are listed below.

- a. Static method, the equilibrium pressure in a thermostatic vessel is directly measured by use of pressure gauges: diaphragm gauge (Ambrose et al. 1975), Rodebush gauge (Sears and Hopke 1947), inclined-piston gauge (Osborn and Douslin 1975);
- b. Dynamic method (or boiling point) for measuring relatively high vapor pressure, eg., comparative ebulliometry (Ambrose 1981);
- c. Effusion methods, torsion and weight-loss (Balson 1947, Bradley and Cleasby 1953, Hamaker and Kerlinger 1969, De Kruif 1980);
- d. Gas saturation or transpiration methods (Spencer and Cliath 1970, 1972, Sinke 1974, Macknick and Prausnitz 1979, Westcott et al. 1981, Rordorf 1985a,b, 1986);
- e. Dynamic coupled-column liquid chromatographic method- a gas saturation method (Sonnefeld et al. 1983);
- f. Calculation from evaporation rates and vapor pressures of a reference compound (Gückel et al. 1974, 1982, Dobbs and Grant 1980, Dobbs and Cull 1982);
- g. Calculation from GC retention time data (Hamilton 1980, Westcott and Bidleman 1982, Bidleman 1984, Kim et al. 1984, Foreman and Bidleman 1985, Burkhard et al. 1985a, Hinckley et al. 1990).

The greatest difficulty and uncertainty arises when determining the vapor pressure of chemicals of low volatility, i.e., those with vapor pressures below 1.0 Pa. Vapor pressures are strongly dependent on temperature, thus accurate temperature control is essential. Data are often regressed against temperature and reported as Antoine or Clapeyron constants. Care

must be taken if the Antoine or other equations are used to extrapolate data beyond the temperature range specified. It must be clear if the data apply to the solid or liquid phase of the chemical.

1.3.3 OCTANOL-WATER PARTITION COEFFICIENT K_{OW}

The experimental approaches are similar to those for solubility, i.e., employing shake flask or generator-column techniques. Concentrations in both the water and octanol phases may be determined after equilibration. Both phases can then be analyzed by the instrumental methods discussed above and the partition coefficient is calculated from the concentration ratio C_O/C_W . This is actually the ratio of solute concentration in octanol saturated with water to that in water saturated with octanol.

As with solubility, K_{OW} is a function of the presence of electrolytes and for dissociating chemicals it is a function of pH. Accurate values can generally be measured up to about 10^7 , but accurate measurement beyond this requires meticulous technique. A common problem is the presence of small quantities of emulsified octanol in the water phase. The high concentration of chemical in that emulsion causes an erroneously high apparent water phase concentration.

Considerable success has been achieved by calculating K_{OW} from molecular structure; thus, there has been a tendency to calculate K_{OW} rather than measure it, especially for “difficult” hydrophobic chemicals. These calculations are, in some cases, extrapolations and can be in serious error. Any calculated log K_{OW} value above 7 should be regarded as suspect, and any experimental or calculated value above 8 should be treated with extreme caution.

For many hydrophilic compounds such as the alcohols, K_{OW} is low and can be less than 1.0, resulting in negative values of log K_{OW} . In such cases, care should be taken when using correlations developed for more hydrophobic chemicals since partitioning into biota or organic carbon phases may be primarily into aqueous rather than organic media.

Details of experimental methods are described by Fujita et al. (1964), Leo et al. (1971), Hansch and Leo (1979), Rekker (1977), Chiou et al. (1977), Miller et al. (1984, 1985), Bowman and Sans (1983), Woodburn et al. (1984), Doucette and Andren (1987), and De Bruijn et al. (1989).

1.3.4 HENRY'S LAW CONSTANT

The Henry's law constant is essentially an air-water partition coefficient which can be determined by measurement of solute concentrations in both phases. This raises the difficulty of accurate analytical determination in two very different media which usually requires different techniques. Accordingly, effort has been devoted to devising techniques in which concentrations are measured in only one phase and the other concentration is deduced from a mass balance. These methods are generally more accurate. The principal difficulty arises with hydrophobic, low-volatility chemicals which can establish only very small concentrations in both phases.

Henry's law constant can be regarded as a ratio of vapor pressure to solubility, thus it is subject to the same effects that electrolytes have on solubility. Temperature affects both properties. Some methods are as follows:

- a. Volatility measurement of dilute aqueous solutions (Butler et al. 1935, Burnett 1963, Buttery et al. 1969);
- b. Multiple equilibration method (McAuliffe 1971, Munz and Roberts 1987);
- c. Equilibrium batch stripping (Mackay et al. 1979, Dunnivant et al. 1988, Betterton and Hoffmann 1988, Zhou and Mopper 1990);
- d. GC-determined distribution coefficients (Leighton and Calo 1981);
- e. GC analysis of both air/water phases (Vejrosta et al. 1982, Jönsson et al. 1982);
- f. EPICS (Equilibrium Partitioning In Closed Systems) method (Lincoff and Gossett 1984, Gossett 1987, Ashworth et al. 1988);
- g. Wetted-wall column (Fendinger and Glotfelty 1988, 1989, 1990);
- h. Headspace analyses (Hussam and Carr 1985);
- i. Calculation from vapor pressure and solubility (Mackay and Shiu 1981);
- j. GC retention volume/time determined activity coefficient at infinite dilution γ^∞ (Karger et al. 1971a,b, Sugiyama et al. 1975, Tse et al. 1992).

When using vapor pressure and solubility data, it is essential to ensure that both properties apply to the same chemical phase, i.e., both are of the liquid, or of the solid. Occasionally, a solubility is of a solid while a vapor pressure is extrapolated from higher temperature liquid phase data.

As was discussed earlier under solubility, for miscible chemicals it is necessary to determine the Henry's law constant directly, since solubilities are not measurable.

1.3.5 OCTANOL-AIR PARTITION COEFFICIENT K_{OA}

As was discussed earlier the octanol-air partition coefficient is increasingly used as a descriptor of partitioning between the atmosphere and organic phases in soils and vegetation. A generator column technique is generally used in which an inert gas is flowed through a column containing a substance dissolved in octanol. The concentration in the equilibrated gas leaving the column is then measured (Harner and Mackay 1995). More recent methods have been described by Harner and Bidleman (1996) and Shoeib and Harner (2002). Su et al (2002) have described a GC retention time method.

1.4 QUANTITATIVE STRUCTURE-PROPERTY RELATIONSHIPS (QSPRs)

1.4.1 OBJECTIVES OF QSPRs

Because of the large number of chemicals of actual and potential concern, the difficulties and cost of experimental determinations, and scientific interest in elucidating the fundamental molecular determinants of physical-chemical properties, considerable effort has been devoted to generating quantitative structure-property relationships (QSPRs). This concept of structure-property relationships or structure-activity relationships (QSARs) is based on observations of linear free-energy relationships, and usually takes the form of a plot or regression of the property of interest as a function of an appropriate molecular descriptor which can be calculated using only a knowledge of molecular structure or a readily accessible molecular property.

Such relationships have been applied to solubility, vapor pressure, K_{OW} , K_{AW} , K_{OA} , Henry's law constant, reactivities, bioconcentration data and several other environmentally relevant partition coefficients. Of particular value are relationships involving various manifestations of toxicity, but these are beyond the scope of this handbook. These relationships are valuable because they permit values to be checked for "reasonableness" and (with some caution) interpolation is possible to estimate undetermined values. They may be used (with extreme caution!) for extrapolation.

A large number of descriptors have been, and are being, proposed and tested. Dearden (1990) and the compilations by Karcher and Devillers (1990) and Hermens and Opperhuizen (1991) give comprehensive accounts of descriptors and their applications.

A valuable source of up-to-date information is the proceedings of the biennial QSAR conferences. The QSAR 2002 conference proceedings have been edited by Breton et al. (2003). A set of critical reviews has been edited by Walker (2003). Of particular note is the collection of estimation methods developed by the Syracuse Research Corporation with US EPA support and available on the internet at www.syrres.com under "estimation methods."

Among the most commonly used molecular descriptors are molecular weight and volume, the number of specific atoms (e.g., carbon or chlorine), surface areas (which may be defined in various ways), refractivity, parachor, steric parameters, connectivities and various topological parameters. Several quantum chemical parameters can be calculated from molecular orbital calculations including charge, electron density and superdelocalizability. It is likely that existing and new descriptors will continue to be tested, and that eventually a generally preferred set of readily accessible parameters will be adopted for routine use for correlating purposes.

From the viewpoint of developing quantitative correlations it is desirable to seek a linear relationship between descriptor and property, but a nonlinear or curvilinear relationship is adequate for illustrating relationships and interpolating purposes. In this handbook we have elected to use the simple descriptor of molar volume at the normal boiling point as estimated by the Le Bas method (Reid et al. 1987). This parameter is very easily calculated and proves to be adequate for the present purposes of plotting property versus relationship without seeking linearity.

The Le Bas method is based on a summation of atomic volumes with adjustment for the volume decrease arising from ring formation. The full method is described by Reid et al. (1987), but for the purposes of this compilation, the volumes and rules as listed in Table 1.3.1 are used.

Example: The experimental molar volume of chlorobenzene 115 cm³/mol (Reid et al. 1987). From the above rules, the Le Bas molar volume for chlorobenzene (C₆H₅Cl) is:

$$V = 6 \times 14.8 + 5 \times 3.7 + 24.6 - 15 = 117 \text{ cm}^3/\text{mol}$$

Accordingly, plots are presented at the end of each chapter for solubility, vapor pressure, K_{OW} , and Henry's law constant versus Le Bas molar volume.

TABLE 1.3.1
Le Bas molar volume

	increment, cm ³ /mol
Carbon	14.8
Hydrogen	3.7
Oxygen	7.4
In methyl esters and ethers	9.1
In ethyl esters and ethers	9.9
Join to S, P, or N	8.3
Nitrogen	
Doubly bonded	15.6
In primary amines	10.5
In secondary amines	12.0
Bromine	27.0
Chlorine	24.6
Fluorine	8.7
Iodine	37.0
Sulfur	25.6
Rings	
Three-membered	−6.0
Four-membered	−8.5
Five-membered	−11.5
Six-membered	−15.0
Naphthalene	−30.0
Anthracene	−47.5

As was discussed earlier in Section 1.2.8 a complication arises in that two of these properties (solubility and vapor pressure) are dependent on whether the solute is in the liquid or solid state. Solid solutes have lower solubilities and vapor pressures than they would have if they had been liquids. The ratio of the (actual) solid to the (hypothetical supercooled) liquid solubility or vapor pressure is termed the fugacity ratio F and can be estimated from the melting point and the entropy of fusion. This “correction” eliminates the effect of melting point, which depends on the stability of the solid crystalline phase, which in turn is a function of molecular symmetry and other factors. For solid solutes, the correct property to plot is the calculated or extrapolated supercooled liquid solubility. This is calculated in this handbook using where possible a measured entropy of fusion, or in the absence of such data the Walden’s Rule relationship suggested by Yalkowsky (1979) which implies an entropy of fusion of 56 J/mol·K or 13.5 cal/mol·K (e.u.)

$$F = C_S^S/C_L^S = P_S^S/P_L^S = \exp\{6.79(1 - T_M/T)\}$$

where C^S is solubility, P^S is vapor pressure, subscripts S and L refer to solid and liquid phases, T_M is melting point and T is the system temperature, both in absolute (K) units. The fugacity ratio is given in the data tables at 25°C, the usual temperature at which physical-chemical property data are reported. For liquids, the fugacity ratio is 1.0.

The usual approach is to compile data for the property in question for a series of structurally similar molecules and plot the logarithm of this property versus molecular descriptors, on a trial-and-error basis seeking the descriptor which best characterizes the variation in the property. It may be appropriate to use a training set to obtain a relationship and test this relationship on another set. Generally a set of at least ten data points is necessary before a reliable QSPR can be developed.

1.4.2 EXAMPLES OF QSARs AND QSPRs

There is a continuing effort to extend the long-established concept of quantitative-structure-activity-relationships (QSARs) to quantitative-structure-property relationships (QSPRs) to compute all relevant environmental physical-chemical properties (such as aqueous solubility, vapor pressure, octanol-water partition coefficient, Henry’s law constant, bioconcentration factor (BCF), sorption coefficient and environmental reaction rate constants from molecular structure).

Examples are Burkhard (1984) and Burkhard et al. (1985a), who calculated solubility, vapor pressure, Henry's law constant, K_{OW} and K_{OC} for all PCB congeners. Hawker and Connell (1988) also calculated $\log K_{OW}$; Abramowitz and Yalkowsky (1990) calculated melting point and solubility for all PCB congeners based on the correlation with total surface area (planar TSAs). Doucette and Andren (1988b) used six molecular descriptors to compute the K_{OW} of some chlorobenzenes, PCBs and PCDDs. Mailhot and Peters (1988) employed seven molecular descriptors to compute physical-chemical properties of some 300 compounds. Isnard and Lambert (1988, 1989) correlated solubility, K_{OW} and BCF for a large number of organic chemicals. Nirmalakhandan and Speece (1988a,b, 1989) used molecular connectivity indices to predict aqueous solubility and Henry's law constants for 300 compounds over 12 logarithmic units in solubility. Kamlet and co-workers (1986, 1987, 1988) have developed the "solvatochromic" parameters with the intrinsic molar volume to predict solubility, $\log K_{OW}$ and toxicity of organic chemicals. Warne et al. (1990) correlated solubility and K_{OW} for lipophilic organic compounds with 39 molecular descriptors and physical-chemical properties. Atkinson (1987, 1988) has used the structure-activity relationship (SAR) to estimate gas-phase reaction rate constants of hydroxyl radicals for organic chemicals. Mabey et al. (1984) have reviewed the estimation methods from SAR correlation for reaction rate constants and physical-chemical properties in environmental fate assessment. Other correlations are reviewed by Lyman et al. (1982) and Yalkowsky and Banerjee (1992). As Dearden (1990) has pointed out, "new parameters are continually being devised and tested, although the necessity of that may be questioned, given the vast number already available." It must be emphasized, however, that regardless of how accurate these predicted or estimated properties are claimed to be, ultimately they have to be confirmed or verified by experimental measurement.

A fundamental problem encountered in these correlations is the mismatch between the accuracy of experimental data and the molecular descriptors which can be calculated with relatively high precision, usually within a few percent. The accuracy may not always be high, but for correlation purposes precision is more important than accuracy. The precision and accuracy of the experimental data are often poor, frequently ranging over a factor of two or more. Certain isomers may yield identical descriptors, but have different properties. There is thus an inherent limit to the applicability of QSPRs imposed by the quality of the experimental data, and further efforts to improve descriptors, while interesting and potentially useful, may be unlikely to yield demonstrably improved QSPRs.

One of the most useful and accessible set of QSARs is that developed primarily by Howard and Meylan at the Syracuse Research Corporation, NY. These estimation methods are available as the EPISuite set from their website at www.syrres.com.

For correlation of solubility, the correct thermodynamic quantities for correlation are the activity coefficient γ , or the excess Gibbs free energy ΔG , as discussed by Pierotti et al. (1959) and Tsonopoulos and Prausnitz (1971). Examples of such correlations are given below.

1. Carbon number or carbon plus chlorine number (Tsonopoulos and Prausnitz 1971, Mackay and Shiu 1977);
2. Molar volume cm^3/mol
 - a. Liquid molar volume - from density (McAuliffe 1966, Lande and Banerjee 1981, Chiou et al. 1982, Abernethy et al. 1988, Wang et al. 1992);
 - b. Molar volume by additive group contribution method, e.g., Le Bas method, Schroeder method (Reid et al. 1987, Miller et al. 1985);
 - c. Intrinsic molar volume, V_i , cm^3/mol - from van der Waals radius with solvatochromic parameters α and β (Leahy 1986, Kamlet et al. 1987, 1988);
 - d. Characteristic molecular volume, m^3/mol (McGowan and Mellors 1986);
3. Group contribution method (Irmann 1965, Korenman et al. 1971, Polak and Lu 1973, Klopman et al. 1992);
4. Molecular volume - $\text{\AA}^3/\text{molecule}$ (cubic Angstrom per molecule)
 - a. van der Waals volume (Bondi 1964);
 - b. Total molecular volume (TMV) (Pearlman et al. 1984, Pearlman 1986);
5. Total surface area (TSA) - $\text{\AA}^2/\text{molecule}$ (Hermann 1971, Amidon et al. 1975, Yalkowsky and Valvani 1976, Yalkowsky et al. 1979, Iwase et al. 1985, Pearlman 1986, Andren et al. 1987, Hawker and Connell 1988, Dunnivant et al. 1992);
6. Molecular connectivity indices (MCI) or χ (Kier and Hall 1976, Andren et al. 1987, Nirmalakhandan and Speece 1988b, 1989);
7. Boiling point (Almgren et al. 1979);
8. Melting point (Amidon and Williams 1982);
9. Melting point and TSA (Abramowitz and Yalkowsky 1990);
10. High-pressure liquid chromatography (HPLC) - retention data (Locke 1974, Whitehouse and Cooke 1982, Brodsky and Ballschmiter 1988);

11. Adsorbability index (AI) (Okouchi et al. 1992);
12. Fragment solubility constants (Wakita et al. 1986).

Several workers have explored the linear relationship between octanol-water partition coefficient and solubility as a means of estimating solubility.

Hansch et al. (1968) established the linear free-energy relationship between aqueous and octanol-water partition of organic liquid. Others, such as Tulp and Hutzinger (1978), Yalkowsky et al. (1979), Mackay et al. (1980), Banerjee et al. (1980), Chiou et al. (1982), Bowman and Sans (1983), Miller et al. (1985), Andren et al. (1987) and Doucette and Andren (1988b) have all presented similar but modified relationships.

The UNIFAC (UNIQUAC Functional Group Activity Coefficient) group contribution (Fredenslund et al. 1975, Kikic et al. 1980, Magnussen et al. 1981, Gmehling et al. 1982 and Hansen et al. 1991) is widely used for predicting the activity coefficient in nonelectrolyte liquid mixtures by using group-interaction parameters. This method has been used by Kabadi and Danner (1979), Banerjee (1985), Arbuckle (1983, 1986), Banerjee and Howard (1988) and Al-Sahhaf (1989) for predicting solubility (as a function of the infinite dilution activity coefficient, γ^∞) in aqueous systems. Its performance is reviewed by Yalkowsky and Banerjee (1992).

HPLC retention time data have been used as a pseudo-molecular descriptor by Whitehouse and Cooke (1982), Hafkenscheid and Tomlinson (1981), Tomlinson and Hafkenscheid (1986) and Swann et al. (1983).

The octanol-water partition coefficient K_{OW} is widely used as a descriptor of hydrophobicity. Variation in K_{OW} is primarily attributable to variation in activity coefficient in the aqueous phase (Miller et al. 1985); thus, the same correlations used for solubility in water are applicable to K_{OW} . Most widely used is the Hansch-Leo compilation of data (Leo et al. 1971, Hansch and Leo 1979) and related predictive methods. Examples of K_{OW} correlations are:

1. Molecular descriptors
 - a. Molar volumes: Le Bas method; from density; intrinsic molar volume; characteristic molecular volume (Abernethy et al. 1988, Chiou 1985, Kamlet et al. 1988, McGowan and Mellors 1986);
 - b. TMV (De Bruijn and Hermens 1990);
 - c. TSA (Yalkowsky et al. 1979, 1983, Pearlman 1980, 1986, Pearlman et al. 1984, Hawker and Connell 1988);
 - d. Molecular connectivity indices (Doucette and Andren 1988b);
 - e. Molecular weight (Doucette and Andren 1988b).
2. Group contribution methods
 - a. π -constant or hydrophobic substituent method (Hansch et al. 1968, Hansch and Leo 1979, Doucette and Andren 1988b);
 - b. Fragment constants or f-constant (Rekker 1977, Yalkowsky et al. 1983);
 - c. Hansch and Leo's f-constant (Hansch and Leo 1979; Doucette and Andren 1988b).
3. From solubility - K_{OW} relationship
4. HPLC retention data
 - a. HPLC- k' capacity factor (Könemann et al. 1979, McDuffie 1981);
 - b. HPLC-RT retention time (Veith et al. 1979, Rapaport and Eisenreich 1984, Doucette and Andren 1988b);
 - c. HPLC-RV retention volume (Garst 1984);
 - d. HPLC-RT/MS HPLC retention time with mass spectrometry (Burkhard et al. 1985c).
5. Reversed-phase thin-layer chromatography (TLC) (Ellgehausen et al. 1981, Bruggeman et al. 1982).
6. Molar refractivity (Yoshida et al. 1983).
7. Combination of HPLC retention data and molecular connectivity indices (Finizio et al. 1994).
8. Molecular orbital methods (Reddy and Locke 1994).

As with solubility and octanol-water partition coefficient, vapor pressure can be estimated with a variety of correlations as discussed in detail by Burkhard et al. (1985a) and summarized as follows:

1. Interpolation or extrapolation from equation for correlating temperature relationships, e.g., the Clausius-Clapeyron, Antoine equations (Burkhard et al. 1985a);
2. Carbon or chlorine numbers (Mackay et al. 1980, Shiu and Mackay 1986);
3. Le Bas molar volume (Shiu et al. 1987, 1988);
4. Boiling point T_b and heat of vaporization ΔH_v (Mackay et al. 1982);
5. Group contribution method (Macknick and Prausnitz 1979);

6. UNIFAC group contribution method (Jensen et al. 1981, Yair and Fredenslund 1983, Burkhard et al. 1985a, Banerjee et al. 1990);
7. Molecular weight and Gibbs' free energy of vaporization ΔG_v (Burkhard et al. 1985a);
8. TSA and ΔG_v (Amidon and Anik 1981, Burkhard et al. 1985a, Hawker 1989);
9. Molecular connectivity indices (Kier and Hall 1976, 1986, Burkhard et al. 1985a);
10. Melting point T_M and GC retention index (Bidleman 1984, Burkhard et al. 1985a);
11. Solvatochromic parameters and intrinsic molar volume (Banerjee et al. 1990).

As described earlier, Henry's law constants can be calculated from the ratio of vapor pressure and aqueous solubility. Henry's law constants do not show a simple linear pattern as solubility, K_{OW} or vapor pressure when plotted against simple molecular descriptors, such as numbers of chlorine or Le Bas molar volume, e.g., PCBs (Burkhard et al. 1985b), pesticides (Suntio et al. 1988), and chlorinated dioxins (Shiu et al. 1988). Henry's law constants can be estimated from:

1. UNIFAC-derived infinite dilution activity coefficients (Arbuckle 1983);
2. Group contribution and bond contribution methods (Hine and Mookerjee 1975, Meylan and Howard 1991);
3. Molecular connectivity indices (Nirmalakhandan and Speece 1988b, Sabljic and Güsten 1989, Dunnivant et al. 1992);
4. Total surface area - planar TSA (Hawker 1989);
5. Critical reviews by Mackay and Shiu 1981, Shiu and Mackay 1986 and Suntio et al. 1988.

For water-miscible compounds the use of aqueous solubility data is obviously impossible.

Bioconcentration Factors:

1. Correlation with K_{OW} (Neely et al. 1974, Könnemann and van Leeuwen 1980, Veith et al. 1980, Chiou et al. 1977, Mackay 1982, Briggs 1981, Garten and Trabalka 1983, Davies and Dobbs 1984, Zaroogian et al. 1985, Oliver and Niimi 1988, Isnard and Lambert 1988);
2. Correlation with solubility (Kenaga 1980, Kenaga and Goring 1980, Briggs 1981, Garten and Trabalka 1983, Davies and Dobbs 1984, Isnard and Lambert 1988);
3. Correlation with K_{OC} (Kenaga 1980, Kenaga and Goring 1980, Briggs 1981);
4. Calculation with HPLC retention data (Swann et al. 1983);
5. Calculation with solvatochromic parameters (Hawker 1989, 1990b).

Sorption Coefficients:

1. Correlation with K_{OW} (Karickhoff et al. 1979, Schwarzenbach and Westall 1981, Mackay 1982, Oliver 1984);
2. Correlation with solubility (Karickhoff et al. 1979);
3. Molecular connectivity indices (Gerstl and Helling 1984; Sabljic 1984, 1987, Bahnick and Doucette 1988, Sabljic et al. 1989, Meylan et al. 1992);
4. Estimation from molecular connectivity index/fragment contribution method (Meylan et al. 1992, Lohninger 1994);
5. From HPLC retention data (Swann et al. 1983, Szabo et al. 1990).
6. Molecular orbital method (Reddy and Locke 1994).

Octanol-Air Partition coefficient.

The molecular descriptors used for K_{OW} , solubility in water and vapor pressure can potentially be applied to K_{OA} .

1.5 MASS BALANCE MODELS OF CHEMICAL FATE

1.5.1 EVALUATIVE ENVIRONMENTAL CALCULATIONS

When conducting assessments of how a chemical is likely to behave in the environment and especially how different chemicals behave in the same environment, there is incentive to standardize the evaluations using "evaluative" environmental models. The nature of these calculations has been described in a series of papers, notably Mackay (1979),

Paterson and Mackay (1985), Mackay and Paterson (1990, 1991), and a recent text (Mackay 2001). Only the salient features are presented here. Three evaluations are completed for each chemical, namely the Level I, II and III fugacity calculations. These calculations can also be done in concentration format instead of fugacity, but for this type of evaluation the fugacity approach is simpler and more instructive. The mass balance models of the types described below can be downloaded for the web site www.trentu.ca/cemc

1.5.2 LEVEL I FUGACITY CALCULATIONS

The Level I calculation describes how a given amount of chemical partitions at equilibrium between six media: air, water, soil, bottom sediment, suspended sediment and fish. No account is taken of reactivity. Whereas most early evaluative environments have treated a one square kilometre region with about 70% water surface (simulating the global proportion of ocean surface), it has become apparent that a more useful approach is to treat a larger, principally terrestrial area similar to a jurisdictional region such as a US state. The area selected is 100,000 km² or 10¹¹ m², which is about the area of Ohio, Greece or England. This environment was used in previous editions of this Handbook and is identical to the EQC or Equilibrium Criterion model described by Mackay et al. (1996).

The atmospheric height is selected as an arbitrary 1000 m reflecting that region of the troposphere which is most affected by local air emissions. A water surface area of 10% or 10,000 km² is used, with a water depth of 20 m. The water volume is thus 2 × 10¹¹ m³. The soil is viewed as being well mixed to a depth of 10 cm and is considered to be 2% organic carbon. It has a volume of 9 × 10⁹ m³. The bottom sediment has the same area as the water, a depth of 1 cm and an organic carbon content of 4%. It thus has a volume of 10⁸ m³.

For the Level I calculation both the soil and sediment are treated as simple solid phases with the above volumes, i.e., the presence of air or water in the pores of these phases is ignored.

Two other phases are included for interest. Suspended matter in water is often an important medium when compared in sorbing capacity to that of water. It is treated as having 20% organic carbon and being present at a volume fraction in the water of 5 × 10⁻⁶, i.e., it is about 5 to 10 mg/L. The volume is thus 10⁶ m³. Fish is also included at an entirely arbitrary volume fraction of 10⁻⁶ and are assumed to contain 5% lipid, equivalent in sorbing capacity to octanol. The volume is thus 2 × 10⁵ m³. These two phases are small in volume and rarely contain an appreciable fraction of the chemical present, but it is in these phases that the highest concentration of chemical often exists.

Another phase which is introduced later in the Level III model is aerosol particles with a volume fraction in air of 2 × 10⁻¹¹, i.e., approximately 30 µg/m³. Although negligible in volume, an appreciable fraction of the chemical present in the air phase may be associated with aerosols. Aerosols are not treated in Level I or II calculations because their capacity for the chemical at equilibrium is usually negligible when compared with soil.

These dimensions and properties are summarized in Tables 1.5.1 and 1.5.2. The user is encouraged to modify these dimensions to reflect conditions in a specific area of interest.

The amount of chemical introduced in the Level I calculation is an arbitrary 100,000 kg or 100 tonnes. If dispersed entirely in the air, this amount yields a concentration of 1 µg/m³ which is not unusual for ubiquitous contaminants such as hydrocarbons. If dispersed entirely in the water, the concentration is a higher 500 µg/m³ or 500 ng/L, which again is reasonable for a well-used chemical of commerce. The corresponding value in soil is about 0.0046 µg/g. Clearly for restricted chemicals such as PCBs, this amount is too large, but it is preferable to adopt a common evaluative amount

TABLE 1.5.1
Compartment dimensions and properties for Levels I and II calculations

Compartment	Air	Water	Soil	Sediment	Suspended sediment	Fish
Volume, V (m ³)	10 ¹⁴	2 × 10 ¹¹	9 × 10 ⁹	10 ⁸	10 ⁶	2 × 10 ⁵
Depth, h (m)	1000	20	0.1	0.01	—	—
Area, A (m ²)	100 × 10 ⁹	10 × 10 ⁹	90 × 10 ⁹	10 × 10 ⁹	—	—
Fraction OC	—	—	0.02	0.04	0.2	—
Density, ρ (kg/m ³)	1.2	1000	2400	2400	1500	1000
Adv. Residence	100	1000	—	50,000	—	—
Time, t (hours)						
Adv. flow, G (m ³ /h)	10 ¹²	2 × 10 ⁸	—	2000	—	—

TABLE 1.5.2
Bulk compartment dimensions and volume fractions (v) for Level III calculations

Compartment		Volume
Air	Total volume	10^{14} m^3 (as above)
	Air phase	10^{14} m^3
	Aerosol phase	2000 m^3 ($v = 2 \times 10^{-11}$)
Water	Total volume	$2 \times 10^{11} \text{ m}^3$
	Water phase	$2 \times 10^{11} \text{ m}^3$ (as above)
	Suspended sediment phase	10^6 m^3 ($v = 5 \times 10^{-6}$)
	Fish phase	$2 \times 10^5 \text{ m}^3$ ($v = 1 \times 10^{-6}$)
Soil	Total volume	$18 \times 10^9 \text{ m}^3$
	Air phase	$3.6 \times 10^9 \text{ m}^3$ ($v = 0.2$)
	Water phase	$5.4 \times 10^9 \text{ m}^3$ ($v = 0.3$)
	Solid phase	$9.0 \times 10^9 \text{ m}^3$ ($v = 0.5$) (as above)
Sediment	Total volume	$500 \times 10^6 \text{ m}^3$
	Water phase	$400 \times 10^6 \text{ m}^3$ ($v = 0.8$)
	Solid phase	$100 \times 10^6 \text{ m}^3$ ($v = 0.2$) (as above)

TABLE 1.5.3
Equations for phase Z values used in Levels I, II and bulk phase values used in Level III

Compartment	Z values
Air	$Z_1 = 1/RT$
Water	$Z_2 = 1/H = C^S/P^S$
Soil	$Z_3 = Z_2 \cdot \rho_3 \cdot \phi_3 \cdot K_{OC}/1000$
Sediment	$Z_4 = Z_2 \cdot \rho_4 \cdot \phi_4 \cdot K_{OC}/1000$
Suspended Sediment	$Z_5 = Z_2 \cdot \rho_5 \cdot \phi_5 \cdot K_{OC}/1000$
Fish	$Z_6 = Z_2 \cdot \rho_6 \cdot L \cdot K_{OW}/1000$
Aerosol	$Z_7 = Z_1 \cdot 6 \times 10^6 / P_L^S$ or $0.1 Z_1 K_{OA}$
where	R = gas constant ($8.314 \text{ J/mol} \cdot \text{K}$) T = absolute temperature (K) C^S = solubility in water (mol/m^3) P^S = vapor pressure (Pa) H = Henry's law constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$) P_L^S = liquid vapor pressure (Pa) K_{OA} = octanol-air partition coefficient K_{OW} = octanol-water partition coefficient ρ_i = density of phase i (kg/m^3) ϕ_i = mass fraction organic-carbon in phase i (g/g) L = lipid content of fish

Note for solids $P_L^S = P^S / \exp\{6.79(1 - T_M/T)\}$, where T_M is melting point (K) of the solute and T is 298 K. An experimental entropy of fusion should be used if available.

for all substances. No significance should, of course, be attached to the absolute values of the concentrations which are deduced from this arbitrary amount. Only the relative values have significance.

The Level I calculation proceeds by deducing the fugacity capacities or Z values for each medium (see Table 1.5.3), following the procedures described by Mackay (2001). These working equations show the necessity of having data on molecular mass, water solubility, vapor pressure, and octanol-water partition coefficient. The fugacity f (Pa) common to all media is deduced as

$$f = M / \sum V_i Z_i$$

where M is the total amount of chemical (mol), V_i is the medium volume (m^3) and Z_i is the corresponding fugacity capacity for the chemical in each medium. It is noteworthy that Z values contain all the necessary partition information. The partition coefficient K_{12} is simply the ratio of Z values, i.e., Z_1/Z_2 . Definition of the Z values starts in the air compartment then proceeds to other compartments using the appropriate partition coefficients.

The molar concentration C (mol/m^3) can then be deduced as Zf mol/m^3 or as WZf g/m^3 or $1000 WZf/\rho$ $\mu\text{g}/\text{g}$, where ρ is the phase density (kg/m^3) and W is the molecular mass (g/mol). The amount m_i in each medium is $C_i V_i$ mol, and the total in all media is M mol. The information obtained from this calculation includes the concentrations, amounts and distribution.

Note that this simple treatment assumes that the soil and sediment phases are entirely solid, i.e., there are no air or water phases present to “dilute” the solids. Later in the Level III calculation these phases and aerosols are included (see Table 1.5.4).

Correction for Dissociation

As discussed earlier in Section 1.2.4, for dissociating or ionizing organic chemicals in aqueous solution, it is necessary to consider the effect of pH and thus the degree of dissociation, and to calculate the concentrations of both ionic and non-ionic species. The EQC model does not address dissociation.

The Z values are calculated using the conventional equations at the pH of the experimental data (i.e., the system pH). The total Z value in water is then separated into its ionic and non-ionic contributions, i.e., fractions of $I/(I+1)$ and $1/(I+1)$. The Z value for the non-ionic form in water is assumed to apply at all pHs i.e., including the environmental pH, but an additional and possibly different ionic Z value in water is deduced at the environmental pH using I calculated at that pH. The total Z values in water are then calculated. Z values in other media are unaffected.

The calculation is illustrated in Table 1.5.5 for pentachlorophenol. The experimental aqueous solubility is $14.0 \text{ g}/\text{m}^3$ at a pH of 5.1. The environmental pH is 7. Higher environmental pH increases the extent of dissociation, thus increasing the Z value in water, increasing the apparent solubility, decreasing the apparent K_{OW} and Henry's law constant and the air-water partition coefficient, and decreasing the soil-water partition coefficient.

Note: At pH of 5.1, K_{OW} is 112200 and is the ratio of concentration in octanol to total concentration in water comprising fractions $1/(1+I)$ or $1/(1+2.29)$ or 0.304 of neutral and 0.696 of ionic species. K_{OW} is thus $112200/0.304$ or 369000 for the neutral species and zero for the ionic species. For the neutral species K_{OC} is assumed to be $0.41 \cdot K_{\text{OW}}$ or 151300, thus K_p is $151300 \times 0.02 \text{ L}/\text{kg}$, i.e., 3027 for a soil of 2% organic carbon. K_{SW} is thus 3027×2.4 where 2.4 is the solid density (kg/L) or 7265. Z_s for the neutral species is thus $7265 \times Z_w$ or 27970. At pH of 7, the neutral species Z values are unaffected, but the Z value for water increases to 704 because of the greater extent of dissociation. K_{SW} thus decreases to $27970/704$ or 39.72.

TABLE 1.5.4

Bulk phase Z values, Z_{Bi} deduced as $\sum v_i Z_i$, in which the coefficients, e.g., 2×10^{-11} , are the volume fractions v_i of each pure phase as specified in Table 1.5.2

Compartment	Bulk Z values		
Air	$Z_{\text{B1}} = Z_1 + 2 \times 10^{-11} Z_7$	(approximately $30 \mu\text{g}/\text{m}^3$ aerosols)	
Water	$Z_{\text{B2}} = Z_2 + 5 \times 10^{-6} Z_5 + 1 \times 10^{-6} Z_6$	(5 ppm solids, 1 ppm fish by volume)	
Soil	$Z_{\text{B3}} = 0.2 Z_1 + 0.3 Z_2 + 0.5 Z_3$	(20% air, 30% water, 50% solids)	
Sediment	$Z_{\text{B4}} = 0.8 Z_2 + 0.2 Z_4$	(80% water, 20% solids)	

TABLE 1.5.5

Calculated Z values at different experimental and environmental pHs of pentachlorophenol. Z values at 25°C , $\log K_{\text{OW}}$ is 5.05, $\text{p}K_a$ 4.74, at data pH of 5.1 and environmental pH of 7.0 for air, water and soil of fraction organic carbon 0.02 and density of soil $2.4 \text{ kg}/\text{L}$

	At data pH of 5.1 ($I = 2.29$)			At environ. pH of 7 ($I = 182$)		
	Neutral	Ionic	Total	Neutral	Ionic	Total
Air	4.03×10^{-4}	0	4.03×10^{-4}	4.03×10^{-4}	0	4.03×10^{-4}
Water	3.85	8.82	12.67	3.85	700.4	704.2
Soil solids	27970	0	27970	27970	0	27970

TABLE 1.5.6

Calculated Z_w values and some partition coefficients at different environmental pHs for pentachlorophenol (PCP), 2,4-dichlorophenol (2,4-DCP), 2,4,6-trichlorophenol (2,4,6-TCP) and *p*-cresol at 25°C. K_{AW} is the air-water partition coefficient and K_{SW} is the soil-water partition coefficient

At pH	Z values in water				Partitioning properties			
	Neutral	Ionic	Total Z_w	Fraction x_N	S_T g/m ³	H_T Pa·m ³ /mol	K_{AW}	K_{SW}
<i>PCP</i>								
4	3.849	0.7004	4.549	0.846	16.55	0.224	8.9×10^{-5}	6147
6	3.849	70.04	73.89	0.052	268.8	0.0135	5.46×10^{-6}	378.5
7	3.849	700.4	704.2	0.0055	2562	0.00142	5.73×10^{-7}	39.7
<i>2,4,6-TCP</i>								
4	1.7677	0.0140	1.7817	0.992	434	0.5612	2.26×10^{-4}	105.2
6	1.7677	1.4041	3.1718	0.557	772	0.315	1.272×10^{-4}	59.09
7	1.7677	14.041	15.8088	0.118	3644	0.172	6.945×10^{-5}	11.86
<i>2,4-DCP</i>								
4	3.063	0.000386	3.063	1.0	6000	0.326	0.000132	31.24
6	3.063	0.0386	3.101	0.988	6073	0.322	0.000130	30.85
7	3.063	0.386	3.448	0.888	6760	0.290	0.000117	27.75
<i>p</i> -Cresol								
4	11.97	0	11.948	1.0	22000	0.0836	3.37×10^{-5}	1.968
7	11.97	0.0066	11.975	1.0	22000	0.0836	3.35×10^{-5}	1.968

This is further demonstrated in Table 1.5.6 which shows the effects of environmental pH on the partitioning behavior of 2,4-dichlorophenol ($pK_a = 7.90$, solubility of 6000 g/m³ at pH of 5.1 and $\log K_{OW} = 3.20$), 2,4,6-trichlorophenol ($pK_a = 6.10$, solubility of 430 g/m³ at pH of 5.1 and $\log K_{OW} = 3.69$), pentachlorophenol ($pK_a = 4.74$, solubility of 14.0 g/m³ at pH of 5.1 and $\log K_{OW} = 5.05$) and *p*-cresol ($pK_a = 10.26$, a solubility of 22000 g/m³ and $\log K_{OW} = 2.0$) in the multimedia environment at 25°C. For environmental pH from 4 to 7, there is no significant effect for *p*-cresol (or for chemicals for which $pK_a \gg pH$), very little effect for 2,4-dichlorophenol (and chemicals with pK_a ranging between 7–10). There is some effect on 2,4,6-trichlorophenol (and chemicals with pK_a of 6–7) and a large effect for pentachlorophenol.

A similar treatment can be applied to other dissociating compounds such as the carboxylic acids, nitrophenols. For bases such as amines the pK_a is defined as $(14 - pK_b)$, and the extent of dissociation is estimated as above.

1.5.3 LEVEL II FUGACITY CALCULATIONS

The Level II calculation simulates a situation in which a chemical is continuously discharged into the multimedia environment and achieves a steady-state and equilibrium condition, at which input and output rates are equal. The task is to deduce the rates of loss by reaction and advection and the prevailing concentrations and masses.

The reaction rate data developed for each chemical in the tables are used to select a reactivity class as described earlier, and hence a first-order rate constant for each medium. Often these rates are in considerable doubt; thus the quantities selected should be used with extreme caution because they may not be widely applicable. The rate constants k_i h⁻¹ are used to calculate reaction D values for each medium D_{Ri} as $V_i Z_i k_i$. The rate of reactive loss is then $D_{Ri} f$ mol/h.

For advection, it is necessary to select flow rates. This is conveniently done in the form of advective residence times, t in hour (h); thus the advection rate G_i is V_i/t m³/h for each medium. For air, a residence time of 100 hours is used (approximately 4 days), which is probably too long for the geographic area considered, but shorter residence times tend to cause air advective loss to be a dominant mechanism. For water, a figure of 1000 hours (42 days) is used, reflecting a mixture of rivers and lakes. For sediment burial (which is treated as an advective loss), a time of 50,000 hours or 5.7 years is used. Only for very persistent, hydrophobic chemicals is this process important. No advective loss from soil is included. The D value for loss by advection D_{Ai} is $G_i Z_i$, and the rates are $D_{Ai} f$ mol/h.

There may thus be losses caused by both reaction and advection D values for the four primary media. These loss processes are not included for fish or suspended matter. At steady-state and equilibrium conditions, the input rate E mol/h can be equated to the sum of the output rates, from which the common fugacity can be calculated as follows

$$E = f \cdot \Sigma D_{Ai} + f \cdot \Sigma D_{Ri}$$

thus,

$$f = E / (\Sigma D_{Ai} + \Sigma D_{Ri})$$

The common assumed emission rate is 1000 kg/h or 1 tonne/h. To achieve an amount equivalent to the 100 tonnes in the Level I calculation requires an overall residence time of 100 hours. Again, the concentrations and amounts m_i and Σm_i or M can be deduced, as well as the reaction and advection rates. These rates obviously total to give the input rate E . Of particular interest are the relative rates of these loss processes, and the overall persistence or residence time, which is calculated as

$$t_o = M/E$$

where M is the total amount present. It is also useful to calculate a reaction and an advection persistence t_R and t_A as

$$t_R = M / \Sigma D_{Ri} f \quad t_A = M / \Sigma D_{Ai} f$$

Obviously,

$$1/t_o = 1/t_R + 1/t_A$$

These persistences indicate the likelihood of the chemical being lost by reaction as distinct from advection. The percentage distribution of chemical between phases is identical to that in Level I. A pie chart depicting the distribution of losses can be drawn.

1.5.4 LEVEL III FUGACITY CALCULATIONS

Whereas the Levels I and II calculations assume equilibrium to prevail between all media, this is recognized as being excessively simplistic and even misleading. In the interests of algebraic simplicity, only the four primary media are treated for this level. The task is to develop expressions for intermedia transport rates by the various diffusive and non-diffusive processes as described by Mackay (2001). This is done by selecting values for 12 intermedia transport velocity parameters which have dimensions of velocity (m/h or m/year), are designated as U_i m/h and are applied to all chemicals. These parameters are used to calculate seven intermedia transport D values.

It is desirable to calculate new “bulk phase” Z values for the four primary media which include the contribution of dispersed phases within each medium as described by Mackay and Paterson (1991) and as listed earlier. The air is now treated as an air-aerosol mixture, water as water plus suspended particles and fish, soil as solids, air and water, and sediment as solids and porewater. The Z values thus differ from the Level I and Level II “pure phase” values. The necessity of introducing this complication arises from the fact that much of the intermedia transport of the chemicals occurs in association with the movement of chemical in these dispersed phases. To accommodate this change the same volumes of the soil solids and sediment solids are retained, but the total phase volumes are increased. These Level III volumes are also given in Table 1.5.2. The reaction and advection D values employ the generally smaller bulk phase Z values but the same residence times; thus the G values are increased and the D values are generally larger.

Intermedia D Values

The justification for each intermedia D value follows. It is noteworthy that, for example, air-to-water and water-to-air values differ because of the presence of one-way non-diffusive processes. A fuller description of the background to these calculations is given by Mackay (2001).

1. Air to Water (D_{12})

Four processes are considered: diffusion (absorption), dissolution in rain of gaseous chemical, and wet and dry deposition of particle-associated chemical.

For diffusion, the conventional two-film approach is taken with water-side (k_w) and air-side (k_A) mass transfer coefficients (m/h) being defined. Values of 0.05 m/h for k_w and 5 m/h for k_A are used. The absorption D value is then

$$D_{vw} = 1/[1/(k_A A_w Z_1) + 1/(k_w A_w Z_2)]$$

where A_w is the air-water area (m^2) and Z_1 and Z_2 are the pure air and water Z values. The velocities k_A and k_w are designated as U_1 and U_2 .

For rain dissolution, a rainfall rate of 0.876 m/year is used, i.e., U_R or U_3 is 10^{-4} m/h. The D value for rain dissolution D_{RW} is then

$$D_{RW} = U_R A_w Z_2 = U_3 A_w Z_2$$

For wet deposition, it is assumed that the rain scavenges Q (the scavenging ratio) or about 200,000 times its volume of air. Using a particle concentration (volume fraction) v_Q of 2×10^{-11} , this corresponds to the removal of Qv_Q or 4×10^{-6} volumes of aerosol per volume of rain. The total rate of particle removal by wet deposition is then $Qv_Q U_R A_w$ m^3/h , thus the wet "transport velocity" $Qv_Q U_R$ is 4×10^{-10} m/h.

For dry deposition, a typical deposition velocity U_Q of 10 m/h is selected yielding a rate of particle removal of $U_Q v_Q A_w$ or $2 \times 10^{-10} A_w$ m^3/h corresponding to a transport velocity of 2×10^{-10} m/h. Thus,

$$U_4 = Qv_Q U_R + U_Q v_Q = v_Q (Q U_R + U_Q)$$

The total particle transport velocity U_4 for wet and dry deposition is thus 6×10^{-10} m/h (67% wet and 33% dry) and the total D value D_{QW} is

$$D_{QW} = U_4 A_w Z_7$$

where Z_7 is the aerosol Z value.

The overall D value is given by

$$D_{12} = D_{vw} + D_{RW} + D_{QW}$$

2. Water to Air (D_{21})

Evaporation is treated as the reverse of absorption; thus D_{21} is simply D_{vw} as before.

3. Air to Soil (D_{13})

A similar approach is adopted as for air-to-water transfer. Four processes are considered with rain dissolution (D_{RS}) and wet and dry deposition (D_{QS}) being treated identically except that the area term is now the air-soil area A_s .

For diffusion, the approach of Jury et al. (1983, 1984a,b,c) is used as described by Mackay and Stiver (1991) and Mackay (1991) in which three diffusive processes are treated. The air boundary layer is characterized by a mass transfer coefficient k_s or U_7 of 5 m/h, equal to that of the air-water mass transfer coefficient k_A used in D_{12} .

For diffusion in the soil air-pores, a molecular diffusivity of 0.02 m^2/h is reduced to an effective diffusivity using a Millington-Quirk type of relationship by a factor of about 20 to $10^{-3} m^2/h$. Combining this with a path length of 0.05 m gives an effective air-to-soil mass transfer coefficient k_{SA} of 0.02 m/h, which is designated as U_5 .

Similarly, for diffusion in water a molecular diffusivity of $2 \times 10^{-6} m^2/h$ is reduced by a factor of 20 to an effective diffusivity of $10^{-7} m^2/h$, which is combined with a path length of 0.05 m to give an effective soil-to-water mass transfer coefficient of k_{SW} 2×10^{-6} m/h.

It is probable that capillary flow of water contributes to transport in the soil. For example, a rate of 7 cm/year would yield an equivalent water velocity of 8×10^{-6} m/h, which exceeds the water diffusion rate by a factor of four. For illustrative purposes we thus select a water transport velocity or coefficient U_6 in the soil of 10×10^{-6} m/h, recognizing that this will vary with rainfall characteristics and soil type. These soil processes are in parallel with boundary layer diffusion in series, so the final equations are

$$D_{VS} = 1/[1/D_s + 1/(D_{SW} + D_{SA})]$$

where

$$D_S = U_7 A_S Z_1 \quad (U_7 = 5 \text{ m/h})$$

$$D_{SW} = U_6 A_S Z_2 \quad (U_6 = 10 \times 10^{-6} \text{ m/h})$$

$$D_{SA} = U_5 A_S Z_1 \quad (U_5 = 0.02 \text{ m/h})$$

where A_S is the soil horizontal area.

Air-soil diffusion thus appears to be much slower than air-water diffusion because of the slow migration in the soil matrix. In practice, the result will be a nonuniform composition in the soil with the surface soil (which is much more accessible to the air than the deeper soil) being closer in fugacity to the atmosphere.

The overall D value is given as

$$D_{13} = D_{VS} + D_{QS} + D_{RS}$$

4. Soil to Air (D_{31})

Evaporation is treated as the reverse of absorption, thus the D value is simply D_{VS} .

5. Water to Sediment (D_{24})

Two processes are treated, diffusion and deposition.

Diffusion is characterized by a mass transfer coefficient U_8 of 10^{-4} m/h, which can be regarded as a molecular diffusivity of 2×10^{-6} m²/h divided by a path length of 0.02 m. In practice, bioturbation may contribute substantially to this exchange process, and in shallow water current-induced turbulence may also increase the rate of transport. Diffusion in association with organic colloids is not included. The D value is thus given as $U_8 A_W Z_2$.

Deposition is assumed to occur at a rate of 5000 m³/h, which corresponds to the addition of a depth of solids of 0.438 cm/year; thus 43.8% of the solids resident in the accessible bottom sediment is added each year. This rate is about 12 cm³/m²-day, which is high compared to values observed in large lakes. The velocity U_9 , corresponding to the addition of 5000 m³/h over the area of 10^{10} m², is thus 5×10^{-7} m/h.

It is assumed that of this 5000 m³/h deposited, 2000 m³/h or 40% is buried (yielding the advective flow rate in [Table 1.5.1](#)), 2000 m³/h or 40% is resuspended (as discussed later) and the remaining 20% is mineralized organic matter. The organic carbon balance is thus only approximate.

The transport velocities are thus:

deposition U_9	5.0×10^{-7} m/h or 0.438 cm/y
resuspension U_{10}	2.0×10^{-7} m/h or 0.175 cm/y
burial U_B	2.0×10^{-7} m/h or 0.175 cm/y
(included as an advective residence time of 50,000 h)	

The water-to-sediment D value is thus

$$D_{24} = U_8 A_W Z_2 + U_9 A_W Z_5$$

where Z_5 is the Z value of the particles in the water column.

6. Sediment to Water (D_{42})

This is treated similarly to D_{24} giving:

$$D_{42} = U_8 A_W Z_2 + U_{10} A_W Z_4$$

where U_{10} is the sediment resuspension velocity of 2.0×10^{-7} m/h and Z_4 is the Z value of the sediment solids.

7. Sediment Advection or Burial (D_{A4})

This D value is $U_B A_W Z_4$, where U_B , the sediment burial rate, is 2.0×10^{-7} m/h. It can be viewed as $G_B Z_{B4}$, where G_B is the total burial rate specified as V_S/t_B where t_B (residence time) is 50,000 h, and V_S (the sediment volume) is the product of sediment depth (0.01 cm) and area A_W . Z_4 , Z_{B4} are the Z values of the sediment solids and of the bulk sediment, respectively. Since there are 20% solids, Z_{B4} is about 0.2 Z_4 . There is a slight difference between these approaches because in the advection approach (which is used here) there is burial of water as well as solids.

8. Soil to Water Run-Off (D_{32})

It is assumed that there is run-off of water at a rate of 50% of the rain rate, i.e., the D value is

$$D = 0.5 U_3 A_S Z_2 = U_{11} A_S Z_2$$

thus the transport velocity term U_{11} is $0.5U_3$ or 5×10^{-5} m/h.

For solids run-off it is assumed that this run-off water contains 200 parts per million by volume of solids; thus the corresponding velocity term U_{12} is $200 \times 10^{-6}U_{11}$, i.e., 10^{-8} m/h. This corresponds to the loss of soil at a rate of about 0.1 mm per year. If these solids were completely deposited in the aquatic environment (which is about 1/10th the soil area), they would accumulate at about 0.1 cm per year, which is about a factor of four less than the deposition rate to sediments. The implication is that most of this deposition is of naturally generated organic carbon and from sources such as bank erosion.

Summary

The twelve intermedia transport parameters are listed in Table 1.5.7 and the equations are summarized in Table 1.5.8.

Algebraic Solution

Four mass balance equations can be written, one for each medium, resulting in a total of four unknown fugacities, enabling simple algebraic solution as shown in Table 1.5.9. From the four fugacities, the concentration, amounts and rates of all transport and transformation processes can be deduced, yielding a complete mass balance.

The new information from the Level III calculations are the intermedia transport data, i.e., the extent to which chemical discharged into one medium tends to migrate into another. This migration pattern depends strongly on the proportions of the chemical discharged into each medium; indeed, the relative amounts in each medium are largely a reflection of the locations of discharge. It is difficult to interpret these mass balance diagrams because, for example, chemical depositing from air to water may have been discharged to air, or to soil from which it evaporated, or even to water from which it is cycling to and from air.

To simplify this interpretation, it is best to conduct three separate Level III calculations in which unit amounts (1000 kg/h) are introduced individually into air, soil and water. Direct discharges to sediment are unlikely and are not

TABLE 1.5.7
Intermedia transport parameters

U		m/h	m/year
1	Air side, air-water MTC*, k_A	5	43,800
2	Water side, air-water MTC, k_W	0.05	438
3	Rain rate, U_R	10^{-4}	0.876
4	Aerosol deposition	6×10^{-10}	5.256×10^{-6}
5	Soil-air phase diffusion MTC, k_{SA}	0.02	175.2
6	Soil-water phase diffusion MTC, k_{SW}	10×10^{-6}	0.0876
7	Soil-air boundary layer MTC, k_S	5	43,800
8	Sediment-water MTC	10^{-4}	0.876
9	Sediment deposition	5.0×10^{-7}	0.00438
10	Sediment resuspension	2.0×10^{-7}	0.00175
11	Soil-water run-off	5.0×10^{-5}	0.438
12	Soil-solids run-off	10^{-8}	8.76×10^{-5}

*MTC is mass transfer coefficient. Scavenging ratio Q is 2×10^5 , dry deposition velocity U_Q is 10 m/h and sediment burial rate U_B is 2.0×10^{-7} m/h

TABLE 1.5.8
Intermedia transport D value equations

Air-Water	$D_{12} = D_{vw} + D_{rw} + D_{qw}$ $D_{vw} = A_w/(1/U_1Z_1 + 1/U_2Z_2)$ $D_{rw} = U_3A_wZ_2$ $D_{qw} = U_4A_wZ_7$
Water-Air	$D_{21} = D_{vw}$
Air-Soil	$D_{13} = D_{vs} + D_{rs} + D_{qs}$ $D_{vs} = 1/(1/D_s + 1/(D_{sw} + D_{sa}))$ $D_s = U_7A_sZ_1$ $D_{sa} = U_5A_sZ_1$ $D_{sw} = U_6A_sZ_2$ $D_{rs} = U_3A_sZ_2$ $D_{qs} = U_4A_sZ_7$
Soil-Air	$D_{31} = D_{vs}$
Water-Sediment	$D_{24} = U_8A_wZ_2 + U_9A_wZ_5$
Sediment-Water	$D_{42} = U_8A_wZ_2 + U_{10}A_wZ_4$
Soil-Water	$D_{32} = U_{11}A_sZ_2 + U_{12}A_sZ_3$

TABLE 1.5.9
Level III solutions to mass balance equations

Compartment	Mass balance equations
Air	$E_1 + f_2D_{21} + f_3D_{31} = f_1D_{T1}$
Water	$E_2 + f_1D_{12} + f_3D_{32} + f_4D_{42} = f_2D_{T2}$
Soil	$E_3 + f_1D_{13} = f_3D_{T3}$
Sediment	$E_4 + f_2D_{24} = f_4D_{T4}$
where	E_i is discharge rate, E_4 usually being zero. $D_{T1} = D_{R1} + D_{A1} + D_{12} + D_{13}$ $D_{T2} = D_{R2} + D_{A2} + D_{21} + D_{23} + D_{24}, (D_{23} = 0)$ $D_{T3} = D_{R3} + D_{A3} + D_{31} + D_{32}, (D_{A3} = 0)$ $D_{T4} = D_{R4} + D_{A4} + D_{42}$
Solutions:	$f_2 = [E_2 + J_1J_4/J_3 + E_3D_{32}/D_{T3} + E_4D_{42}/D_{T4}]/(D_{T2} - J_2J_4/J_3 - D_{24} \cdot D_{42}/D_{T4})$ $f_1 = (J_1 + f_2J_2)/J_3$ $f_3 = (E_3 + f_1D_{13})/D_{T3}$ $f_4 = (E_4 + f_2D_{24})/D_{T4}$
where	$J_1 = E_1/D_{T1} + E_3D_{31}/(D_{T3} \cdot D_{T1})$ $J_2 = D_{21}/D_{T1}$ $J_3 = 1 - D_{31} \cdot D_{13}/(D_{T1} \cdot D_{T3})$ $J_4 = D_{12} + D_{32} \cdot D_{13}/D_{T3}$

considered here. These calculations show clearly the extent to which intermedia transport occurs. If, for example, the intermedia D values are small compared to the reaction and advection values, the discharged chemical will tend to remain in the discharge or "source" medium with only a small proportion migrating to other media. Conversely, if the intermedia D values are relatively large, the chemical becomes very susceptible to intermedia transport. This behavior is observed for persistent substances such as PCBs, which have very low rates of reaction.

A direct assessment of multimedia behavior is thus possible by examining the proportions of chemical found at steady state in the "source" medium and in other media. For example, when discharged to water, an appreciable fraction of the benzene is found in air, whereas for atrazine, only a negligible fraction of atrazine reaches air.

Linear Additivity or Superposition of Results

Because these equations are entirely linear, the solutions can be scaled linearly. The concentrations resulting from a discharge of 2000 kg/h are simply twice those of 1000 kg/h. Further, if discharge of 1000 kg/h to air causes 500 kg in water and discharge of 1000 kg/h to soil causes 100 kg in water, then if both discharges occur simultaneously, there will be 600 kg in water. If the discharge to soil is increased to 3000 kg/h, the total amount in the water will rise to (500 + 300) or 800 kg. It is thus possible to deduce the amount in any medium arising from any combination of discharge rates by scaling and adding the responses from the unit inputs. This “linear additivity principle” is more fully discussed by Stiver and Mackay (1989).

The persistence or residence time of the chemical is independent of the emission rate, but it does depend on the “mode of entry, i.e., into which compartment the chemical is emitted.”

In the diagrams presented later, these three-unit (1000 kg/h) responses are given. Also, an illustrative “three discharge” mass balance is given in which a total of 1000 kg/h is discharged, but in proportions judged to be typical of chemical use and discharge to the environment. For example, benzene is believed to be mostly discharged to air with minor amounts to soil and water.

Also given in the tables are the rates of reaction, advection and intermedia transport for each case.

The reader can deduce the fate of any desired discharge pattern by appropriate scaling and addition. It is important to emphasize that because the values of transport velocity parameters are only illustrative, actual environmental conditions may be quite different; thus, simulation of conditions in a specific region requires determination of appropriate parameter values as well as the site-specific dimensions, reaction rate constants and the physical-chemical properties which prevail at the desired temperature.

In total, the aim is to convey an impression of the likely environmental behavior of the chemical in a readily assimilable form.

1.6 DATA SOURCES AND PRESENTATION

1.6.1 DATA SOURCES

Most physical properties such as molecular weight (MW, g/mol), melting point (m.p., °C), boiling point (b.p., °C), and density have been obtained from commonly used handbooks such as the *CRC Handbook of Chemistry and Physics* (Weast 1972, 1982; Lide 2003), Lange's *Handbook of Chemistry* (Dean 1979, 1985, 1992), Dreisbach's *Physical Properties of Chemical Compounds*, Vol. I, II and III (1955, 1959, 1961), Organic Solvents, Physical Properties and Methods of Purification (Riddick et al. 1986), *The Merck Index* (Windholz 1983, Budavari 1989) and several handbooks and compilations of chemical property data for pesticides. Notable are the text by Hartley and Graham-Bryce (1980), the *Agrochemicals Handbook* (Hartley and Kidd 1987), the *Pesticide Manual* (Worthing and co-workers 1983, 1987, 1991, Tomlin 1994), the *CRC Handbook of Pesticides* (Milne 1995), the *Agrochemicals Desk Reference* (Montgomery 1993) and the SCS/ARS/CES Pesticide Properties Database by Wauchope and co-workers (Wauchope et al. 1992, Augustijn-Beckers et al. 1994, Hornsby et al. 1996). Other physical-chemical properties such as aqueous solubility, vapor pressure, octanol-water partition coefficient, Henry's law constant, bioconcentration factor and sorption coefficient have been obtained from scientific journals or other environmental handbooks, notably Verschueren's *Handbook of Environmental Data on Organic Chemicals* (1977, 1983) and Howard and co-workers' *Handbook of Environmental Fate and Exposure Data*, Vol. I, II, III and IV (1989, 1990, 1991 and 1993). Other important sources of vapor pressure are the *CRC Handbook of Chemistry and Physics* (Weast 1972, 1982), Lange's *Handbook of Chemistry* (Dean 1992), the *Handbook of Vapor Pressures and Heats of Vaporization of Hydrocarbons and Related Compounds* (Zwolinski and Wilhoit 1971), the *Vapor Pressure of Pure Substances* (Boublik et al. 1973, 1984), the *Handbook of the Thermodynamics of Organic Compounds* (Stephenson and Malanowski 1987). For aqueous solubilities, valuable sources include the *IUPAC Solubility Data Series* (Barton 1984, Horvath and Getzen 1985, Shaw 1989a,b) and Horvath's *Halogenated Hydrocarbons, Solubility-Miscibility with Water* (Horvath 1982). Octanol-water partition coefficients are conveniently obtained from the compilation by Leo et al. (1971), Hansch and Leo (1979), Hansch et al. (1995), and Sangster (1989, 1993), or can be calculated from molecular structure by the methods of Hansch and Leo (1979) or Rekker (1977). Lyman et al. (1982) and Boethling and Mackay (2000) also outline methods of estimating solubility, K_{ow} , vapor pressure, and the bioconcentration factor for organic chemicals. The recent *Handbook of Environmental Degradation Rates* by Howard et al. (1991) is a valuable source of rate constants and half-lives.

The most reliable sources of data are the original citations of valuable experimental data in the reviewed scientific literature. Particularly reliable are those papers which contain a critical review of data from a number of sources as well as independent experimental determinations. Calculated or correlated values are viewed as being less reliable. The aim

in this work has been to gather sufficient experimental data with a list of citations to interpret them and select a “best” or “most likely” value.

1.6.2 DATA PRESENTATION

Chemical Properties.

The emphasis in this handbook is on experimentally determined values rather than estimated values. The latter are included when there is a lack of experimental data. Included in the experimental data are indirect measurements using GC or HPLC retention times.

The names, formula, melting and boiling point and density data are self-explanatory.

The molar volumes are in some cases at the stated temperature and in other cases at the normal boiling point. Certain calculated molecular volumes are also used; thus the reader is cautioned to ensure that when using a molar volume in any correlation, it is correctly selected. In the case of polynuclear aromatic hydrocarbons, the Le Bas molar volume is regarded as suspect because of the compact nature of the multi-ring compounds. It should thus be regarded as merely an indication of relative volume, not an absolute volume.

Heats of fusion, ΔH_{fus} , are generally expressed in kcal/mol or kJ/mol and entropies of fusion, ΔS_{fus} in cal/mol·K (e.u. or entropy unit) or J/mol·K. The fugacity ratio F , as discussed in Section 1.2.8, is used to calculate the supercooled liquid vapor pressure or solubility for correlation purposes. In the case of liquids such as benzene, it is 1.0. For solids it is a fraction representing the ratio of solid-to-liquid solubility or vapor pressure.

A wide variety of solubilities (in units of g/m³ or the equivalent mg/L) have been reported. Experimental data have the method of determination indicated. In other compilations of data the reported value has merely been quoted from another secondary source. In some cases the value has been calculated. The abbreviations are generally self-explanatory and usually include two entries, the method of equilibration followed by the method of determination. From these values a single value is selected for inclusion in the summary data table. Vapor pressures and octanol-water partition coefficients are selected similarly.

The reader is advised to consult the original reference when using these values of bioconcentration factors (BCF), bioaccumulation factors (BAF), K_{OC} and K_{OM} , to ensure that conditions are as close as possible to those of specific interest.

The “Environmental Fate Rate Constants” refer to specific degradation processes rather than media. As far as possible the original numerical quantities are given and thus there is a variety of time units with some expressions being rate constants and others half-lives. The conversion is that the rate constant k is $0.693/t_{1/2}$ where $t_{1/2}$ is the half-life.

From these data a set of medium-specific degradation reaction half-lives is selected for use in Levels II and III calculations. Emphasis is placed on the fastest and the most plausible degradation process for each of the environmental compartments considered. Instead of assuming an equal half-life for both the water and soil compartment as suggested by Howard et al. (1991), a slower active class (in the reactivity table described earlier) was assigned for soil and sediment compared to that of the water compartment. This is in part because the major degradation processes are often photolysis (or photooxidation) and biodegradation. There is an element of judgment in this selection, and it is desirable to explore the implications of selecting other values.

The “Half-life in the Environment” data reflect observations of the rate of disappearance of the chemical from a medium, without necessarily identifying the cause of mechanism of loss. For example, loss from water may be a combination of evaporation, biodegradation and photolysis. Clearly these times are highly variable and depend on factors such as temperature, meteorology and the nature of the media. Again, the reader is urged to consult the original references.

1.7 ILLUSTRATIVE QSPR PLOTS AND FATE CALCULATIONS

Illustrative QSPR plots and their interpretation are given in this section, followed by examples of Levels I, II and III fate calculations. A relatively simple evaluation of benzene is given first followed by the more complex evaluation of pentachlorophenol.

1.7.1 QSPR PLOTS FOR MONONUCLEAR AROMATIC HYDROCARBONS

The physical-chemical data for mononuclear aromatics are plotted in the appropriate QSPR plots on [Figures 1.7.1 to 1.7.5](#) (which are also [Figures 3.2.1 to 3.2.5](#) for the mononuclear aromatic hydrocarbons in [Chapter 3](#)). These plots show that the data are relatively “well-behaved,” there being consistency among the reported values for this homologous series. In the case of benzene this QSPR plot is of little value because this is a well-studied chemical, but for other less-studied chemicals the plots are invaluable as a means of checking the reasonableness of data. The plots can also be used,

with appropriate caution, to estimate data for untested chemicals. We do not develop linear regressions of these data since we suggest that the plots be used directly for data estimation purposes. This enables the user to assess into account the values of similarly structured compounds and it gives a direct impression of likely error. We discuss, below, the general nature of the relationships and in particular the slopes of the QSPR plots.

Figures 1.7.1 to 1.7.4 show the dependence of the physical-chemical properties on Le Bas molar volume. Figure 1.7.1 shows that the solubilities of the monoaromatics decrease steadily with increasing molar volume. The vapor pressure data in Figure 1.7.2 are similar, but $\log K_{ow}$ in Figure 1.7.3 increases with increasing molar volume also in a linear fashion.

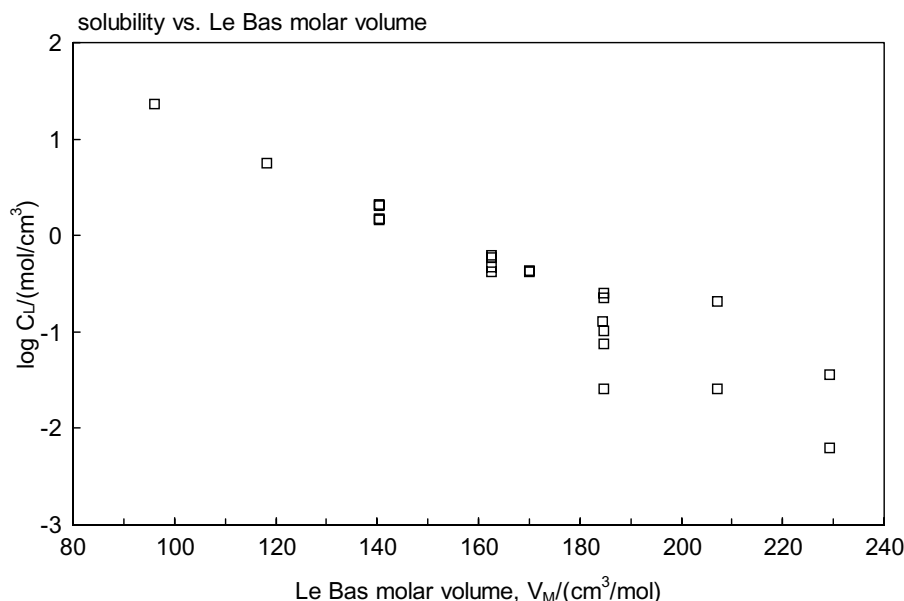


FIGURE 1.7.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.

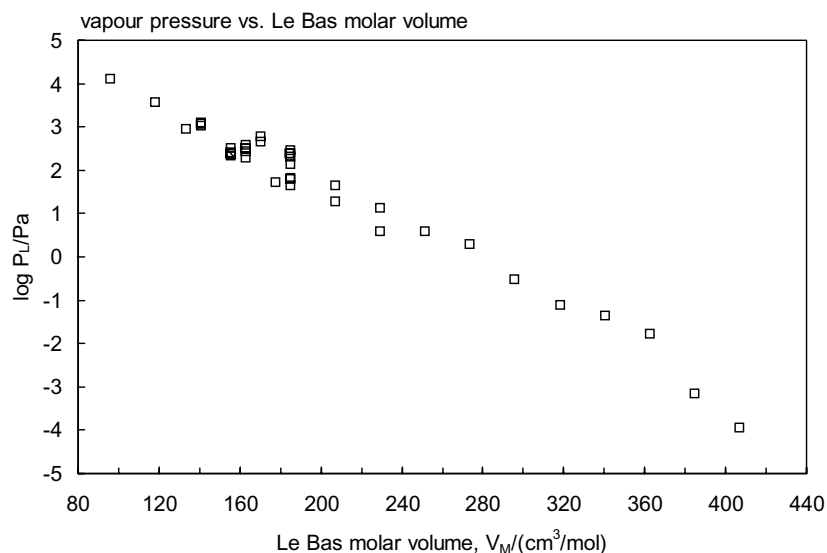


FIGURE 1.7.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.

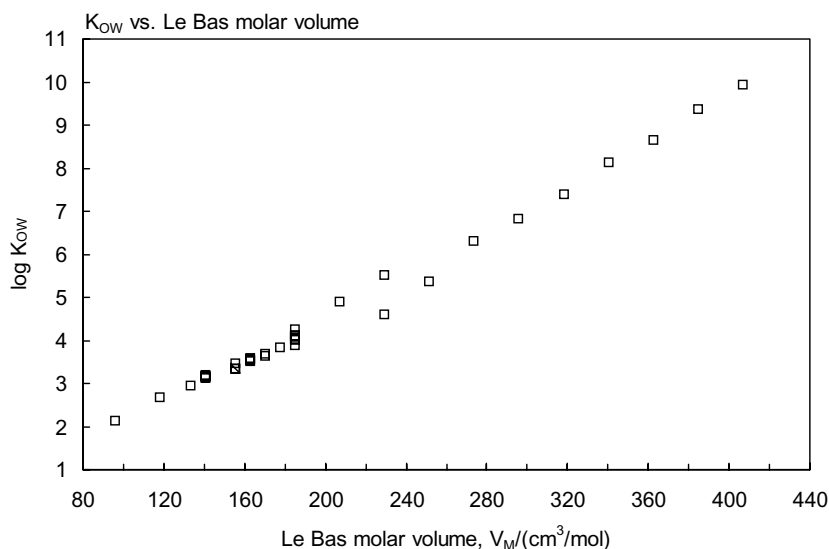


FIGURE 1.7.3 Octanol-water partition coefficient versus Le Bas molar volume for mononuclear aromatic hydrocarbons.

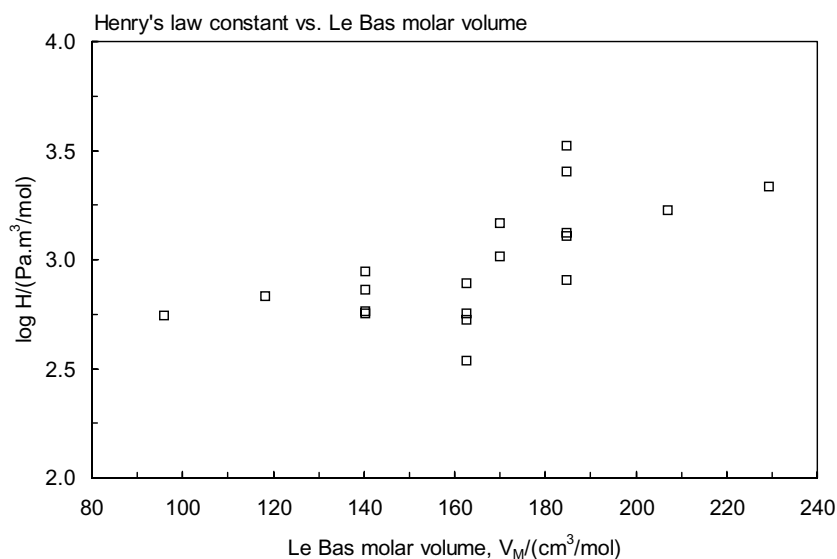


FIGURE 1.7.4 Henry's law constant versus Le Bas molar volume for mononuclear aromatic hydrocarbons.

The plot between Henry's law constant and molar volume (Figure 1.7.4) is more scattered. [Figure 1.7.5](#) shows the often-reported inverse relationship between octanol-water partition coefficient and the supercooled liquid solubility.

The QSPR plots show that an increase in molar volume by 100 cm³/mol generally causes:

- (i) A decrease in log solubility by 2.5 units, i.e., a factor of 10^{2.5} or 316;
- (ii) A decrease in log vapor pressure by 2.2 units, i.e., a factor of 10^{2.2} or 159;
- (iii) An increase in log Henry's law constant of 0.3 (i.e., 2.5 – 2.2) or a factor of 10^{0.3} or 2.0;
- (iv) An increase in log K_{OW} by 2.0 units, i.e., a factor of 100.

The plot of log K_{OW} versus log solubility thus has a slope of approximately 2.0/2.5 or 0.8. This slope of less than 1.0 has been verified experimentally by Chiou et al. (1982) and Bowman and Sans (1983). Its theoretical basis has been discussed in detail by Miller et al. (1985).

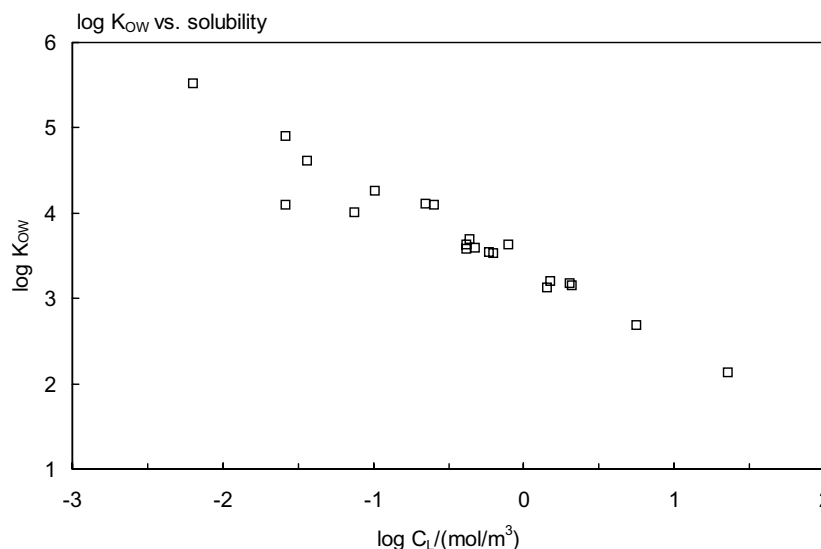


FIGURE 1.7.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for mononuclear aromatic hydrocarbons.

Similar inferences can be made for other homologous series such as the chlorobenzenes and PCBs. In such cases the property change caused by substitution of one chlorine can be deduced as is illustrated later for chlorophenols.

The “Half-life in the Environment” and “Environmental Fate Rate Constants” are medium-specific degradation reaction half-lives selected for use in Level II and Level III calculations. As discussed earlier, emphasis was based on the fastest and the most plausible degradation process for each of the environmental compartments considered.

In summary, the physical-chemical and environmental fate data listed result in the tabulated selected values of solubility, vapor pressure, K_{OW} , dissociation constant where appropriate and reaction half-lives at the end of each chapter. These values are used in the evaluative environmental calculations.

1.7.2 EVALUATIVE CALCULATIONS FOR BENZENE

The illustrative evaluative environmental calculations described here are presented in the following format. Levels I, II and III diagrams are assigned to separate pages, and the physical-chemical properties are included in the Level I diagram. Two types of Level III diagrams are given; one depicts the transport processes and the other the distribution among compartments.

Level I

The Level I calculation suggests that if 100,000 kg (100 tonnes) of benzene are introduced into the 100,000 km² environment, 99% will partition into air at a concentration of 9.9×10^{-7} g/m³ or about 1 µg/m³. The water will contain nearly 1% at a low concentration of 4 µg/m³ or equivalently 4 ng/L. Soils would contain 5×10^{-6} µg/g and sediments about 9.7×10^{-6} µg/g. These values would normally be undetectable as a result of the very low tendency of benzene to sorb to organic matter in these media. The fugacity is calculated to be 3.14×10^{-5} Pa. The dimensionless soil-water and sediment-water partition coefficients or ratios of Z values are 2.6 and 5.3 as a result of a K_{OC} of about 55 and a few percent organic carbon in these media. There is little evidence of bioconcentration with a very low fish concentration of 3.0×10^{-5} µg/g. The pie chart in Figure 1.7.6 clearly shows that air is the primary medium of accumulation.

Level II

The Level II calculation includes the half-lives of 17 h in air, 170 h in water, 550 h in soil and 1700 h in sediment. No reaction is included for suspended sediment or fish. The input of 1000 kg/h results in an overall fugacity of 6×10^{-6} Pa, which is about 20% of the Level I value. The concentrations and amounts in each medium are thus about 20% of the Level I values. The relative mass distribution is identical to Level I. The primary loss mechanism is reaction in air, which accounts for 802 kg/h or 80.2% of the input. Most of the remainder is lost by advective outflow. The water, soil and sediment loss processes are unimportant largely because so little of the benzene is present in these media, but also

Chemical name: Benzene
 Fugacity Level I calculations: (six-compartment model)

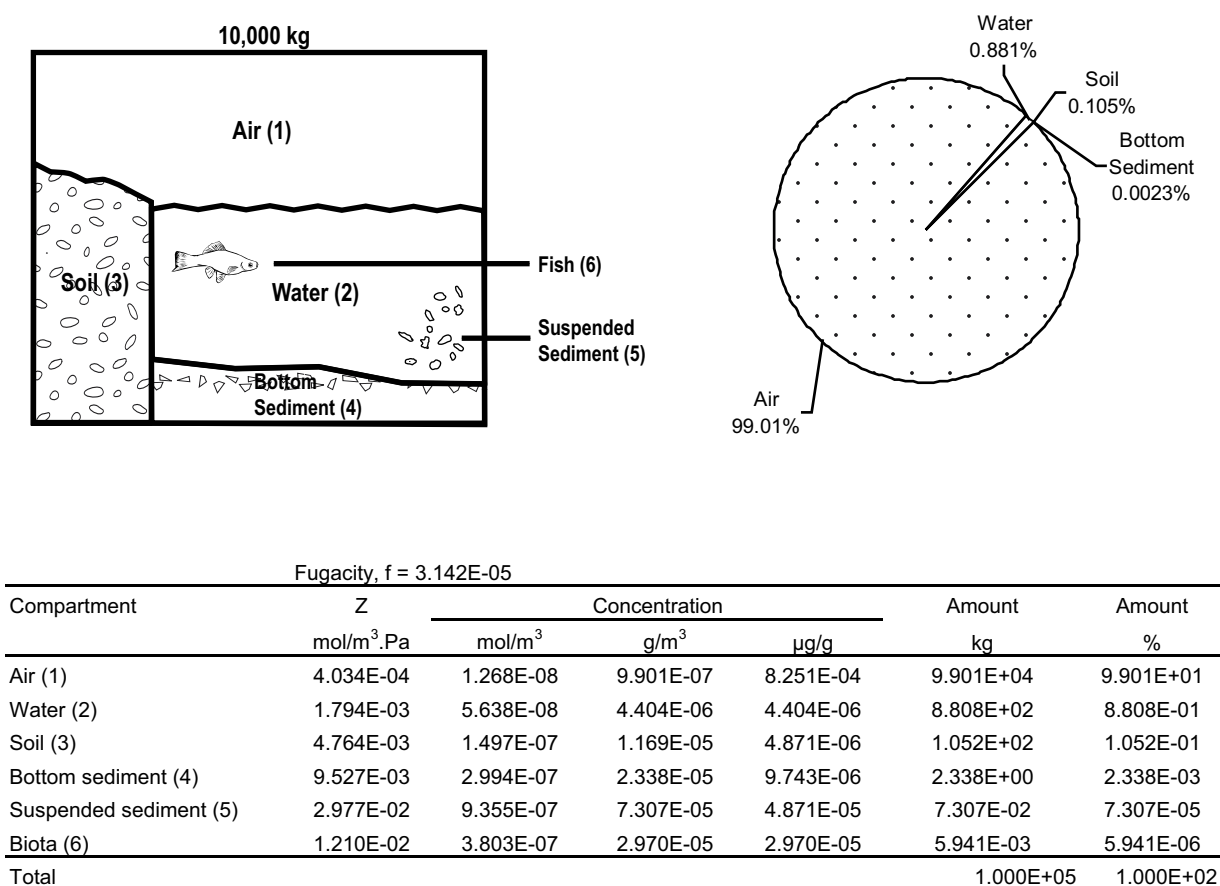


FIGURE 1.7.6 Level I fugacity calculations for benzene in a generic environment.

because of the slower reaction and advection rates. The overall residence time is 19.9 h; thus, there is an inventory of benzene in the system of 19.9×1000 or 19900 kg. The pie chart in Figure 1.7.7 illustrates the dominance of air reaction and advection.

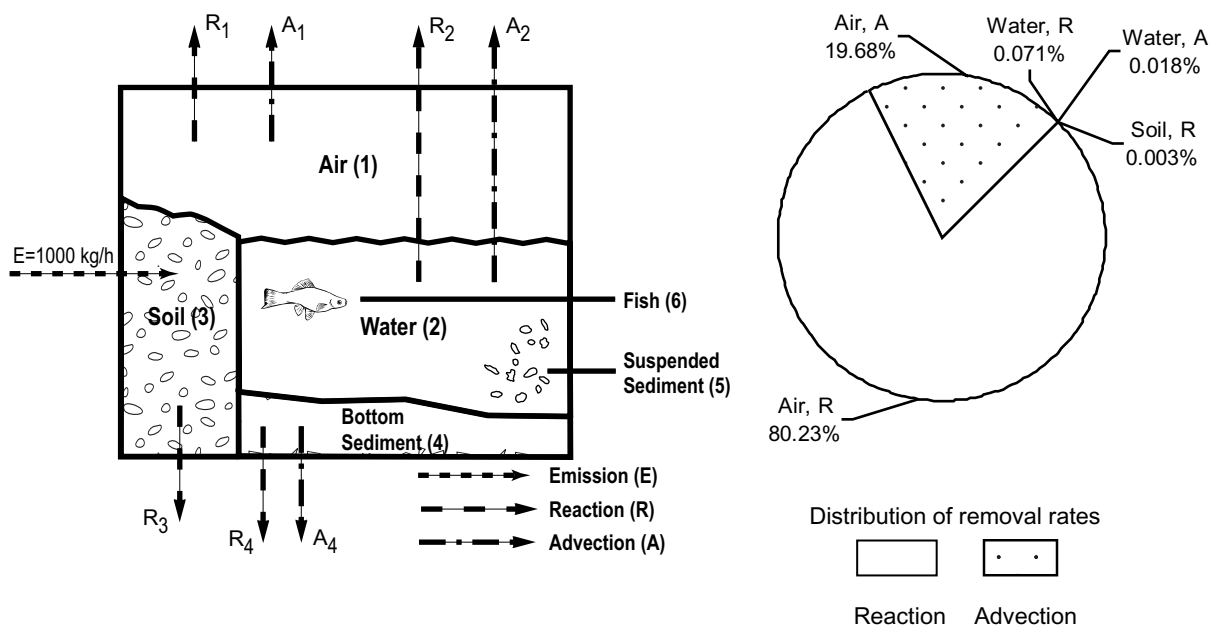
If the primary loss mechanism of atmospheric reaction is accepted as having a 17h half-life, the D value is 1.6×10^9 mol/Pa·h. For any other process to compete with this would require a value of at least 10^8 mol/Pa·h. This is achieved by advection (4×10^8), but the other processes range in D value from 19 (advection in bottom sediment) to 1.5×10^6 (reaction in water) and are thus a factor of over 100 or less. The implication is that the water reaction rate constant would have to be increased 100-fold to become significant. The soil rate constant would require an increase by 10^4 and the sediment by 10^6 . These are inconceivably large numbers corresponding to very short half-lives, thus the actual values of the rate constants in these media are relatively unimportant in this context. They need not be known accurately. The most sensitive quantity is clearly the atmospheric reaction rate.

The amounts in the compartments can be calculated easily from the total amount and the percentages of mass distribution in Level I. For example, the amount in water is 0.881% of 19877 kg or 175 kg.

Level III

The Level III calculation includes an estimation of intermedia transport. Examination of the magnitude of the intermedia D values given in the fate diagram (Figure 1.7.8) suggests that air-water and air-soil transport are most important with water-sediment and soil-water transport being negligible in potential transfer rate. The magnitude of these larger intermedia

Chemical name: Benzene
Fugacity Level II calculations: (six-compartment model)



Compartment	Half-life h	D Value		Concentration mol/m ³	Loss		Total Removal %
		Reaction mol/Pa.h	Advection mol/Pa.h		Reaction kg/h	Advection kg/h	
Air (1)	17	1.645E+09	4.034E+08	2.520E-09	8.023E+02	1.968E+02	9.991E+01
Water (2)	170	1.463E+06	3.589E+05	1.121E-08	7.137E-01	1.751E-01	8.888E-02
Soil (3)	550	5.402E+04	-	2.975E-08	2.635E-02	-	2.635E-03
Bottom sediment (4)	1700	3.884E+02	1.905E+01	5.950E-08	1.895E-04	9.296E-06	1.988E-05
Suspended sediment (5)	170	1.214E+02	2.977E+01	1.859E-07	5.921E-05	1.452E-05	7.373E-06
Biota (6)	170	9.867E+00	2.421E+00	7.559E-08	4.814E-06	1.181E-06	5.995E-07

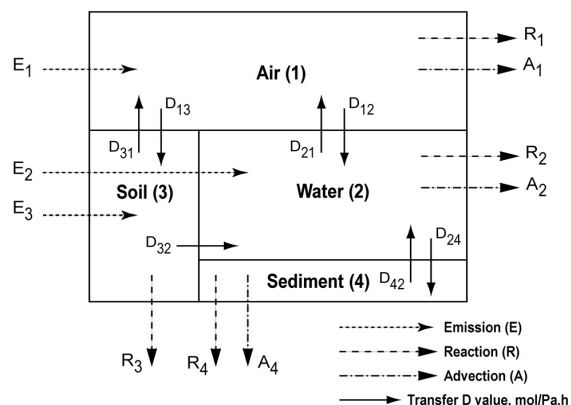
Fugacity, f 6.246E-06 Pa
Total amount, M 2.545E+05 mol
Total amount 1.988E+04 kg
Total reaction D value, D_R 1.646E+09 mol/Pa.h
Total advection D value, D_A 4.038E+08 mol/Pa.h
Total D value, D_T 2.050E+09 mol/Pa.h
Total loss by reaction 8.030E+02 kg/h
Total loss by advection 1.970E+02 kg/h
Total loss 1.000E+03 kg/h
Reaction residence time, t_R 2.475E+01 h
Advection residence time, t_A 1.009E+02 h
Overall residence time, t_O 1.988E+01 h

FIGURE 1.7.7 Level II fugacity calculations for benzene in a generic environment.

transport D values (approximately $10^6 \text{ mol/Pa}\cdot\text{h}$) compared to the atmospheric reaction and advection values of 10^8 to 10^9 suggests that reaction and advection will be very fast relative to transport.

The bulk Z values are similar for air and water to the values for the “pure” phases in Levels I and II, but they are lower for soil and sediment because of the “dilution” of the solid phase with air or water.

Chemical name: Benzene
Fugacity Level III calculations: (four-compartment model)



Phase Properties and Rates:

Compartment	Bulk Z mol/m ³ .Pa	Half-life h	D Value	
			Reaction mol/Pa.h	Advection mol/Pa.h
Air (1)	4.034E-04	1.700E+01	1.645E+09	4.034E+08
Water (2)	1.795E-03	1.700E+02	1.463E+06	3.589E+05
Soil (3)	3.001E-03	5.500E+02	6.806E+04	-
Sediment (4)	3.341E-03	1.700E+03	6.810E+02	3.341E+01

Residence time (h)	Emission to			
	(A)ir Only	(W)ater Only	(S)oil Only	A+W+S
Overall residence time	1.977E+01	1.407E+02	8.675E+01	6.274E+01
Reaction residence time	2.462E+01	1.752E+02	1.058E+02	7.796E+01
Advection residence time	1.004E+02	7.142E+02	4.813E+02	3.212E+02

Phase Properties, Compositions, and Transport and Transformation Rates:

Emission Scenario	Emission (kg/h)			Fugacity (Pa)				Concentration (g/m ³)				Amount (kg)				Total Amount (kg)
	E ₁	E ₂	E ₃	f ₁	f ₂	f ₃	f ₄	C ₁	C ₂	C ₃	C ₄	w ₁	w ₂	w ₃	w ₄	
(A)ir Only	1000	0	0	6.249E-06	2.023E-06	5.781E-06	1.556E-06	1.969E-07	2.836E-07	1.355E-06	4.059E-07	1.969E+04	5.673E+01	2.439E+01	2.030E-01	1.977E+04
(W)ater Only	0	1000	0	2.002E-06	4.775E-03	1.852E-06	3.671E-03	6.308E-08	6.693E-04	4.341E-07	9.579E-04	6.308E+03	1.339E+05	7.814E+00	4.790E+02	1.407E+05
(S)oil Only	0	0	1000	5.676E-06	4.999E-05	1.599E-02	3.843E-05	1.788E-07	7.007E-06	3.748E-03	1.003E-05	1.788E+04	1.401E+03	6.746E+04	5.015E+00	8.675E+04
A+W+S	600	300	100	4.918E-06	1.439E-03	1.603E-03	1.106E-03	1.550E-07	2.017E-04	3.757E-04	2.886E-04	1.550E+04	4.033E+04	6.763E+03	1.443E+02	6.274E+04

Emission Scenario	Emission (kg/h)			Loss by Reaction (kg/h)				Loss by Advection (kg/h)			Intermedia Rate of Transport (kg/h)						
	E ₁	E ₂	E ₃	R ₁	R ₂	R ₃	R ₄	A ₁	A ₂	A ₄	T ₁₂	T ₂₁	T ₁₃	T ₃₁	T ₃₂	T ₂₄	T ₄₂
(A)ir Only	1000	0	0	8.028E+02	2.312E-01	3.073E-02	8.274E-05	1.969E+02	5.673E-02	4.059E-06	4.202E-01	1.358E-01	3.617E-01	3.273E-01	3.648E-03	3.071E-04	2.203E-04
(W)ater Only	0	1000	0	2.572E+02	5.457E+02	9.845E-03	1.952E-01	6.308E+01	1.339E+02	9.579E-03	1.346E-01	3.204E+02	1.159E-01	1.049E-01	1.169E-03	7.248E-01	5.200E-01
(S)oil Only	0	0	1000	7.290E+02	5.713E+00	8.499E+01	2.044E-03	1.788E+02	1.401E+00	1.003E-04	3.816E-01	3.354E+00	3.285E-01	9.052E+02	1.009E+01	7.588E-03	5.444E-03
A+W+S	600	300	100	6.317E+02	1.644E+02	8.521E+00	5.883E-02	1.550E+02	4.033E+01	2.886E-03	3.306E-01	9.653E+01	2.846E-01	9.075E+01	1.011E+00	2.184E-01	1.567E-01

FIGURE 1.7.8 Level III fugacity calculations for benzene in a generic environment.

The first row describes the condition if 1000 kg/h is emitted into the air. The result is similar to the Level II calculation with 19700 kg in air, 57 kg in water, 24 kg in soil and only 0.2 kg in sediment. It can be concluded that benzene discharged to the atmosphere has very little potential to enter other media. The rates of transfer from air to water and air to soil are both only about 0.4 kg/h. Even if the transfer coefficients were increased by a factor of 10, the rates would remain negligible. The reason for this is the value of the mass transfer coefficients which control this transport process. The overall residence time is 19.8 hours, similar to Level II.

If 1000 kg/h of benzene is discharged to water, as in the second row, there is predictably a much higher concentration in water (by a factor of over 2000). There is reaction of 546 kg/h in water, advective outflow of 134 kg/h and transfer to air of 320 kg/h with negligible loss to sediment. The amount in the water is 134000 kg; thus the residence time in the water is 134 h and the overall environmental residence time is a longer 140 hours. The key processes are thus reaction in water (half-life 170 h), evaporation (half-life 290 h) and advective outflow (residence time 1000 h). The evaporation half-life can be calculated as $(0.693 \times \text{mass in water})/\text{rate of transfer}$, i.e., $(0.693 \times 133863)/320 = 290$ h. Clearly, competition between reaction and evaporation in the water determines the overall fate. Ninety-five percent of the benzene discharged is now found in the water, and the concentration is a fairly high 6.7×10^{-4} g/m³, or 670 ng/L.

The third row shows the fate if discharge is to soil. The amount in soil is 67460 kg, reflecting an overall 87 h residence time. The rate of reaction in soil is only 85 kg/h and there is no advection; thus, the primary loss mechanism is transfer to air (T_{31}) at a rate of 905 kg/h, with a relatively minor 10 kg/h to water by run-off. The net result is that the air concentrations are similar to those for air discharge and the soil acts only as a reservoir. The soil concentration of 3.75×10^{-3} g/m³ or 2.5×10^{-3} µg/g or 2.5 ng/g is controlled almost entirely by the rate at which the benzene can evaporate.

The net result is that benzene behaves entirely differently when discharged to the three media. If discharged to air it reacts rapidly and advects with a residence time of 20 h with little transport to soil or water. If discharged to water it reacts and evaporates to air with a residence time of 140 h. If discharged to soil it mostly evaporates to air with a residence time in soil of 53 h.

The final scenario is a combination of discharges, 600 kg/h to air, 300 kg/h to water, and 100 kg/h to soil. The concentrations, amounts and transport and transformation rates are merely linearly combined versions of the three initial scenarios. For example, the rate of reaction in air is now 632 kg/h. This is 0.6 of the first (air emission) rate of 803 kg/h, i.e., 482 kg/h, plus 0.3 of the second (water emission) rate of 257 kg/h, i.e., 77 kg/h and 0.1 of the third (soil emission) rate of 729 kg/h, i.e., 73 kg yielding a total of $(482 + 77 + 73)$ or 632 kg/h. It is also apparent that the amount in the air of 15500 kg causing a concentration of 0.155 µg/m³ is attributable to emissions to air (0.6×0.197) or 0.118 µg/m³, emissions to water (0.3×0.063) or 0.019 µg/m³ and emissions to soil (0.1×0.179) or 0.018 µg/m³. The concentration in water of 2.0×10^{-4} g/m³ or 202 µg/m³ or ng/L is largely attributable to the discharges to water, which alone cause 0.3×669 or 200 µg/m³. Although more is emitted to air, it contributes less than 1 µg/m³ to the water with soil emissions accounting for about 1 µg/m³. Similarly, the prevailing soil concentration is controlled by the rate of discharge to the soil.

In this multimedia discharge scenario the overall residence time is 59 hours, which can be viewed as 60% of the air residence time of 19.7 h, 30% of the water residence time of 140 h and 10% of the overall soil residence time of 53 h. The overall amount in the environment of 59,000 kg is thus largely controlled by the discharges to water, which account for (0.3×133863) or 40,000 kg.

Figure 1.7.9 shows the distributions of mass and removal process rates for these four scenarios. Clearly, when benzene is discharged into a specific medium, most of the chemical is found in that medium. Only in the case of discharges to soil is an appreciable fraction found in another compartment, namely air. This is because benzene evaporates fairly rapidly from soil without being susceptible to reaction or advection.

Finally, it is interesting to note that the fugacity in this final case (in units of mPa) are for the four media 5.0×10^{-3} , 1.4, 1.6 and 1.1. The soil, sediment and water are fairly close to equilibrium, with the air notably “under-saturated” by a factor of about 200. This is the result of the rapid loss processes from air.

1.7.3 QSPR PLOTS FOR CHLOROPHENOLS AND ALKYLPHENOLS

These QSPR (quantitative structure-property relationship) plots display the usual approximately linear relationships similar to those of the alkyl and chlorinated aromatic hydrocarbons.

Most acid dissociation constants pK_a exceed environmental pH values, the exceptions being the highly chlorinated phenols. As a result, these substances tend to have higher apparent solubilities in water because of dissociation. The structure-property relationships apply to the un-ionized or protonated species; thus, experimental data should preferably be “corrected” to eliminate the effect of ionization, thus eliminating pH effects.

Chemical name: Benzene
Level III Distribution

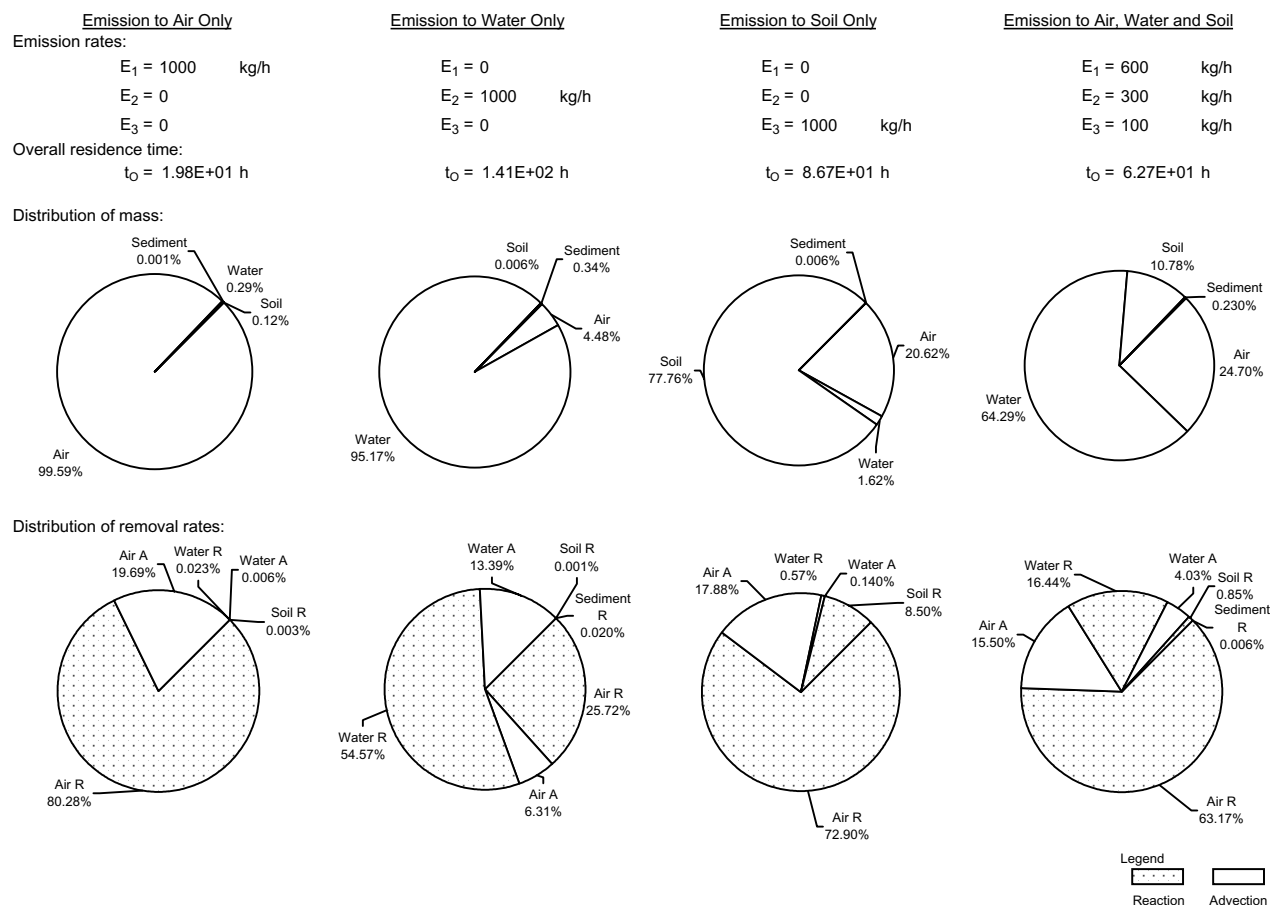


FIGURE 1.7.9 Level III fugacity distributions of benzene for four emission scenarios.

Figure 1.7.10 shows that the chlorophenol solubilities behave similarly to other chemical series with slopes of about 0.62 log units per 20.9 cm³/mol, which is the volume difference resulting from substitution by one chlorine. The result is a factor of 10^{0.62} or 4.2 drop in solubility per chlorine. The alkylphenols have a lower slope of about 0.5 per CH₂ and usually have higher solubilities at the same molar volume. The two sets of data are, however, generally similar.

The vapor pressure data in Figure 1.7.11 show a slope of about 0.60 log units per 20.9 cm³/mol (i.e., a factor of 4.0) per chlorine. There is a lower slope for the alkylphenols, and they usually have higher vapor pressures, especially for the larger molecules.

The K_{OW} data in Figure 1.7.12 show that the chlorophenols and alkylphenols differ in properties, there being more uncertainty about the K_{OW} of the longer-chain phenols. The chlorophenols tend to partition more into octanol at the same molar volume and are thus expected to be more bioaccumulative. The slope of the chlorophenol line is about 0.78 log units per chlorine or a factor of 6.0. The alkylphenol slope is lower and about 0.36 log units per CH₂, i.e., a factor of 2.3.

The Henry's law constant data calculated as the ratio of vapor pressure to solubility in Figure 1.7.13 are quite scattered. There is little systematic variation with molar volume. Most values of log H lie between -0.1 to -0.8, i.e., H lies between 0.8 and 0.08, and the resulting air-water partition coefficient K_{AW} or H/RT thus lies between 3 × 10⁻⁴ and 3 × 10⁻⁵.

Figure 1.7.14, the plot of log K_{OW} versus log solubility, shows a relatively high slope of 1.25 for the chlorophenols and a lower slope of 0.70 for the alkylphenols.

Addition of a chlorine causes a drop in chlorophenol solubility in water by about 0.62 log units, and K_{OW} increases by about 0.78 log units. For the alkylphenols, addition of a methylene causes about a 0.50 log unit drop in solubility in water, and K_{OW} increases by only about 0.36 log units. The slope of the log K_{OW} versus solubility lines are thus about 0.78/0.62 or 1.25 for the chlorophenols and 0.36/0.5 or 0.72 for the alkylphenols. An implication is that since K_{OW} can

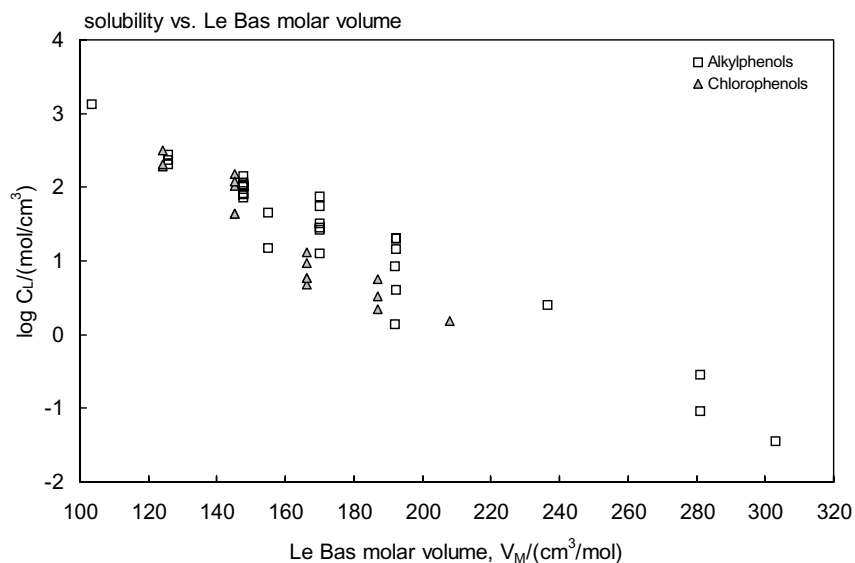


FIGURE 1.7.10 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alkylphenols and chlorophenols.

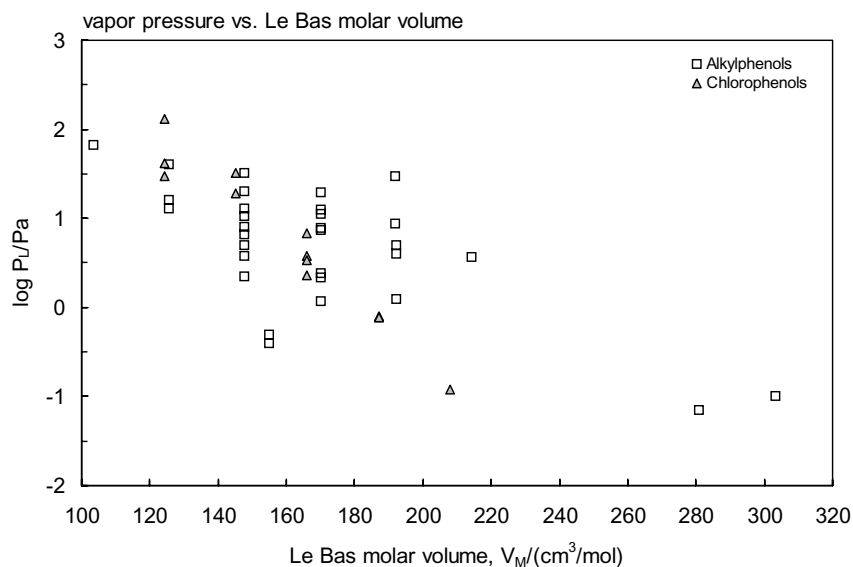


FIGURE 1.7.11 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alkylphenols and chlorophenols.

be viewed as a ratio of “solubility” in octanol and solubility in water, the solubility of the chlorophenols in octanol increases by $(0.78 - 0.62)$ or 0.16 log unit per chlorine, while for the alkylphenols the corresponding change is $(0.36 - 0.50)$ or -0.14 log unit, or a decrease of a factor of 1.4. The reasons for this difference are not known. The chlorophenols thus appear to have an unusually strong tendency to partition into octanol. Whether or not this tendency applies to lipid phases in biota or to organic carbon is not certain, but such a tendency is obviously of considerable interest when interpreting the toxicity and fate of these chemicals.

These data show clearly that the structure-property relationships which apply to hydrophobic organic chemicals such as the chloro- and alkyl-aromatics also apply to the phenols, but the relationships are more scattered and less well defined. The absolute values of properties differ greatly. This scatter is probably attributable, in part, to insufficient experimental data or errors in experimental measurements, to dissociation and to the greater polar character of these chemicals. It is not recommended that correlations developed for non-polar organic chemicals be applied to the phenols. Separate treatment of each homologous series is required.

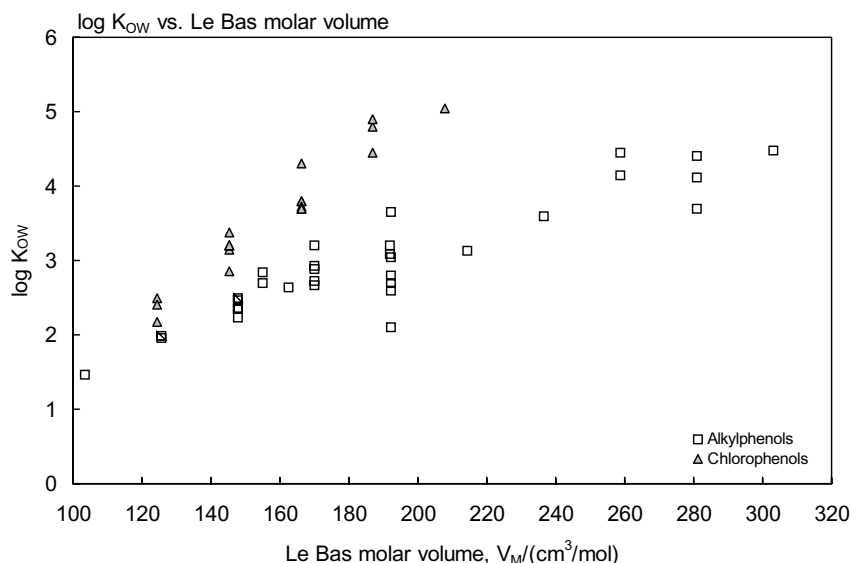


FIGURE 1.7.12 Octanol-water partition coefficient versus Le Bas molar volume for alkylphenols and chlorophenols.

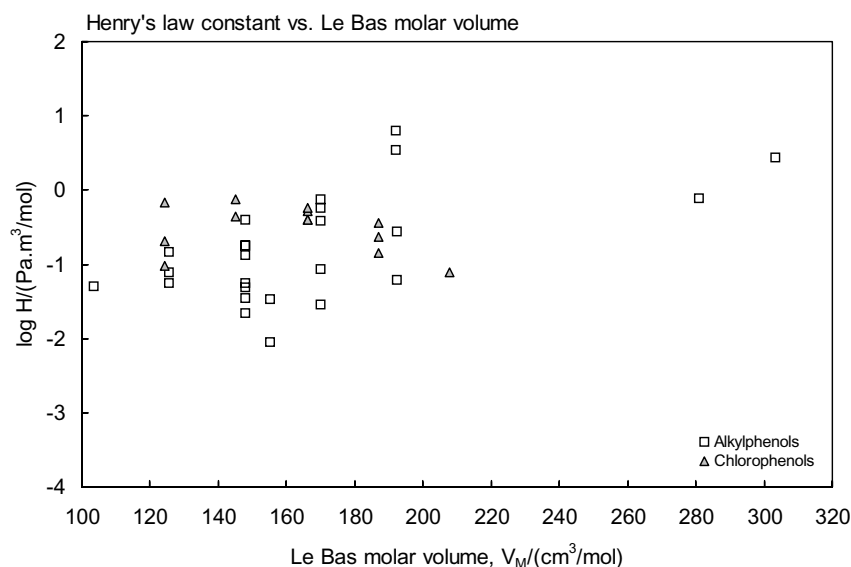


FIGURE 1.7.13 Henry's law constant versus Le Bas molar volume for alkylphenols and chlorophenols.

1.7.4 EVALUATIVE CALCULATIONS FOR PENTACHLOROPHENOL

For dissociating compounds the environmental pH is specified and the calculation of Z values has been modified to include ionic species as discussed in Section 1.2.4. Generally, if discharge is to a compartment such as water, most chemical will be found in that compartment, and will react there, but a quantity does migrate to other compartments and is lost from these media. Three pie charts corresponding to discharges of 1000 kg/h to air, water and soil are included. The percentage emission in each medium in this case has been selected to be 5, 25 and 70% discharged to air, water and soil, respectively. A fourth pie chart with discharges to all three compartments is also given. This latter chart is in principle the linear sum of the first three, but since the overall residence times differ, the diagram with the longer residence time, and greater resident mass, tends to dominate.

Figures 1.7.15 to 1.7.18 show the mass distributions obtained in Level I calculations and the removal distribution from Level II fugacity calculation of pentachlorophenol (PCP) at two different environmental pHs for the generic

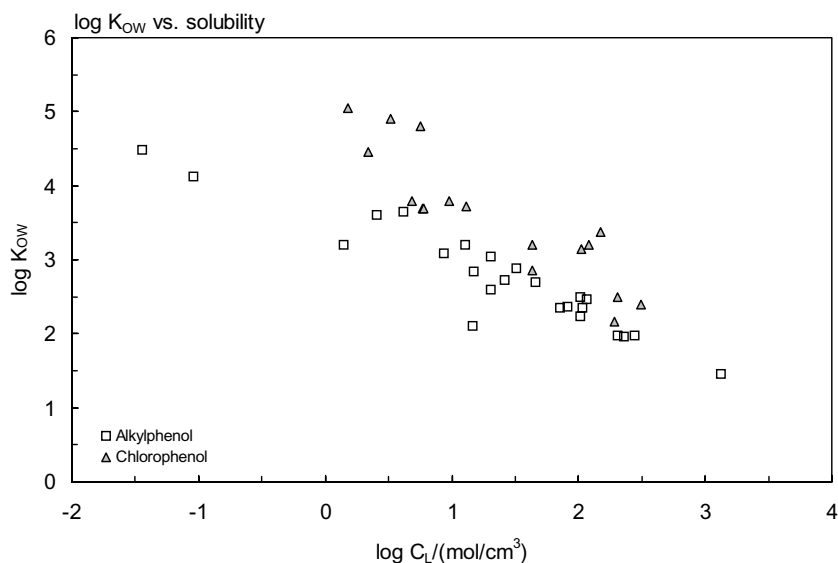


FIGURE 1.7.14 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alkylphenols and chlorophenols.

environment. Figures 1.7.19 to 1.7.22 show the corresponding Level III fugacity calculations. Both mass and removal distributions are shown in these figures for the four scenarios of discharges to air, water, soil, and mixed compartments.

Level I

The Level I calculations for environmental pHs of 5.1 and 7 suggest that if 100,000 kg (100 tonnes) of pentachlorophenol (PCP) are introduced into the 100,000 km² environment, most PCP will tend to be associated with soil. This is especially the case at low pH when the protonated form dominates. Very little partitions into air and only about 1% partitions into water. Soil contains most of the PCP. Sediments contain about 2%. There is evidence of bioconcentration with a rather high fish concentration. Note that only four media (air, water, soil and bottom sediment) are depicted in the pie chart; therefore, the sum of the percent distribution figures is slightly less than 100%. The air-water partition coefficient is very low. As pH increases, dissociation increases and there is a tendency for partitioning to water to become more important. Essentially, the capacity of water for the chemical increases. Partitioning to air is always negligible.

Level II

The Level II calculations at pH 5.1 include the reaction half-lives of 550 h in air, 550 h in water, 1700 h in soil and 5500 h in sediment. No reaction is included for suspended sediment or fish. The steady-state input of 1000 kg/h results in an overall fugacity of 3.43×10^{-8} Pa, which is about 24 times the Level I value. The concentrations and amounts in each medium are thus about 24 times the Level I values. The relative mass distribution is identical to Level I. The primary loss mechanism is reaction in soil, which accounts for 936 kg/h, or 94% of the input. Most of the remainder is lost by reaction and advection in water. The air and sediment loss processes are unimportant largely because so little of the PCP is present in these media. The overall residence time is 2373 h; thus, there is an inventory of PCP in the system of 2373×1000 or 2,373,000 kg.

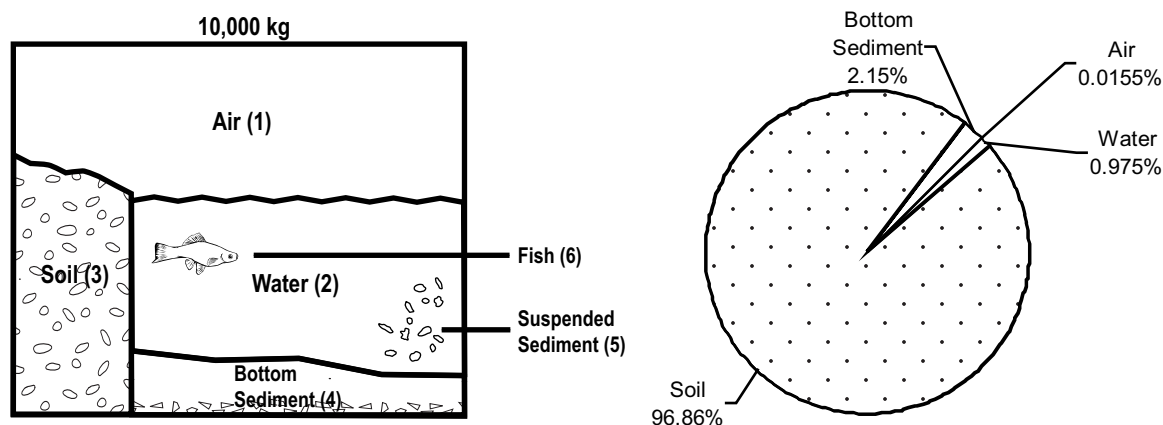
The primary loss mechanism of soil reaction has a D value of 1.03×10^{11} ; thus, for any other process to compete with this would require a D value of at least 10^{10} mol/Pa·h. The next largest D values are 3.19×10^9 and 2.53×10^9 for reaction and advection in water, which are about a factor of 30 smaller. Only if the water advection or reaction rates are increased by about this factor will these processes become significant. As pH increases, reaction in, and advection from, water increase in importance.

Level III

The Level III diagrams (Figures 1.7.19 to 1.7.22 for the two pHs) are regarded as the most realistic depictions of chemical fate.

This calculation includes an estimation of intermedia transport. Examination of the magnitude of the intermedia D values given in the fate diagrams suggest that water-sediment and air-soil transport are most important, with soil-water, and air-water exchange being slower. This chemical tends to be fairly immobile in terms of intermedia transport.

Chemical name: Pentachlorophenol
 Fugacity Level I calculations: (six-compartment model) at data pH of 5.1



Physical-chemical properties:

Molecular weight (g/mol)
 Melting point ($^{\circ}\text{C}$)
 Solubility (g/m^3)
 Vapor pressure (Pa)
 $\log K_{\text{OW}}$
 Fugacity ratio, F
 Dissociation const, pKa

266.34
 174
 14
 4.15E-03
 5.05
 3.36E-02
 4.74

Partition coefficients:

Henry's law constant
 Air/water
 Organic carbon, K_{OC}
 Bioconcentration factor, BCF
 Soil/water
 Sediment/water
 Suspended sediment/water
 Aerosol/water

7.90E-02
 3.19E-05
 4.60E+04
 5.61E+03
 2.21E+03
 4.42E+03
 1.38E+04
 4.86E+07

Z values in water:

at data pH
 neutral
 ionic
 total
 at environ. pH
 neutral
 ionic
 total

Compartment	Z mol/m ³ .Pa	Concentration			Amount	
		mol/m ³	g/m ³	μg/g	kg	%
Air (1)	4.03E-04	5.82E-13	1.55E-10	1.31E-07	1.55E+01	1.55E-02
Water (2)	1.27E+01	1.83E-08	4.87E-06	4.87E-06	9.74E+02	9.74E-01
Soil (3)	2.80E+04	4.04E-05	1.08E-02	4.48E-03	9.68E+04	9.68E+01
Bottom sediment (4)	5.59E+04	8.80E-05	2.15E-02	8.96E-03	2.15E+03	2.15E+00
Suspended sediment (5)	1.75E+05	2.52E-04	6.72E-02	4.48E-02	6.72E+01	6.72E-02
Biota (6)	7.11E+04	1.03E-04	2.73E-02	2.73E-02	5.46E+00	5.46E-03
Total					1.00E+05	1.00E+02

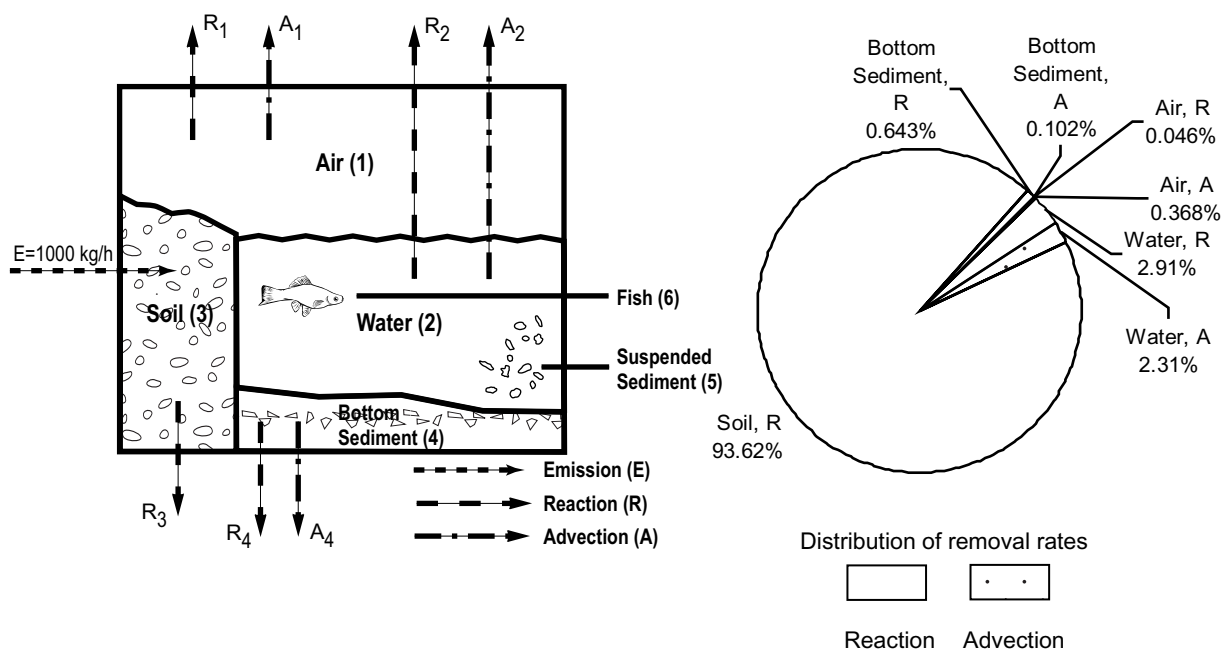
FIGURE 1.7.15 Level I fugacity calculations for PCP at data determination pH of 5.1.

The bulk Z values are similar for air and water to the values for the “pure” phases in Level I and II, but they are lower for soil and sediment because of the “dilution” of the solid soil and sediment phases with air or water.

The complete discussion of PCP fate as deduced in these calculations is beyond our scope, but to assist the reader we describe the behavior at a pH of 5.1 in some detail below.

These tabulated data are given in numerical and pictorial form in Figures 1.7.19 to 1.7.22. The first row of figures at the foot of Figure 1.7.19 describes the condition if 1000 kg/h is emitted to the air. The result is similar to the Level II calculation with 65780 kg in air, 21070 kg in water, 504700 kg in soil and only 40800 kg in sediment. It can be concluded that PCP discharged to the atmosphere has fairly high potential to enter other media. The rate of transfer from air to

Chemical name: Pentachlorophenol
Fugacity Level II calculations: (six-compartment model) at data pH of 5.1



Compartment	Half-life h	D Value		Concentration mol/m ³	Loss		Total Removal %
		Reaction mol/Pa.h	Advection mol/Pa.h		Reaction kg/h	Advection kg/h	
Air (1)	550	5.08E+07	4.03E+08	1.38E-11	4.64E-01	3.68E+00	4.14E-01
Water (2)	550	3.19E+09	2.53E+09	4.34E-07	2.91E+01	2.31E+01	5.22E+00
Soil (3)	1700	1.03E+11	-	9.58E-04	9.36E+02	-	9.36E+01
Bottom sediment (4)	5500	7.05E+08	1.12E+08	1.92E-03	6.43E+00	1.02E+00	7.45E-01
Suspended sediment (5)	-	-	-	5.99E-03	-	-	-
Biota (6)	-	-	-	2.43E-03	-	-	-

Fugacity, f	3.43E-08 Pa
Total amount, M	8.91E+06 mol
Total amount	2.37E+06 kg
Total reaction D value , D _R	1.06E+11 mol/Pa.h
Total advection D value, D _A	2.94E+09 mol/Pa.h
Total D value, D _T	1.09E+11 mol/Pa.h
Total loss by reaction	9.72E+02 kg/h
Total loss by advection	2.78E+01 kg/h
Total loss	1.00E+03 kg/h
Reaction residence time, t _R	2.44E+03 h
Advection residence time, t _A	8.53E+04 h
Overall residence time, t _O	2.37E+03 h

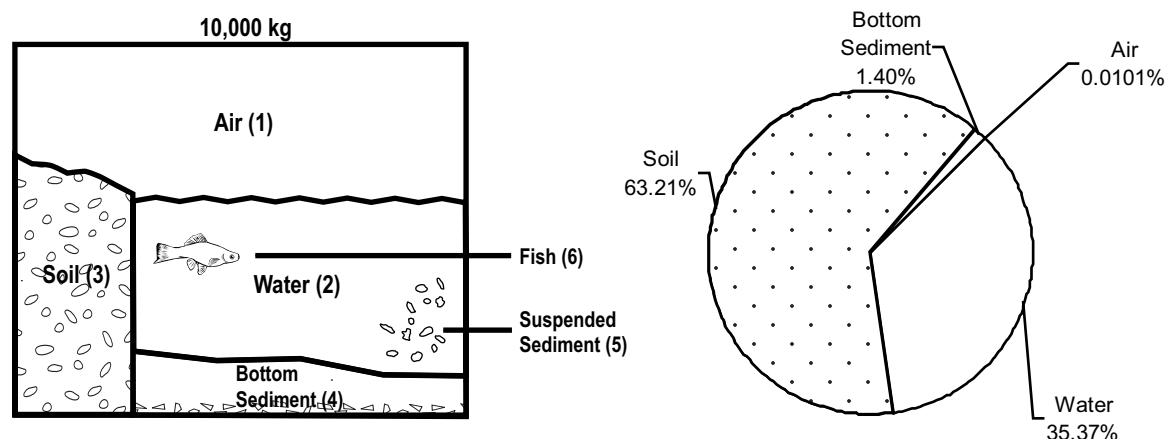
FIGURE 1.7.16 Level II fugacity calculations for PCP at data determination pH of 5.1.

water (T_{12}) is about 54 kg/h and that from air to soil (T_{13}) 206 kg/h. The reason for this is the value of the mass transfer coefficients which control this transport process. The overall residence time is 632 h.

If 1000 kg/h of PCP is discharged to water, as in the second row, there is, as expected, a much higher concentration in water. There is reaction of 494 kg/h in water, advective outflow of 392 kg/h and transfer to air (T_{21}) of 2.90 kg/h with

Chemical name: Pentachlorophenol

Fugacity Level I calculations: (six-compartment model) at environmental pH of 7



Physical-chemical properties:

Molecular weight (g/mol)
Melting point ($^{\circ}\text{C}$)
Solubility (g/m^3)
Vapor pressure (Pa)
 $\log K_{OW}$
Fugacity ratio, F
Dissociation const, pKa

266.34
174
14
4.15E-03
5.05
3.36E-02
4.74

Partition coefficients:

Henry's law constant
Air/water
Organic carbon, K_{OC}
Bioconcentration factor, BCF
Soil/water
Sediment/water
Suspended sediment/water
Aerosol/water

1.42E-03
5.73E-07
4.60E+04
5.61E+03
3.97E+01
7.94E+01
2.48E+02
4.86E+07

Z values in water:

at data pH
neutral
ionic
total
at environ. pH
neutral
ionic
total

5.1
3.849
8.817
12.666
7
3.849
700.379
704.228

Fugacity, $f = 9.43\text{E-}10$

Compartment	Z $\text{mol}/\text{m}^3 \cdot \text{Pa}$	Concentration			Amount	
		mol/m^3	g/m^3	$\mu\text{g}/\text{g}$	kg	%
Air (1)	4.03E-04	3.80E-13	1.01E-10	8.54E-08	1.01E+01	1.01E-02
Water (2)	7.04E+02	6.64E-07	1.77E-04	1.77E-04	3.54E+04	3.54E+01
Soil (3)	2.80E+04	2.64E-05	7.02E-03	2.93E-03	6.32E+04	6.32E+01
Bottom sediment (4)	5.59E+04	5.27E-05	1.40E-02	5.85E-03	1.40E+03	1.40E+00
Suspended sediment (5)	1.75E+05	1.65E-04	4.39E-02	2.93E-02	4.39E+01	4.39E-02
Biota (6)	7.11E+04	6.70E-05	1.78E-02	1.78E-02	3.57E+00	3.57E-03
Total					1.00E+05	1.00E+02

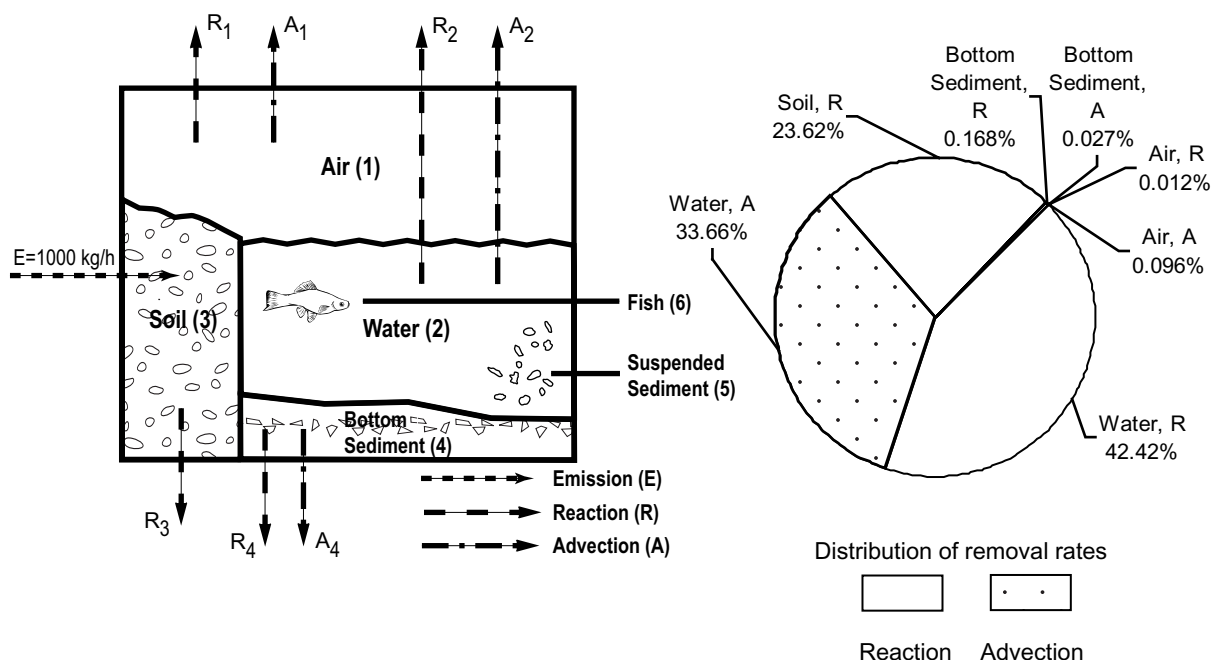
FIGURE 1.7.17 Level I fugacity calculations for PCP at environmental pH of 7.

substantial loss of 128 kg/h to sediment. The amount in the water is 392,200 kg; thus, the residence time in the water is 392 h, and the overall environmental residence time is a longer 1153 h. The key processes are thus reaction in water (half-life 550 h) and advective outflow (residence time 1000 h). The evaporation half-life can be calculated as $(0.693 \times \text{mass in water})/\text{rate of transfer}$, i.e., $(0.693 \times 392,200)/2.90 = 93700$ h. Clearly competition between advection and reaction in the water determines the overall fate. Thirty-four percent of the PCP discharged is now found in the water and the concentration is fairly high, namely $1.96 \times 10^{-3} \text{ g}/\text{m}^3$ or $1.96 \mu\text{g}/\text{L}$.

The third row shows the fate if PCP is discharged to soil. The amount in soil is 245100 kg, with only 7.43 kg in air. The overall residence time is 2452 hours, which is largely controlled by the reaction rate in soil. The rate of reaction in soil is 999 kg/h and there is no advection; thus, the other loss mechanism is transfer to air (T_{31}) at a rate of 0.11 kg/h, with a relatively minor 0.8 kg/h to water by run-off. The soil concentration of $0.136 \text{ g}/\text{m}^3$ is controlled almost entirely by the rate at which the PCP reacts.

Chemical name: Pentachlorophenol

Fugacity Level II calculations: (six-compartment model) at environmental pH of 7



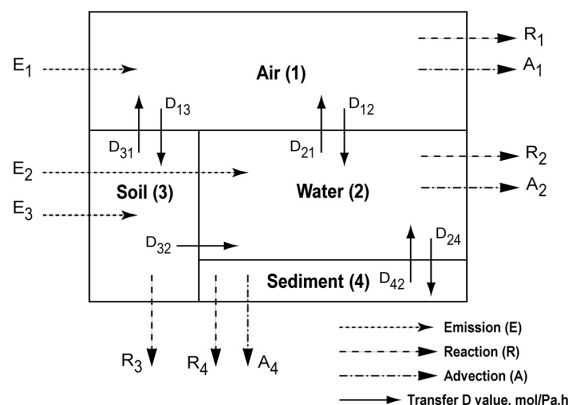
Compartment	Half-life h	D Value		Concentration mol/m ³	Loss		Total Removal %
		Reaction mol/Pa.h	Advection mol/Pa.h		Reaction kg/h	Advection kg/h	
Air (1)	550	5.08E+07	4.03E+08	3.59E-12	1.20E-01	9.56E-01	1.08E-01
Water (2)	550	1.77E+11	1.41E+11	6.26E-06	4.20E+02	3.34E+02	7.54E+01
Soil (3)	1700	1.03E+11	-	2.49E-04	2.34E+02	-	2.43E+01
Bottom sediment (4)	5500	7.05E+08	1.12E+08	4.97E-04	1.67E+00	2.65E-01	1.93E-01
Suspended sediment (5)	-	-	-	1.55E-03	-	-	-
Biota (6)	-	-	-	6.32E-04	-	-	-

Fugacity, f	8.89E-09 Pa
Total amount, M	3.54E+06 mol
Total amount	9.44E+05 kg
Total reaction D value, D_R	2.80E+11 mol/Pa.h
Total advection D value, D_A	1.41E+11 mol/Pa.h
Total D value, D_T	4.21E+11 mol/Pa.h
Total loss by reaction	6.65E+02 kg/h
Total loss by advection	3.35E+02 kg/h
Total loss	1.00E+03 kg/h
Reaction residence time, t_R	1.42E+03 h
Advection residence time, t_A	2.82E+03 h
Overall residence time, t_O	9.44E+02 h

FIGURE 1.7.18 Level II fugacity calculations for PCP at environmental pH of 7.

The net result is that PCP behaves entirely differently when discharged to the three media. If discharged to air, it advects rapidly and reacts with a residence time of 632 h or about 26.3 days, with substantial transport to soil or water. If discharged to water, it reacts and evaporates to air with a residence time of 1153 h or 48 days. If discharged to soil, it mostly reacts with an overall residence time of about 2452 h or 102 days.

Chemical name: Pentachlorophenol
 Fugacity Level III calculations: (four-compartment model) at data pH of 5.1



Phase Properties and Rates:

Compartment	Bulk Z mol/m ³ .Pa	Half-life h	D Value	
			Reaction mol/Pa.h	Advection mol/Pa.h
Air (1)	4.038E-04	5.500E+02	5.09E+07	4.04E+08
Water (2)	1.361E+01	5.500E+02	3.43E+09	2.72E+09
Soil (3)	1.399E+04	1.700E+03	1.03E+11	-
Sediment (4)	1.120E+04	5.500E+03	7.05E+08	1.12E+08

Residence time (h)	Emission to			
	(A)ir Only	(W)ater Only	(S)oil Only	A+W+S
Overall residence time	6.324E+02	1.153E+03	2.452E+03	2.036E+03
Reaction residence time	1.974E+03	1.952E+03	2.453E+03	2.358E+03
Advection residence time	9.304E+02	2.817E+03	6.090E+06	1.491E+04

Phase Properties, Compositions, and Transport and Transformation Rates:

Emission Scenario	Emission (kg/h)			Fugacity (Pa)				Concentration (g/m ³)				Amount (kg)				Total Amount (kg)
	E ₁	E ₂	E ₃	f ₁	f ₂	f ₃	f ₄	C ₁	C ₂	C ₃	C ₄	w ₁	w ₂	w ₃	w ₄	
(A)ir Only	1000	0	0	6.116E-06	2.907E-08	7.526E-09	2.736E-08	6.578E-07	1.054E-04	2.804E-02	8.160E-02	6.578E+04	2.107E+04	5.047E+05	4.080E+04	6.324E+05
(W)ater Only	0	1000	0	1.772E-08	5.410E-07	2.180E-11	5.092E-07	1.905E-09	1.961E-03	8.122E-05	1.519E+00	1.905E+02	3.922E+05	1.462E+03	7.593E+05	1.153E+06
(S)oil Only	0	0	1000	6.909E-10	4.359E-10	3.655E-08	4.103E-10	7.430E-11	1.580E-06	1.362E-01	1.224E-03	7.430E+00	3.160E+02	2.451E+06	6.118E+02	2.452E+06
A+W+S	50	250	700	3.107E-07	1.370E-07	2.597E-08	1.290E-07	3.342E-08	4.966E-04	9.674E-02	3.846E-01	3.342E+03	9.933E+04	1.741E+06	1.923E+05	2.036E+06

Emission Scenario	Emission (kg/h)			Loss by Reaction (kg/h)				Loss by Advection (kg/h)			Intermedia Rate of Transport (kg/h)						
	E ₁	E ₂	E ₃	R ₁	R ₂	R ₃	R ₄	A ₁	A ₂	A ₄	T ₁₂	T ₂₁	T ₁₃	T ₃₁	T ₃₂	T ₂₄	T ₄₂
(A)ir Only	1000	0	0	8.288E+01	2.655E+01	2.06E+02	5.141E+00	6.578E+02	2.107E+01	8.160E-01	5.358E+01	1.557E-01	2.059E+02	2.278E-02	1.647E-01	6.864E+00	9.076E-01
(W)ater Only	0	1000	0	2.401E-01	4.942E+02	5.96E-01	9.567E+01	1.905E+00	3.922E+02	1.519E+01	1.552E-01	2.897E+00	5.965E-01	6.599E-05	4.770E-04	1.278E+02	1.689E+01
(S)oil Only	0	0	1000	9.362E-03	3.982E-01	9.99E+02	7.709E-02	7.430E-02	3.160E-01	1.224E-02	6.052E-03	2.334E-03	2.326E-02	1.106E-01	7.999E-01	1.029E-01	1.361E-02
A+W+S	50	250	700	4.211E+00	1.252E+02	7.10E+02	2.423E+01	3.342E+01	9.933E+01	3.846E+00	2.722E+00	7.337E-01	1.046E+01	7.861E-02	5.863E-01	3.235E+01	4.277E+00

FIGURE 1.7.19 Level III fugacity calculations for PCP at pH of 5.1.

Chemical name: Pentachlorophenol
 Level III Distribution at data pH of 5.1

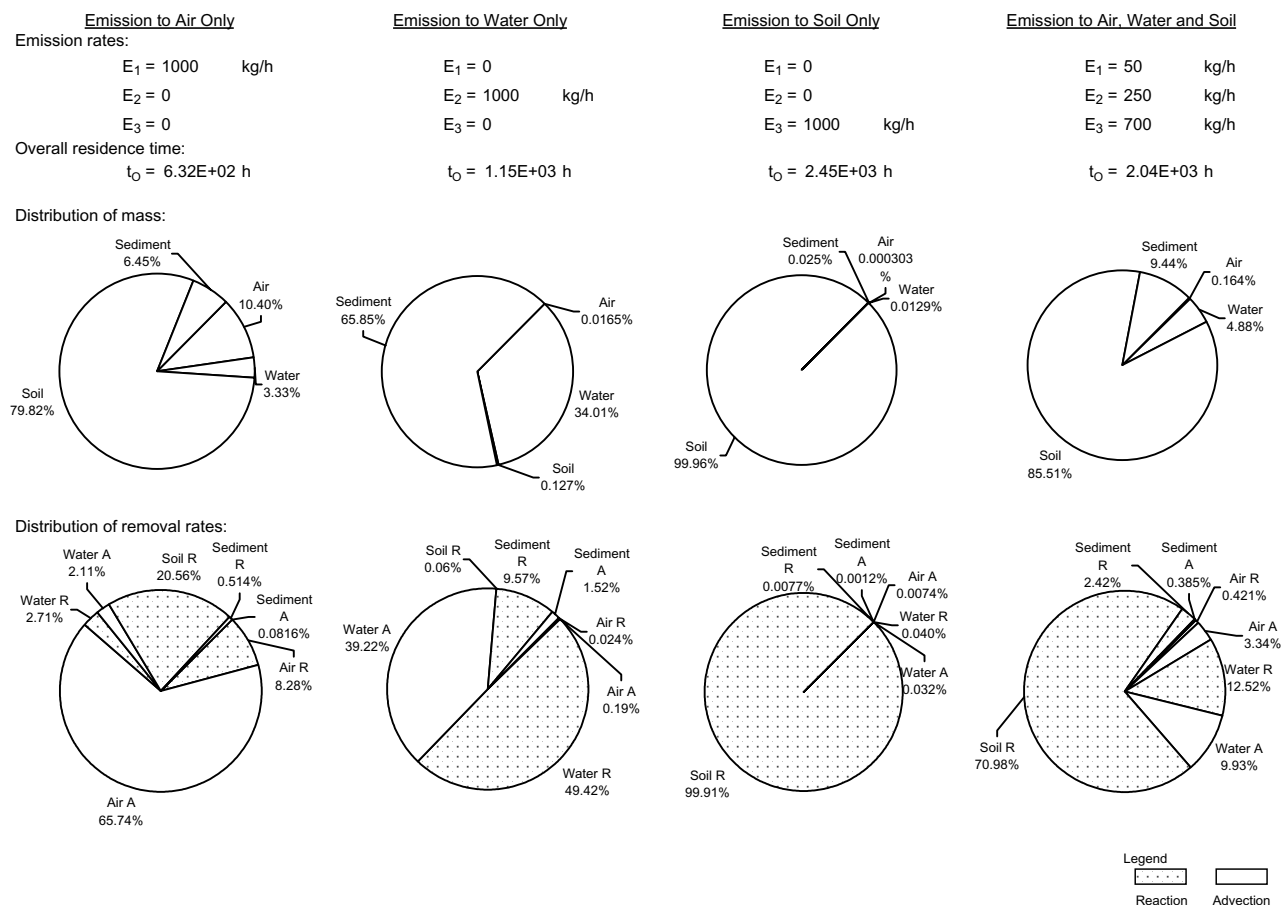


FIGURE 1.7.20 Level III fugacity distributions of PCP for four emission scenarios at pH of 5.1.

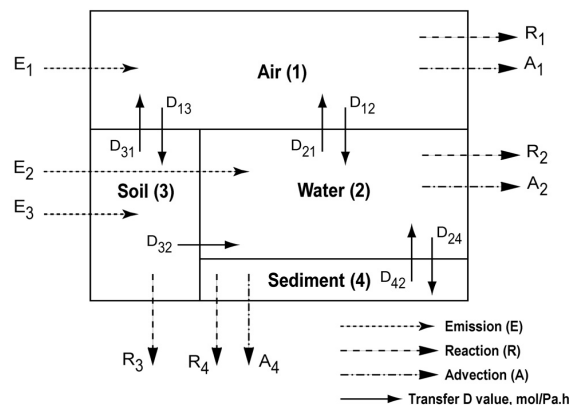
The final scenario is a combination of discharges, 50 kg/h to air, 250 kg/h to water, and 700 kg/h to soil (which are different from the often assumed equal emissions). The concentrations, amounts and transport and transformation rates are merely linearly combined versions of the three initial scenarios. For example, the rate of reaction in air is now 4.21 kg/h. This is 0.05 of the first (air emission) rate of 82.9 kg/h, i.e., 4.14 kg/h, plus 0.25 of the second (water emission) rate of 0.24 kg/h, i.e., 0.06 kg/h and 0.7 of the third (soil emission) rate of 0.0094 kg/h, i.e., 0.0066 kg/h yielding a total of $(4.14 + 0.06 + 0.0066)$ or 4.21 kg/h. It is also apparent that the amount in the air of 3342 kg causing a concentration of 3.342×10^{-8} g/m³ or 33 ng/m³ is attributable to emissions to air (0.05×658 or 33 ng/m³), emissions to water (0.25×1.9 or 0.5 ng/m³) and emissions to soil (0.7×0.0743 or 0.052 μ g/m³). The concentration in water of 4.97×10^{-4} g/m³, or 497 ng/L, is largely attributable to the discharges to water, which alone cause $0.25 \times 1.96 \times 10^{-3}$ g/m³ or 4.9×10^{-4} g/m³ or 490 μ g/m³, or 490 ng/L. Although more is emitted to soil, it contributes only about 1.1 μ g/m³ to the water with air emissions accounting for about 5.27 μ g/m³. Similarly, the prevailing soil concentration is controlled by the rate of discharge to the soil.

In this multimedia discharge scenario the overall residence time is 2036 h, which can be viewed as the sum of 5% of the air emission residence time of 632 h, 25% of the water emission residence time of 1153 h and 70% of the soil emission residence time of 2452 h. The overall amount in the environment of 2.04×10^6 kg is thus largely controlled by the discharges to soil and water.

Finally, it is interesting to note that the fugacities in this final case (in units of μ Pa) are for the four media: 0.31 (air), 0.137 (water), 0.026 (soil) and 0.129 (sediment). The media are fairly close to equilibrium, i.e., within a factor of about 5 of the average value.

At pH 7, Figure 1.7.21, the capacity of water for PCP increases; thus, the water compartment becomes more important as do intermedia transport processes involving water such as wet deposition in dissolved form and run-off

Chemical name: Pentachlorophenol
 Fugacity Level III calculations: (four-compartment model) at environmental pH of 7



Phase Properties and Rates:

Compartment	Bulk Z mol/m ³ .Pa	Half-life h	D Value	
			Reaction mol/Pa.h	Advection mol/Pa.h
Air (1)	4.038E-04	5.500E+02	5.09E+07	4.04E+08
Water (2)	7.052E+02	5.500E+02	1.78E+11	1.41E+11
Soil (3)	1.420E+04	1.700E+03	1.04E+11	-
Sediment (4)	1.175E+04	5.500E+03	7.40E+08	1.18E+08

Residence time (h)	Emission to			
	(A)ir Only	(W)ater Only	(S)oil Only	A+W+S
Overall residence time	2.074E+03	4.588E+02	2.393E+03	1.894E+03
Reaction residence time	2.319E+03	8.218E+02	2.426E+03	2.164E+03
Advection residence time	1.961E+04	1.039E+03	1.805E+05	1.515E+04

Phase Properties, Compositions, and Transport and Transformation Rates:

Emission Scenario	Emission (kg/h)			Fugacity (Pa)				Concentration (g/m ³)				Amount (kg)				Total Amount (kg)
	E ₁	E ₂	E ₃	f ₁	f ₂	f ₃	f ₄	C ₁	C ₂	C ₃	C ₄	w ₁	w ₂	w ₃	w ₄	
(A)ir Only	1000	0	0	4.907E-07	1.408E-09	2.958E-08	1.328E-09	5.278E-08	2.645E-04	1.118E-01	4.158E-03	5.278E+03	5.290E+04	2.013E+06	2.078E+03	2.074E+06
(W)ater Only	0	1000	0	3.097E-11	1.175E-08	1.867E-12	1.108E-08	3.331E-12	2.207E-03	7.060E-06	3.467E-02	3.331E-01	4.413E+05	1.271E+02	1.733E+04	4.588E+05
(S)oil Only	0	0	1000	6.453E-10	3.510E-10	3.497E-08	3.309E-10	6.940E-11	6.592E-05	1.322E-01	1.036E-03	6.940E+00	1.318E+04	2.380E+06	5.178E+02	2.393E+06
A+W+S	50	250	700	2.500E-08	3.253E-09	2.596E-08	3.067E-09	2.688E-09	6.110E-04	9.814E-02	9.600E-03	2.688E+02	1.222E+05	1.766E+06	4.800E+03	1.894E+06

Emission Scenario	Emission (kg/h)			Loss by Reaction (kg/h)				Loss by Advection (kg/h)			Intermedia Rate of Transport (kg/h)						
	E ₁	E ₂	E ₃	R ₁	R ₂	R ₃	R ₄	A ₁	A ₂	A ₄	T ₁₂	T ₂₁	T ₁₃	T ₃₁	T ₃₂	T ₂₄	T ₄₂
(A)ir Only	1000	0	0	6.650E+00	6.665E-02	8.21E+02	2.618E-01	5.278E+01	5.290E+01	4.156E-02	9.470E+01	7.565E-03	8.470E+02	1.112E+00	2.517E+01	5.920E-01	2.886E-01
(W)ater Only	0	1000	0	4.197E-04	5.561E+02	5.18E-02	2.184E+00	3.331E-03	4.413E+02	3.467E-01	5.977E-03	6.312E-02	5.346E-02	7.020E-05	1.589E-03	4.939E+00	2.408E+00
(S)oil Only	0	0	1000	8.745E-03	1.661E+01	9.70E+02	6.525E-02	6.940E-02	1.318E+01	1.036E-02	1.245E-01	1.885E-03	1.114E+00	1.315E+00	2.975E+01	1.475E-01	7.193E-02
A+W+S	50	250	700	3.387E-01	1.540E+02	7.20E+02	6.048E-01	2.688E+00	1.222E+02	9.600E-02	4.823E+00	1.748E-02	4.314E+01	9.758E-01	2.208E+01	1.368E+00	6.667E-01

FIGURE 1.7.21 Level III fugacity calculations for PCP at pH of 7.

Chemical name: Pentachlorophenol
 Level III Distribution at environmental pH of 7

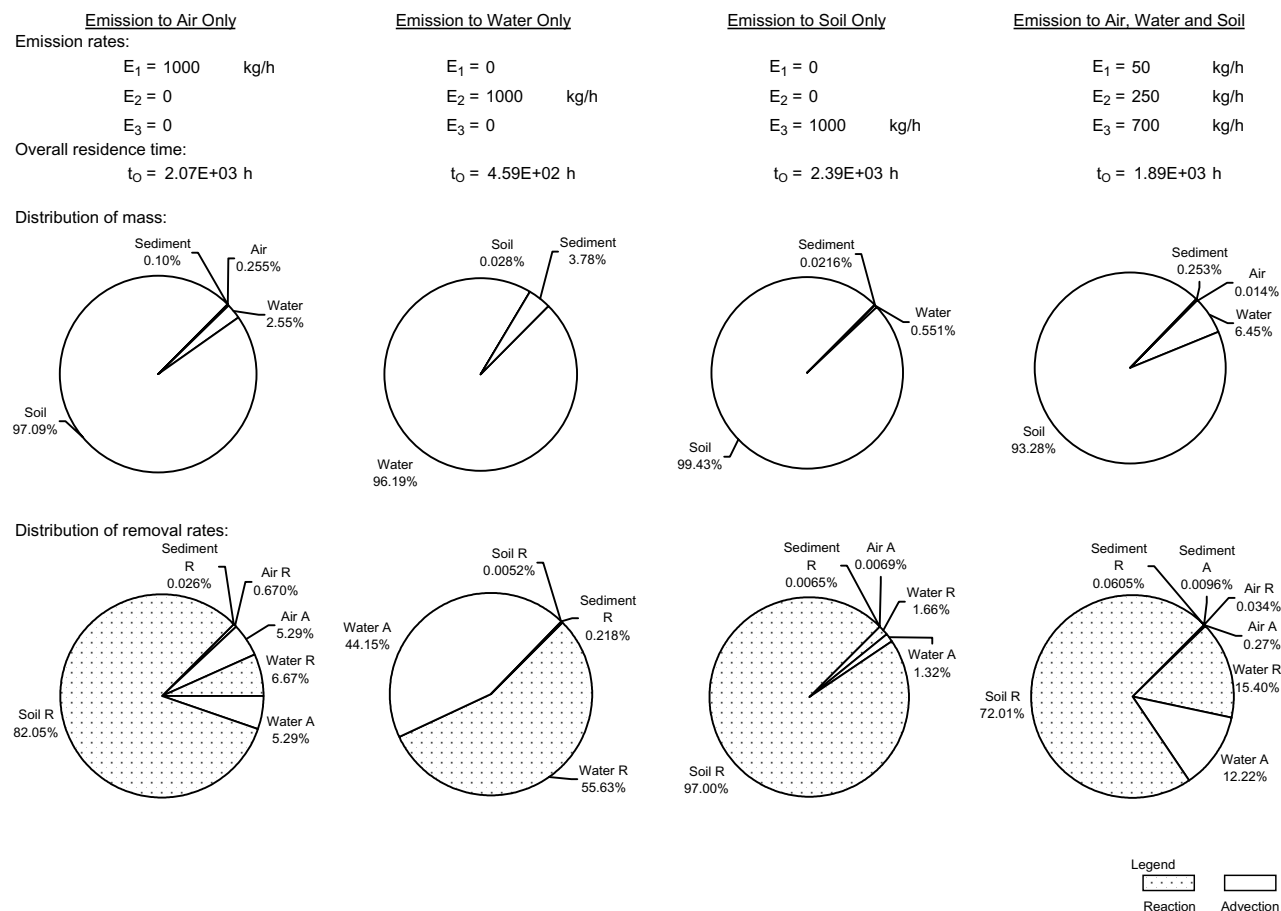


FIGURE 1.7.22 Level III fugacity distributions of PCP for four emission scenarios at pH of 7.

from soil to water. The net effect is that if discharged to air, the amounts transferred to soil and water increase as does the overall residence time. If discharged to water, there is less water to sediment transfer because of the reduced apparent hydrophobicity, and the residence time decreases. If discharged to soil, there is little effect of the pH increase because the PCP tends to remain there.

Similar diagrams could be prepared for other phenolic compounds at a range of pH values. The results suggest that the same broad patterns of behavior apply as for PCP but the residence times are generally shorter because of reduced hydrophobicity and more rapid reactions. The lower chlorinated phenols are relatively short-lived and are not subject to appreciable intermedia transport, i.e., when discharged to a medium they tend to remain there until degraded or advected. The longest persistence occurs when the chemical is present in soils.

Such simulations suggest that because of their relatively high water solubility which in combination with low vapor pressure causes low air-water partition coefficients, the phenols tend to remain in water or in soil and show little tendency to evaporate. Their environmental fate tends to be dominated by reaction in soil and water, and for the more sorptive species, in sediments. Their half-lives are relatively short, because of their susceptibility to degradation.

It is believed that examining these three behavior profiles, and their combination in the fourth, illustrate and explain the environmental fate characteristics of this and other chemicals. Important intermedia transport processes and levels in various media that arise from discharges into other media become clear. It is believed that the broad characteristics of environmental fate as described in the generic environment are generally applicable to other environments, albeit with differences attributable to changes in volumes, temperature, flow rates and compartment compositions.

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2.1 LIST OF CHEMICALS AND DATA COMPILATIONS

2.1.1 SATURATED HYDROCARBONS

2.1.1.1 Alkanes

2.1.1.1.1 Isobutane (2-Methylpropane)



Common Name: Isobutane

Synonym: 2-methylpropane

Chemical Name: 2-methylpropane

CAS Registry No: 75-28-5

Molecular Formula: C₄H₁₀

Molecular Weight: 58.122

Melting Point (°C):

−159.4 (Weast 1984; Lide 2003)

Boiling Point (°C):

−11.73 (Lide 2003)

Density (g/cm³ at 20°C):

0.5490 (Weast 1984)

0.5571, 0.5509 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

105.9 (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

96.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

19.121, 21.297 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.540 (Dreisbach 1959; Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

48.9 (shake flask-GC at atmospheric pressure, McAuliffe 1963, 1966)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

101783* (−11.609°C, static method-manometer, measured range −85.5 to −11.609°C, Aston et al. 1940)

101325* (−11.7°C, summary of literature data, temp range −109.2 to −11.7°C, Stull 1947)

348100 (calculated from determined exptl. data, Dreisbach 1959)

log (P/mmHg) = 6.74808 − 882.80/(240.0 + t/°C); temp range −75 to 30°C (Antoine eq. for liquid state, Dreisbach 1959)

357000 (interpolated-Antoine eq., temp range −86.57 to 18.88°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.91048 − 946.35/(246.68 + t/°C); temp range −86.57 to 18.88°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [−0.2185 × 5084.4/(T/K)] + 7.250; temp range −115 to −34°C (Antoine eq., Weast 1972–73)

log (P/mmHg) = [−0.2185 × 5416.2/(T/K)] + 7.349085; temp range −109.5 to 137.5°C (Antoine eq., Weast 1972–73)

312486, 313702* (21.07, 21.22°C, vapor-liquid equilibrium, measured range 4.580–71.17°C, Steele et al. 1976)

356600 (extrapolated-Antoine eq., temp range −87 to 7°C, Dean 1985, 1992)

log (P/mmHg) = 6.90148 − 946.35/(246.68 + t/°C); temp range −87 to 7°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 6.00272 − 947.54/(248.87 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

351130 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.03538 - 946.35/(-26.47 + T/\text{K})$; temp range 186–280 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.83572 - 1470.08/(3.99 + T/\text{K})$; temp range 121–187 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.93028 - 907.164/(-30.14 + T/\text{K})$; temp range 263–306 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.26924 - 1102.296/(-2.12 + T/\text{K})$; temp range 301–366 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.95371 - 1648.648/(77.939 + T/\text{K})$; temp range 361–408 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 31.2541 - 1.9532 \times 10^3/(T/\text{K}) - 8.806 \cdot \log (T/\text{K}) + 8.9246 \times 10^{-11} \cdot (T/\text{K}) + 5.7501 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 114–408 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

118640	(converted from $1/K_{\text{AW}} = C_{\text{W}}/C_{\text{A}}$ reported as exptl., Hine & Mookerjee 1975)
100980, 22090	(calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
120000	(calculated-P/C, Mackay & Shiu 1981)
116700	(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.76	(shake flask-GC, Leo et al. 1975)
2.76	(recommended, Sangster 1993)
2.76	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}^*(\text{exptl}) = 1.42 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 1.31 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 297 K, measured range 297–499 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{\text{OH}} = 1.28 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at 300 K (Greiner 1967; quoted, Altshuller & Bufalini 1971)

$k_{\text{OH}} = (2.52 \pm 0.05) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)

$k_{\text{O}_3} = 2.0 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, temp range 298–323 K (Atkinson & Carter 1984)

$k_{\text{OH}} = (2.29 \pm 0.06) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{\text{OH}} = (2.34 \pm 0.33) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(24.6 \pm 0.4)^\circ\text{C}$ (Edney et al. 1986)

$k_{\text{OH}}^* = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 9.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (recommended, Atkinson 1990)

$k_{\text{NO}_3}^* = (1.10 \pm 0.2) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–523 K, atmospheric $t_{1/2} = 1750$ h during the night at room temp. (discharge flow system, Bagley et al. 1990)

$k_{\text{OH}} = 7.38 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 6.50 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljić & Güsten 1990)

$k_{\text{NO}_3} = 9.8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1991)

$k_{\text{OH}} = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and an estimated lifetime was 59 h (Altshuller 1991)

$k_{\text{NO}_3}(\text{exptl}) = 9.8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{recommended}) = 9.9 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{calc}) = 7.90 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{\text{OH}}^* = 2.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}^* = 10.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

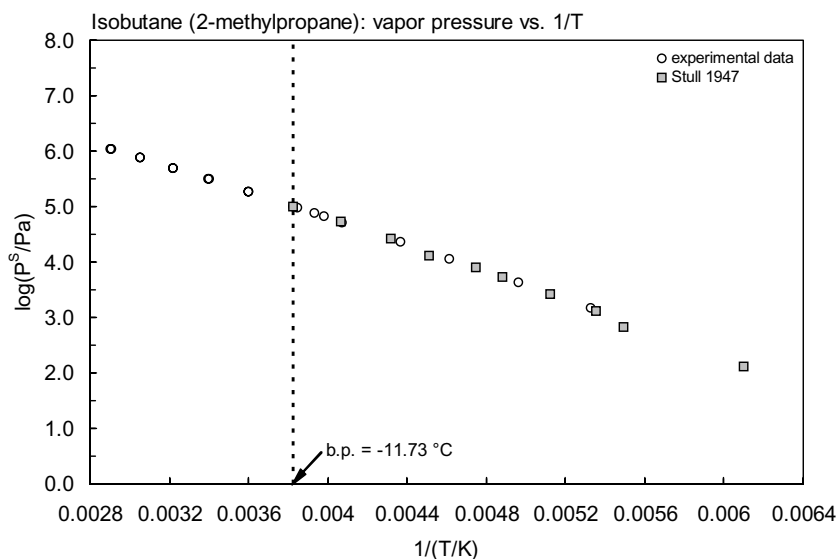
Air: atmospheric $t_{1/2}$ = 1750 h due to reaction with NO_3 radical during the night at room temp., and $t_{1/2}$ = 82 h for reaction with OH radical (Bagley et al. 1990);

atmospheric lifetime was estimated to be 59 h, based on a photooxidation rate constant $k = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in summer daylight with OH radical (Altshuller 1991).

TABLE 2.1.1.1.1

Reported vapor pressures of isobutane (2-methylpropane) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log(T/K)$		(4)			
Aston et al. 1940		Stull 1947		Steele et al. 1976	
static method-manometer		summary of literature data		vapor-liquid equilibrium	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
-85.5	1516	-109.2	133.3	4.580	183196
-71.704	4261	-91.1	666.6	4.620	185019
-56.431	11579	-86.4	1333	21.07	312486
-44.107	23233	-77.9	2666	21.22	313702
-27.576	52132	-68.4	5333	37.55	497811
-22.071	66405	-62.4	7999	37.62	498721
-18.761	76349	-51.4	13332	54.43	762470
-13.328	95476	-41.5	26664	54.50	763484
-11.609	101783	-27.1	53329	71.06	1112244
		-11.7	101325	71.17	1114778
mp/ $^{\circ}\text{C}$	-145	mp/ $^{\circ}\text{C}$	-145		

**FIGURE 2.1.1.1.1** Logarithm of vapor pressure versus reciprocal temperature for isobutane.

2.1.1.1.2 2,2-Dimethylpropane (Neopentane)



Common Name: 2,2-Dimethylpropane

Synonym: neopentane, tetramethylmethane

Chemical Name: 2,2-dimethylpropane

CAS Registry No: 463-82-1

Molecular Formula: C_5H_{12}

Molecular Weight: 72.149

Melting Point ($^{\circ}C$):

−16.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

9.503 (Dreisbach 1959; Stephenson & Malanowski 1987)

9.48 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.5910, 0.5852 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

122.10 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Wang et al. 1992)

117.6 ($20^{\circ}C$, Stephenson & Malanowski 1987)

118.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

21.778, 22.753 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

3.255 (Dreisbach 1959; Chickos et al. 1999)

3.146 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

12.69 (exptl., Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

33.2 (shake flask-GC at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

177930* (Antoine eq. regression, temp range -112 to $9.8^{\circ}C$, Stull 1947)

171350 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.73812 - 950.84/(237.0 + t/^{\circ}C)$; temp range -60 to $55^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

171586* (derived from compiled data, temp range -13.729 to $29.914^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P_s/mmHg) = 7.2034 - 1020.7/(230.0 + t/^{\circ}C)$; temp range -52 to $17.6^{\circ}C$ (Antoine eq., solid, Zwolinski & Wilhoit 1971)

$\log(P_l/mmHg) = 6.60427 - 883.42/(227.782 + t/^{\circ}C)$; temp range -13.729 to $29.914^{\circ}C$ (Antoine eq., liquid, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 5648.6/(T/K)] + 7.263947$; temp range -102 to $152.5^{\circ}C$ (Antoine eq., Weast 1972–73)

169019* ($24.56^{\circ}C$, ebulliometry, measured range -5.128 to $40^{\circ}C$, Osborn & Douslin 1974)

$\log(P/mmHg) = 6.60427 - 883.42/(227.78 + t/^{\circ}C)$; temp range -14 to $29^{\circ}C$ (Antoine eq., Dean 1985, 1992)

171300 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.89316 - 938.234/(235.249 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

171520, 171450 (interpolated-Antoine eq.-III and IV, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 6.3283 - 1020.7/(-43.15 + T/K)$; temp range 223 – $256 K$ (Antoine eq.-I., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 7.07825 - 1372.459/(-8.39 + T/\text{K})$; temp range 223–256 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.76532 - 900.545/(-43.111 + T/\text{K})$; temp range 268–313 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.83935 - 937.641/(-38.071 + T/\text{K})$; temp range 257–315 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.08953 - 1080.237/(-17.896 + T/\text{K})$; temp range 312–385 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.26795 - 2114.713/(128.175 + T/\text{K})$; temp range 382–433 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 26.6662 - 1.9307 \times 10^3/(T/\text{K}) - 7.0448 \cdot \log (T/\text{K}) + 7.4104 \times 10^{-9} \cdot (T/\text{K}) + 3.9463 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 257–434 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

221000	(calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
125640, 334380	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
373000	(calculated-P/C, Mackay & Shiu 1981)
213250	(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.11	(shake flask-GC, Leo et al. 1975; Leo et al. 1971; Hansch & Leo 1979)
2.95, 3.41, 3.22	(calculated-fragment const., Rekker 1977)
3.30, 3.08	(calculated-MO, calculated- π const., Bodor et al. 1989)
3.11	(recommended, Sangster 1989, 1993)
2.98	(calculated- V_M , Wang et al. 1992)
3.11	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^*(\text{exptl}) = 6.50 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 5.27 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–493 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{OH}(\text{exptl}) = 6.50 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 5.37 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 K (Greiner 1970)

$k_{O(3P)} = 5.50 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(^3P)$ atom at room temp. (Herron & Huie 1973)

$k_{OH} = (1.04 \pm 0.17) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)

$k_{OH} = 9.30 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979)

$k_{OH} = 9.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Winer et al. 1979)

$k_{OH}^* = 8.49 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1991)

$k_{OH}^* = 8.48 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 2.1.1.1.2.1

Reported vapor pressures of 2,2-dimethylpropane (neopentane) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\log P = A[1 - \Phi/(T/K)]$	(5)	where $\log A = a + b(T/K) + c(T/K)^2$					
Stull 1947	Zwolinski & Wilhoit 1971		Osborn & Douslin 1974				
summary of literature data	selected values		ebulliometry				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
			solid		liquid		
-102.0	133.3	-52.0	4000	-13.729	39997	-5.128	57818
-85.4	666.6	-48.0	5333	-7.047	53329	-0.301	70121
-76.7	1333	-45.0	6666	-1.570	66661	4.577	84666
-67.2	2666	-41.9	7999	3.112	79993	9.500	101325
-56.1	5333	-37.4	10666	7.224	93326	14.472	120793
-49.0	7999	-33.8	13332	7.991	95992	19.492	143246
-39.1	13332	-27.0	19998	8.742	98659	24.560	169019
-23.7	26667	-21.8	26664	9.112	101325	29.675	198488
-7.10	53329	-17.6	33331	10.199	103991	34.838	232017
9.50	101325			10.906	106658	40.048	270022
		bp/°C	9.478	14.251	119990		
mp/°C	-16.6	Antoine eq.		17.324	133322	Cox eq.	
		eq. 2	P/mmHg	22.829	159987	eq. 5	P/mmHg
		A	7.2034	29.914	199984	Φ	282.650
		B	1020.7	25.0	171586	a	0.802264
		C	230.0			b	-6.70026×10^{-4}
		temp range -52 to -17.6°C		Antoine eq.		c	11.22918×10^{-7}
		pres. range 30–250 mmHg		eq. 2	P/mmHg	for temp range 268–314 K	
				A	6.60427		
		$\Delta H_v/(\text{kJ mol}^{-1}) =$		B	883.42		
		at 25°C	21.85	C	227.782		
		at bp	22.75	temp range -14 to 30°C			
				pressure 300–1800 mmHg			

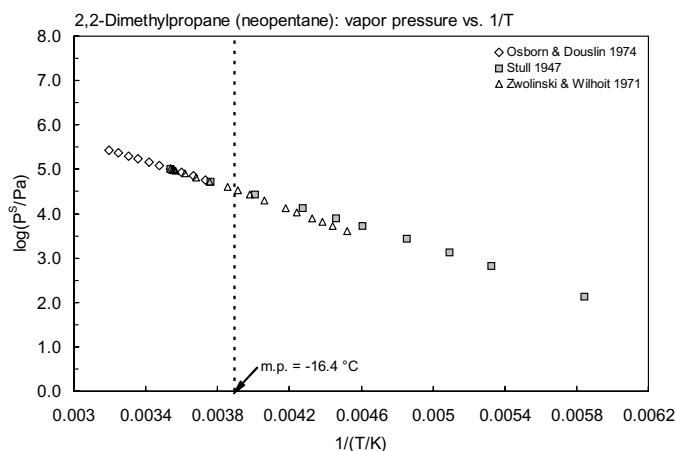


FIGURE 2.1.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2,2-dimethylpropane.

2.1.1.1.3 *n*-ButaneCommon Name: *n*-Butane

Synonym: 1-butane

Chemical Name: *n*-butane

CAS Registry No: 106-97-8

Molecular Formula: C₄H₁₀

Molecular Weight: 58.122

Melting Point (°C):

-138.3 (Lide 2003)

Boiling Point (°C):

-0.50 (Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm³ at 20°C):

0.5788, 0.5730 (20°C, 25°C, Dreisbach 1959)

0.5786, 0.5729 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

100.45, 101.45 (20°C, 25°C, calculated-density)

96.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

21.066, 22.393 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.393 (Parks & Huffman 1931)

4.661 (Dreisbach 1959; Riddick et al. 1986; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

34.56 (exptl., Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

65.6 (shake flask-UV, Morrison & Billett 1952)

67.0 (shake flask-UV, Claussen & Polglase 1952)

72.7 (shake flask-GC, Franks et al. 1966)

61.4 (shake flask-GC, McAuliffe 1963, 1966)

61.66 (shake flask-GC, Coates et al. 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

288200 (extrapolated-Antoine eq. regression, temp range -101.5 to -0.5°C, Stull 1947)

243050 (calculated from determined data, Dreisbach 1959)

log (P/mmHg) = 6.83029 - 945.9/(240.0 + t/°C); temp range -60 to 30°C (Antoine eq. for liquid state, Dreisbach 1959)

242647 (derived from compiled data, temp range -77.62 to 18.88°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.80896 - 935.56/(238.73 + t/°C); temp range -77.62 to 18.88°C (Antoine eq., Zwolinski & Wilhoit 1971)

242840 (extrapolated-Antoine eq., temp range -77 to 19°C, Dean 1985, 1992)

log (P/mmHg) = 6.80896 - 935.86/(238.73 + t/°C); temp range -77 to 19°C (Antoine eq., Dean 1985, 1992)

243000 (lit. average, Riddick et al. 1986)

log (P/kPa) = 5.93266 - 935.773/(238.789 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

242810 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.93386 - 935.86/(-34.52 + T/K); temp range 195-292 K (Antoine eq.-I, Stephenson & Malanowski 1987)log (P_L/kPa) = 7.3327 - 1409.73/(T/K); temp range 135-213 K (Antoine eq.-II, Stephenson & Malanowski 1987)log (P_L/kPa) = 6.07512 - 1007.247/(-25.272 + T/K); temp range 273-321 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.32267 - 1161.1/(-3.107 + T/\text{K})$; temp range 316–383 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.04942 - 1770.348/(84.979 + T/\text{K})$; temp range 375–425 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 27.0441 - 1.9049 \times 10^3/(T/\text{K}) - 7.1805 \cdot \log (T/\text{K}) - 6.6845 \times 10^{-11} \cdot (T/\text{K}) + 4.219 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 135–425 K (vapor pressure eq., Yaws 1994)
 592440 (57.01°C, vapor-liquid equilibrium VLE data, Pasanen et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

94240 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 82080, 22100 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 95900 (calculated-P/C, Mackay & Shiu 1975; Mackay 1981; Mackay & Shiu 1981)
 80210 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 92910 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.89 (shake flask-GC, Leo et al. 1975)
 2.89 (concn. ratio, Cramer 1977)
 2.46, 2.84, 2.96 (calculated-f const., Rekker 1977)
 2.89, 2.76 (Hansch & Leo 1979)
 2.79 (calculated-hydrophobicity const., Iwase et al. 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

1.53 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O_3} = 9.8 \times 10^{-24} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–323 K (Schubert & Pease 1956)

$k_{O(3P)} = 3.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(^3P)$ atom (Herron & Huie 1973)

$k_{OH} = 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1979)

$k_{OH}^*(\text{exptl}) = 1.66 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.54 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–495 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{OH} = 1.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with atmospheric $t_{1/2} = 2.4$ to 24 h at 300 K (Darnall et al. 1976)

$k_{OH} = 1.8 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in polluted atmosphere at $305 \pm 2 \text{ K}$ (relative rate method, Lloyd et al. 1976)

$k_{OH} = 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate at 0.11 d^{-1} for the reaction with OH radical and an average OH concn of $1.2 \times 10^6 \text{ molecules/cm}^3$ (Zafonte & Bonamassa 1977)

$k_{OH}(\text{exptl}) = (2.57 - 4.22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 2.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at atmospheric pressure and 300 K (Darnall et al. 1978)

$k_{OH} = 2.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $299 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1982a, 1984c)

$k_{O_3} < 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 6 \times 10^{-7} \text{ d}^{-1}$, $k_{OH} = 2.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.2 d^{-1} and $k_{NO_3} = 3.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.0007 d^{-1} (Atkinson & Carter 1984; Atkinson 1985)

$k_{OH}^* = 2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}^* = 2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{NO_3} = 6.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson 1990; Altshuller 1991).

$k_{\text{NO}_3}^* = (0.45 \pm 0.06) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–523 K, atmospheric $t_{1/2} = 4300$ h during the night at room temp. (discharge flow system, Bagley et al. 1990)

atmospheric lifetime was estimated to be 54 h, based on the photooxidation reaction rate constant with OH radical during summer daylight hours (Altshuller 1991)

$k_{\text{NO}_3} = (\leq 2.0 - 6.6) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296–298 K (Atkinson 1991)

$k_{\text{NO}_3}(\text{exptl}) = 6.70 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{recommended}) = 4.3 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{\text{OH}}^* = 2.44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}^* = 4.59 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

$k_{\text{OH}}^* = 2.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 6.5$ h in ambient air based on reaction with OH radicals at 300 K (Doyle et al. 1975);

photolysis $t_{1/2} = 2.4$ to 24 h (Darnall et al. 1976);

atmospheric lifetimes $\tau(\text{calc}) = 4 \times 10^7$ h for reaction with O_3 , $\tau = 107$ h with OH radical and $\tau = 32150$ h with NO_3 radical based on reaction rate constants and environmental concentrations of OH, NO_3 radicals and O_3 in the gas phase (Atkinson & Carter 1984);

atmospheric lifetimes $\tau(\text{calc}) = 222$ h for the reaction with OH radical, $\tau = 4 \times 10^7$ h with O_3 and $\tau = 32150$ h with NO_3 radical based on the rate constants and environmental concentrations of OH, NO_3 radicals and O_3 in the gas phase (Atkinson 1985);

atmospheric $t_{1/2} = 4300$ h due to reaction with NO_3 during the night at room temp., and $t_{1/2} = 77$ h for reaction with OH radical (Bagley et al. 1990);

atmospheric lifetime $\tau \sim 54$ h based on a photooxidation reaction rate constant of $2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radicals during summer daylight hours (Altshuller 1991).

2.1.1.1.4 2-Methylbutane (Isopentane)



Common Name: 2-Methylbutane

Synonym: Isopentane

Chemical Name: 2-methylbutane

CAS Registry No: 78-78-4

Molecular Formula: C_5H_{12} ; $CH_3CH(CH_3)CH_2CH_3$

Molecular Weight: 72.149

Melting Point ($^{\circ}C$):

-159.77 (Lide 2003)

Boiling Point ($^{\circ}C$): 27.875

27.88 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.6197, 0.6146 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)0.6193, 0.6142 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)Molar Volume (cm^3/mol):116.5, 117.47 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

118.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.1505 (Dreisbach 1959, Riddick et al. 1986)

5.13 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

45.23, 43.35 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

47.8 (shake flask-GC, McAuliffe 1963,1966)

46.9* ($20^{\circ}C$, shake flask-GC, measured range $20-60^{\circ}C$, Pavlova et al. 1966)72.4; 49.6, 55.2 (0 , $25^{\circ}C$, shake flask-GC, calculated-group contribution, Polak & Lu 1973)

48.0 (shake flask-GC, Price 1976)

48.0 (selected, Riddick et al. 1986)

48.5* (IUPAC recommended best value, temp range $0-60^{\circ}C$, Shaw 1989)52.11* (calculated-liquid-liquid equilibrium LLE data, temp range $273.2-323.2 K$, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

82790 ($22.04^{\circ}C$, Schumann et al. 1942)83720* ($22.44^{\circ}C$, manometer, temp range $16.291-28.587^{\circ}C$, Willingham et al. 1945)log (P/mmHg) = $6.87372 - 1075.816/(233.259 + t/^{\circ}C)$; temp range $16.291-28.587^{\circ}C$ (Antoine eq. from exptl. data, manometer, Willingham et al. 1945)99550* (Antoine eq. regression, temp range -82.9 to $27.8^{\circ}C$, Stull 1947)

91740 (calculated from determined data, Dreisbach 1959)

log (P/mmHg) = $6.78967 - 1020.012/(223.097 + t/^{\circ}C)$; temp range -45 to $75^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)91646* (extrapolated-Antoine eq, temp range -67.03 to $49.14^{\circ}C$, Zwolinski & Wilhoit 1971)log (P/mmHg) = $6.83315 - 1040.73/(235.455C + t/^{\circ}C)$; temp range -67.03 to $49.14^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)log (P/mmHg) = $[-0.2185 \times 6470.8/(T/K)] + 7.544680$; temp range: -82.9 to $180.3^{\circ}C$, (Antoine eq., Weast 1972-73)

91730, 92100 (interpolated, Antoine equations, Boublik et al. 1984)

- $\log (P/\text{kPa}) = 6.04913 - 1081.748/(239.817 + t/^{\circ}\text{C})$; temp range -56 to 22.4°C (Antoine eq. from reported exptl. data of Schumann et al. 1942, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 5.9333 - 1029.602/(234.294 + t/^{\circ}\text{C})$; temp range 16.29 – 28.59°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 91660 (interpolated-Antoine eq., temp range -87 to 7°C , Dean 1985)
 $\log (P/\text{mmHg}) = 6.91048 - 946.35/(246.68 + t/^{\circ}\text{C})$; temp range -87 to 7°C (Antoine eq., Dean 1985, 1992)
 91700 (quoted, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 5.92023 - 1022.88/(233.460 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 91640 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.95805 - 1040.73/(-37.705 + T/\text{K})$; temp range 216 – 323 K (Antoine eq-I., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.32287 - 1279.08/(-4.481 + T/\text{K})$; temp range 300 – 460 K (Antoine eq-II., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.39629 - 1325.048/(1.244 + T/\text{K})$; temp range 320 – 391 K (Antoine eq-III., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.22589 - 1212.803/(-12.958 + T/\text{K})$; temp range 385 – 416 K (Antoine eq-IV., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.09160 - 3167.07/(233.708 + T/\text{K})$; temp range 412 – 460 K (Antoine eq-V., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 29.2963 - 2.1762 \times 10^3/(T/\text{K}) - 7.883 \cdot \log (T/\text{K}) - 4.6512 \times 10^{-11} \cdot (T/\text{K}) + 3.8997 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 113 – 460 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 140000 (calculated-P/C, Mackay et al. 1979; Mackay 1981)
 138000; 140000, 139000, 134700 (recommended; calculated-P/C, Mackay & Shiu 1981))
 138210 (selected, Mills et al. 1982)
 138290 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.30 (calculated- π constant, Hansch et al. 1968)
 2.41 (calculated-MCI χ , Murray et al. 1975)
 2.83 (calculated-molar volume V_M , Wang et al. 1992)
 2.4698 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

- $k_{\text{OH}} = 2.0 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ with atmospheric $t_{1/2} = 2.4$ – 24 h (Lloyd 1976, Darnall et al. 1976)
 $k_{\text{OH}} = (3.78 \pm 0.07) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)
 $k_{\text{OH}} = (3.97 \pm 0.11) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
 $k_{\text{OH}} = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)
 $k_{\text{OH}} = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990, 1991; Altshuller 1991)
 $k_{\text{NO}_3}^* = (1.60 \pm 0.2) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298 – 523 K, atmospheric $t_{1/2} = 1200$ h during the night at room temp. (discharge flow system, Bagley et al. 1990)
 $k_{\text{OH}} = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, estimated atmospheric lifetime of 36 h (Altshuller 1991)

$k_{\text{NO}_3}(\text{exptl}) = 1.56 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{calc}) = 2.49 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{\text{OH}} = 3.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}^* = 1.62 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $2.0 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in air (Darnall et al. 1976; Lloyd et al. 1976) with atmospheric $t_{1/2} = 2.4\text{--}24 \text{ h}$ (Darnall et al. 1976);

atmospheric $t_{1/2} = 1200 \text{ h}$ due to reaction with NO_3 radical during the night at room temp., and $t_{1/2} = 50$ for reaction with OH radical (Bagley et al. 1990);

atmospheric lifetime of 36 h, based on rate constant of $3.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radicals during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.4.1

Reported aqueous solubilities of 2-methylbutane (isopentane) at various temperatures

Pavlova et al. 1966 in IUPAC 1989		Polak & Lu 1973 shake flask-GC/FID		Shaw 1989a IUPAC recommended		Mączyński et al. 2004 calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	46.9	0	72.4	0	72	0	68.14
40	57.7	25	49.6	20	47	20	56.12
50	70.1			25	48.5	25	52.11
60	79.3			30	51	40	52.11
				40	58	50	56.12
				50	70		
				60	79		

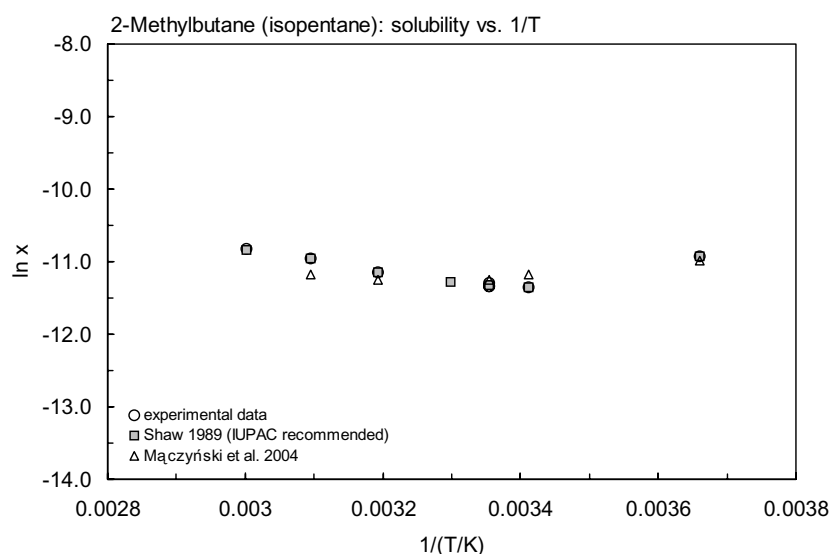


FIGURE 2.1.1.1.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-methylbutane.

TABLE 2.1.1.1.4.2

Reported vapor pressures of 2-methylbutane (isopentane) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$	(5)						
Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971			
ebulliometry		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
16.291	66760	−82.9	133.3	−57.03	1333	25.517	93326
22.435	83722	−65.8	666.6	−47.32	2666	26.320	95992
26.773	97608	−57.0	1333	−41.14	4000	27.156	98659
27.24	99207	−47.3.	2666	−36.49	5333	27.875	101325
27.673	100700	−36.5	5333	−32.74	6666	25.0	91646
28.16	102402	−29.6	7999	−29.56	7999		
28.587	103922	−20.2	13332	−24.35	10666	eq. 2	P/mmHg
		−5.90	26664	−20.11	13332	A	6.83315
bp/°C	27.852	10.5	53329	−11.97	19998	B	1040.73
		27.8	101325	−5.81	26664	C	235.445
eq. 2	P/mmHg			−0.79	33331	bp/°C	28.875
A	6.78967	mp/°C	−159.7	3.47	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
B	1020.012			10.53	53329	at 25°C	24.84
C	233.097			16.293	66661	at bp	24.69
				21.208	79993		

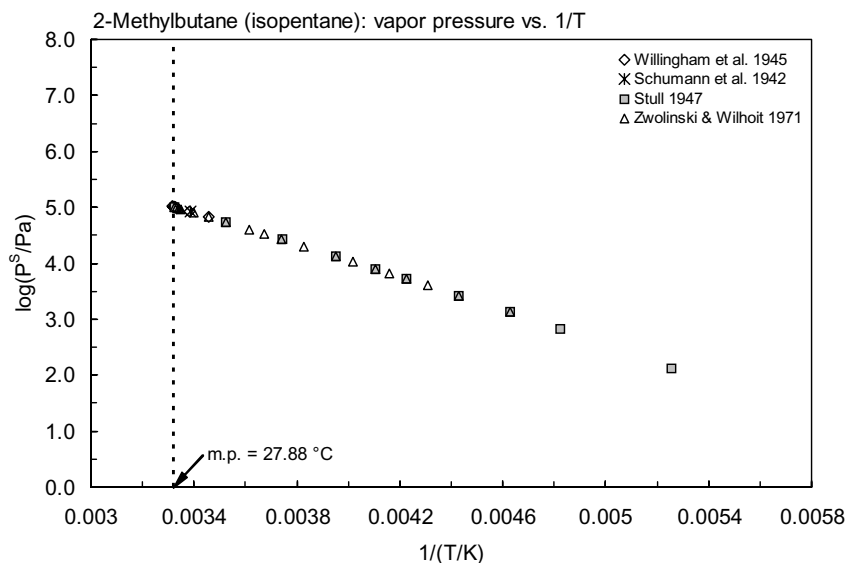


FIGURE 2.1.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methylbutane.

2.1.1.1.5 2,2-Dimethylbutane



Common Name: 2,2-Dimethylbutane

Synonym: neohexane, dimethylpropylmethane

Chemical Name: 2,2-dimethylbutane

CAS Registry No: 75-83-2

Molecular Formula: C_6H_{14} ; $CH_3CH(CH_3)_2CH_2CH_3$

Molecular Weight: 86.175

Melting Point ($^{\circ}C$):

−99.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

49.73 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6492, 0.6445 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

132.74, 133.71 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.791 (Dreisbach 1959; Riddick et al. 1986)

5.4, 0.28, 0.58 (−146.35, −132.35, −98.95 $^{\circ}C$, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

45.88, 42.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

18.4 (shake flask-GC, McAuliffe 1963,1966)

39.4, 23.8 (0, $25^{\circ}C$, shake flask-GC, Polak & Lu 1973)

21.2 (shake flask-GC, Price 1976)

21.2 (shake flask-GC, Krzyzanowska, Szeliga 1978)

18.0 (selected Riddick et al. 1986)

21.0 (IUPAC recommended best value, Shaw 1989)

19.63 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

43320 ($24.47^{\circ}C$, manometer, temp range 15.376 – $50.529^{\circ}C$, Willingham et al. 1945)

$\log(P/mmHg) = 6.75483 - 1081.176/(229.343 + t/^{\circ}C)$; temp range 15.376 – $50.529^{\circ}C$ (Antoine eq. from exptl. data, manometer, Willingham et al. 1945)

43480 (Antoine eq. regression, temp range -69.3 to $49.7^{\circ}C$, Stull 1947)

42570 ($25^{\circ}C$, Nicolini & Laffitte 1949)

42540 (calculated from determined data, Dreisbach 1959; quoted, Hine & Mookerjee 1975)

$\log(P/mmHg) = 6.75483 - 1081.176/(229.343 + t/^{\circ}C)$; temp range -25 to $95^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

42543 (interpolated-Antoine eq., temp range -41.5 to $72.8^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.75483 - 1081.176/(229.343 + t/^{\circ}C)$; temp range -41.5 to $72.8^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 7271.0/(T/K)] + 7.84130$; temp range -69.3 to $49.7^{\circ}C$ (Antoine eq., Weast 1972–73)

42585, 42550 (interpolated-Antoine equations, Boublik et al. 1984)

$\log(P/kPa) = 5.88698 - 1085.038/(229.817 + t/^{\circ}C)$; temp range 15.376 – $50.53^{\circ}C$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

$\log(P/kPa) = 5.87001 - 1080.723/(229.842 + t/^{\circ}C)$; temp range 0 – $45^{\circ}C$ (Antoine eq. from reported exptl. data of Nicolini & Laffitte 1949, Boublik et al. 1984)

- 42540 (interpolated-Antoine eq., temp range -42 to 73°C, Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.75483 - 1081.176/(229.34 + t/^\circ\text{C})$; temp range -42 to 73°C (Antoine eq., Dean 1985, 1992)
 42700 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.87963 - 1081.14/(229.349 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 42560 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.87731 - 1079.789/(-43.978 + T/\text{K})$; temp range 293–324 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 33.1285 - 2.4527 \times 10^3/(T/\text{K}) - 9.2016 \cdot \log(T/\text{K}) - 4.7077 \times 10^{-10} \cdot (T/\text{K}) + 4.1755 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 174–489 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 173000 (calculated-P/C, Mackay & Shiu 1981)
 196800 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 196800, 49430 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 173180 (calculated-P/C, Eastcott et al. 1988)
 188040 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 153890 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.82 (calculated-fragment const., Valvani et al. 1981)
 3.25 (calculated- V_M , Wang et al. 1992)
 3.82 (recommended, Sangster 1993)
 3.82 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$$k_{OH} = (2.66 \pm 0.08) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (relative rate, Atkinson et al. 1984c)}$$

$$k_{OH} = (2.59 - 6.16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 297–299 K (Atkinson 1985)}$$

$$k_{OH}^* = (2.22 - 0.36) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 299 K, measured range 245–328 K (relative rate method, Harris & Kerr 1988; Atkinson 1989)}$$

$$k_{OH}^* = 2.32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1989, 1990)}$$

$$k_{OH}^* = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1997)}$$

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.1.1.6 2,3-Dimethylbutane



Common Name: 2,3-Dimethylbutane

Synonym: diisopropyl

Chemical Name: 2,3-dimethylbutane

CAS Registry No: 79-29-8

Molecular Formula: C_6H_{14} ; $CH_3CH(CH_3)CH(CH_3)CH_3$

Molecular Weight: 86.175

Melting Point ($^{\circ}C$):

−128.10 (Lide 2003)

Boiling Point ($^{\circ}C$):

57.93 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6616, 0.6570 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

0.6616 (Weast 1984)

Molar Volume (cm^3/mol):

130.25, 131.16 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

29.12, 27.275 ($25^{\circ}C$, bp, Dreisbach 1959)

29.125, 27.276 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

0.812 (Dreisbach 1959)

0.7991 (Riddick et al. 1986)

6.43, 2.37, 0.79 (−137.05, −166.15, −127.95 $^{\circ}C$, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

52.96, 37.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

32.9, 22.5 (0, $25^{\circ}C$, shake flask-GC, calculated-group contribution, Polak & Lu 1973)

19.1* (shake flask-GC, measured range 25–149.5 $^{\circ}C$, Price 1976)

11.0 (selected, Riddick et al. 1986)

21.0* (IUPAC tentative value, temp range 0 – 150 $^{\circ}C$, Shaw 1989a)

18.67* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–422.7 K, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

28955* (23.10 $^{\circ}C$, ebulliometry, measured range: 14.256–58.789 $^{\circ}C$, Willingham et al. 1945)

$\log (P/mmHg) = 6.80983 - 1127.187/(228.900 + t/^{\circ}C)$; temp range 14.256–58.789 $^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry, Willingham et al. 1945)

31204* (calculated-Antoine eq. regression, temp range −63.6 to 58 $^{\circ}C$, Stull 1947)

31280 (calculated from determined data, Dreisbach 1959)

$\log (P/mmHg) = 6.90983 - 1127.187/(228.9 + t/^{\circ}C)$; temp range −20 to 100 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

31277* (Antoine eq., temp range −34.9 to 81.3 $^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.80983 - 1127.187/(228.900 + t/^{\circ}C)$; temp range −34.9 to 81.3 $^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = [-0.2185 \times 7120.0/(T/K)] + 7.536008$; temp range −63.6 to 225.5 $^{\circ}C$ (Antoine eq., Weast 1972–73)

- 31280 (interpolated-Antoine equations, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.594371 - 1132.099/(229.494 + t/^\circ\text{C})$; temp range 14.256–58.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
- 32010 (interpolated-Antoine eq., temp range –35 to 81°C, Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.80983 - 1127.83/(228.90 + t/^\circ\text{C})$; temp range –35 to 81°C (Antoine eq., Dean 1985, 1992)
- 31300 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.93941 - 1129.73/(229.215 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
- 31290 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.95181 - 1136.355/(-43.159 + T/\text{K})$; temp range 278–322 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 33.6319 - 2.5524 \times 10^3/(T/\text{K}) - 9.3142 \cdot \log(T/\text{K}) + 1.4759 \times 10^{-10} \cdot (T/\text{K}) + 3.914 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 145–500 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 130000 (recommended, Mackay & Shiu 1981)
 141000 (calculated-P/C, Mackay & Shiu 1981)
 131190 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.85 (shake flask, Hansch & Leo 1979)
 3.85 (calculated-fragment const., Valvani et al. 1981)
 3.85 (recommended, Sangster 1989, 1993)
 2.42; 2.63 (calculated-S, calculated-molar volume, Wang et al. 1992)
 3.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}^*(\text{exptl}) = 5.16 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{correlated}) = 4.49 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K, measured range 300–498 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{\text{O}(^3\text{P})} = 2.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom at room temp. (Herron & Huie 1973)

$k_{\text{OH}} = 5.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979)

$k_{\text{OH}} = 5.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{O}(^3\text{P})} = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O}(^3\text{P})$ atom at room temp. (abstraction mechanism, Gaffney & Levine 1979)

$k_{\text{OH}} = (5.67 \pm 0.29) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)

$k_{\text{OH}} = (6.26 \pm 0.06) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{\text{NO}_3} = 4.06 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (relative rate method, Atkinson et al. 1988)

$k_{\text{OH}}^* = (5.90 - 0.23) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 247–327 K (relative rate method, Harris & Kerr 1988)

$k_{\text{OH}} = 6.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 6.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated atmospheric lifetime of 22 h in air during summer daylight (Altshuller 1991)

$k_{\text{OH}} = 6.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 4.06 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}} = 19.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 4.06 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{\text{NO}_3} = (4.04 - 5.34) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (review, Atkinson 1991)

$k_{\text{OH}} = 6.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 40.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{\text{NO}_3}(\text{exptl}) = 4.08 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{recommended}) = 2.55 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$,
 $k_{\text{NO}_3}(\text{calc}) = 2.55 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{\text{OH}}^* = 5.78 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 4.40 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $6.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radicals and an estimated atmospheric lifetime of 22 h during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.6.1

Reported aqueous solubilities of 2,3-dimethylbutane at various temperatures

Polak & Lu 1973		Price 1976		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC		shake flask-GC/FID		IUPAC tentative values		calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	32.9	25	19.1	0	33	25	18.67
25	22.5	40.1	19.2	25	21	40.1	18.19
		55.1	23.7	30	19	55.1	20.11
		99.1	40.1	41	19	99.1	39.74
		1213	56.8	50	21	121.3	67.03
		137.3	97.9	70	28	137.3	100.5
		149.5	171	90	35	149.5	138.8
				110	46		
				130	75		
				150	180		

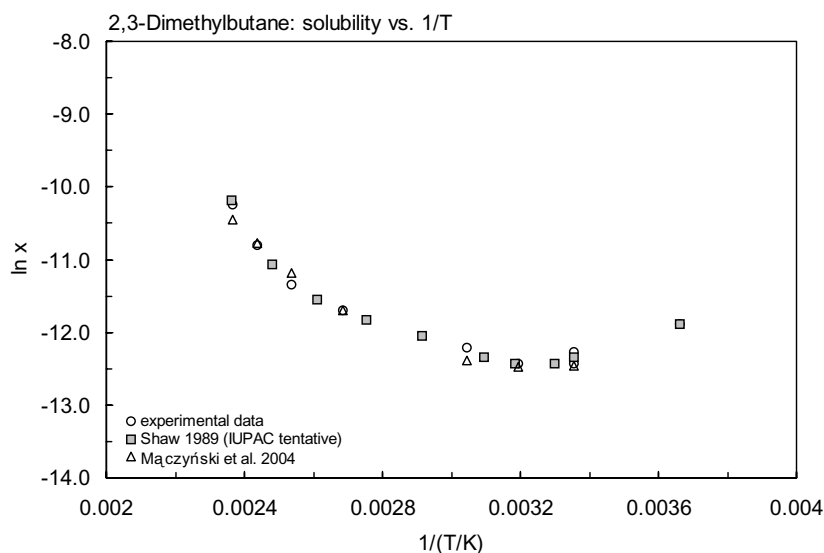


FIGURE 2.1.1.1.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,3-dimethylbutane.

TABLE 2.1.1.1.6.2

Reported vapor pressures of 2,3-dimethylbutane at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971			
ebulliometry		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
14.256	19921	–63.6	133.3	–34.9	1333	57.988	101325
18.044	23451	–44.5	666.6	–24.3	2666	25.0	234.6
23.099	28955	–34.9	1333	–17.5	4000		
27.746	34897	–24.1	2666	–12.5	5333	eq. 2	P/mmHg
33.357	43320	–12.4	5333	–8.4	6666	A	6.80983
39.15	53654	–4.9	7999	–4.9	7999	B	1127.187
45.339	66756	5.40	13332	0.82	10666	C	228.900
52.06	83718	21.1	26664	5.34	13332		
56.806	97604	39.0	53329	14.36	19998	bp/°C	57.998
57.317	99201	58.0	101325	21.097	26664	ΔH _v /(kJ mol ^{–1}) =	
57.79	100693			26.588	33331	at 25°C	29.12
58.32	102390	mp/°C	–128.2	31.257	39997	at bp	27.28
58.789	103907			38.982	53329		
				45.927	66661		
bp/°C	57.988			50.682	79993		
eq. 2	P/mmHg			55.404	93326		
A	6.80983			56.283	95992		
B	1127.187			57.145	98659		
C	228.900			57.568	99992		

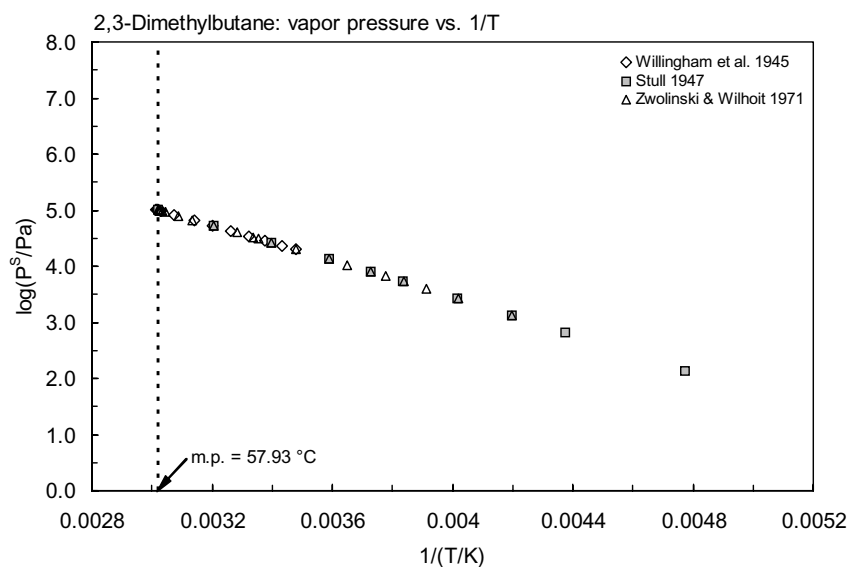


FIGURE 2.1.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylbutane.

2.1.1.1.7 2,2,3-Trimethylbutane



Common Name: 2,2,3-Trimethylbutane

Synonym: triptene

Chemical Name: 2,2,3-trimethylbutane

CAS Registry No: 464-06-2

Molecular Formula: C_7H_{16} ; $CH_3CH(CH_3)_2CH(CH_3)_2$

Molecular Weight: 100.202

Melting Point ($^{\circ}C$):

−24.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

80.86 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6901, 0.6859 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

0.6901 (Weast 1984)

Molar Volume (cm^3/mol):

145.2, 146.1 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.037, 28.94 ($25^{\circ}C$, at normal bp, Dreisbach 1959)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

2.259 (at mp, Dreisbach 1959; Chickos et al. 1999)

2.36, 2.2 (-152.15 , $-25.45^{\circ}C$, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

28.53, 36.7 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.38 (estimated-nomograph of Kabadi & Danner 1979; Brookman et al. 1985)

7.09 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

13840 ($25.3^{\circ}C$, ebulliometry, measured range 12.6 – $81.8^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 6.79230 - 1200.563/(226.650 + t/^{\circ}C)$; temp range 12.6 – $81.8^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

13650 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.79230 - 1200.563/(226.05 + t/^{\circ}C)$; temp range 0 – $125^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

13652 (derived from compiled data, temp range -18.8 – $205.94^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.79230 - 1200.563/(226.050 + t/^{\circ}C)$; temp range -18.8 – $205.94^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

13650, 13660 (interpolated-Antoine equations, Boublik et al. 1984)

$\log(P/kPa) = 5.92699 - 11206.087/(226.731 + t/^{\circ}C)$; temp range 22.7 – $105.6^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 5.92037 - 1202.337/(226.256 + t/^{\circ}C)$; temp range 12.6 – $81.77^{\circ}C$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

13650 (interpolated-Antoine eq., temp range -19 to $106^{\circ}C$, Dean 1985, 1992)

$\log(P/mmHg) = 6.79230 - 1200.563/(226.05 + t/^{\circ}C)$; temp range -19 to $106^{\circ}C$ (Antoine eq., Dean 1985, 1992)

13650 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.9181 - 1201.098/(-47.026 + T/\text{K})$; temp range 284–355 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.18145 - 1390.726/(-20.97 + T/\text{K})$; temp range 353–483 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 32.3633 - 2.6614 \times 10^3/(T/\text{K}) - 8.7743 \cdot \log (T/\text{K}) - 7.687 \times 10^{-10} \cdot (T/\text{K}) + 3.2006 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 249–531 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

241010 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^*(\text{exptl}) = 3.84 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{correlated}) = 3.15 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 296 K, measured range 296–498 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{OH} = (3.6 - 5.05) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296–305 K (Darnall et al. 1978)

$k_{OH} = (4.21 \pm 0.08) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 5.23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, $k_{OH} = 4.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (Atkinson 1985)

$k_{OH}^* = 4.23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{NO_3}(\text{exptl}) = 2.23 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}(\text{calc}) = 1.31 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

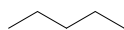
$k_{OH}^* = 4.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}^* = 2.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

2.1.1.1.8 *n*-PentaneCommon Name: *n*-Pentane

Synonym: pentane

Chemical Name: *n*-pentane

CAS Registry No: 109-66-0

Molecular Formula: C₅H₁₂; CH₃(CH₂)₃CH₃

Molecular Weight: 72.149

Melting Point (°C):

-129.67 (Lide 2003)

Boiling Point (°C):

36.06 (Lide 2003)

Density (g/cm³ at 20°C):

0.6262, 0.6214 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm³/mol):

115.22, 116.1 (20° C, 25°C, calculated-density)

118.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

26.42, 25.77 (25°C bp, Dreisbach 1959)

26.427, 25.786 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.393 (Dreisbach 1959; Riddick et al. 1986)

8.4 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

58.59, 63.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

360 (16°C, cloud point, Fühner 1924)

120 (radiotracer method, Black et al. 1948)

38.5 (shake flask-GC, McAuliffe 1963, 1966)

49.7 (vapor saturation-GC, Barone et al. 1966)

40.0 (Baker 1967)

40.3* (shake flask-GC, measured range 4 – 30°C, Nelson & De Ligny 1968)

11.8* (shake flask-GC, measured range 5 – 35°C, Pierotti & Liabastre 1972)

65.7; 47.6, 44.6 (0, 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)

39.5* (shake flask-GC, measured range 25 – 149.5°C, Price 1976)

39.0 (shake flask-GC, Kryzanowska & Szeliga 1978)

40.0 (partition coefficient, Rudakov & Lutsyk 1979)

40.75 (generator column-GC, Tewari et al. 1982a)

36.9 (calculated-activity coeff. γ and K_{ow}, Tewari 1982b)

40.6* (vapor saturation-GC, measured range 15 – 40°C, Jönsson et al. 1982)

38.9 (shake flask-GC, Coates et al. 1985)

38.0 (selected, Riddick et al. 1986)

42.0* (IUPAC recommended best value, temp range 0 – 90°C, Shaw 1989)

$\ln x = -333.59719 + 14358.472/(T/K) + 47.97436 \cdot \ln (T/K)$; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

44.09* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2 – 422.7 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 68213* (24.828°C, static method, measured range -65 to 25°C, Messerly & Kennedy 1940)
 66760* (24.37°C, ebulliometry, measured range 13.282–36.818°C, Willingham et al. 1945)
 $\log(P/\text{mmHg}) = 6.87372 - 1075.816/(233.369 + t/^\circ\text{C})$; temp range 13.282–36.818°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
 71050* (interpolated-Antoine eq. regression, temp range -76.6 to 36.1°C, Stull 1947)
 68330 (calculated from determined data, Dreisbach 1959)
 $\log(P/\text{mmHg}) = 6.85221 - 1064.63/(232.0 + t/^\circ\text{C})$; temp range -35 to 80°C (Antoine eq. for liquid state, Dreisbach 1959)
 68368* (interpolated-Antoine eq., temp range -50.14 to 57.53°C, Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = 6.87632 - 1075.78/(233.205 + t/^\circ\text{C})$; temp range -50.14 to 57.53°C (Antoine eq., Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = [-0.2185 \times 6595.1/(T/\text{K})] + 7.489673$; temp range -76.6 to 191°C (Antoine eq., Weast 1972–73)
 3400* (-30.86°C, gas saturation, measured range -129.54 to -30.86°C, Carruth & Kobayashi 1973)
 57820* (20.57°C, ebulliometric method, measured range -4.4 to 68.218°C, Osborn & Douslin 1974)
 68330 (interpolated-Antoine eq, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.12545 - 1132.518/(239.074 + t/^\circ\text{C})$; temp range -65.2 to 24.83°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.96982 - 1060.916/(231.577 + t/^\circ\text{C})$; temp range 13.28–36.82°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.99028 - 1071.187/(232.766 + t/^\circ\text{C})$; temp range -4.4 to 68.21°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1974, Boublik et al. 1984)
 70915 (interpolated-Antoine eq., temp range -50 to 58°C, Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.85296 - 1064.84/(233.01 + t/^\circ\text{C})$; temp range -50 to 58°C (Antoine eq., Dean 1985, 1992)
 69810, 68880, 68330 (headspace-GC, correlated, Antoine eq., Hussam & Carr 1985)
 68330 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.97786 - 1064.84/(232.012 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 68355 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.6922 - 1686.65/(T/\text{K})$; temp range 143–233 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.99466 - 1073.139/(-40.188 + T/\text{K})$; temp range 223–352 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.98799 - 1070.14/(-40.485 + T/\text{K})$; temp range 269–335 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.28417 - 1260.973/(-14.031 + T/\text{K})$; temp range 350–422 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.47436 - 2414.137/(141.919 + T/\text{K})$; temp range 418–470 K (Antoine eq., Stephenson & Malanowski 1987)
 68340* (recommended, Ruzicka & Majer 1994)
 $\ln[(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/K)/(T/K)] \cdot \exp\{2.73425 - 1.988544 \times 10^{-3} \cdot (T/K) + 2.408406 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_o = 101.325 \text{ kPa}$, $T_o = 309.209 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log(P/\text{mmHg}) = 33.3239 - 2.4227 \times 10^3/(T/\text{K}) - 9.2354 \cdot \log(T/\text{K}) + 9.0199 \times 10^{-11} \cdot (T/\text{K}) + 4.105 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 143–470 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

- 127050 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 115900, 33430 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 128000 (calculated-P/C, Mackay & Shiu 1975, 1990; Bobra et al. 1979; Mackay et al. 1979; Mackay 1981)
 125000 (recommended, Mackay & Shiu 1981)
 128000, 125000, 123000, 122200, 10370 (calculated-P/C, Mackay & Shiu 1981)
 78050, 99075, 126800, 144020, 174480 (14.8, 20.05, 25.1, 30.1, 34.92°C, equilibrium cell-concentration ratio-GC, Jönsson et al. 1982)
 121410* (calculated-temp dependence eq. derived from exptl data, measured range 15–35°C. Jönsson et al. 1982)

$\ln (1/K_{AW}) = 19237.8/(T/K) + 53.671 \cdot \ln (T/K) - 372.214$; temp range: 15 – 35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)

- 127670 (selected, Mills et al. 1982)
- 120970 (calculated-P/C, Eastcott et al. 1988)
- 100980 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 128050 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.50 (shake flask-GC, Hansch et al. 1968)
- 3.39 (shake flask-GC, Leo et al. 1975)
- 2.99, 3.42, 3.48 (calculated-fragment const., Rekker 1977)
- 3.23 (Hansch & Leo 1979)
- 3.64 (calculated-activity coeff. γ , Wasik et al. 1981,1982)
- 3.62 (generator column-GC, Tewari et al. 1982a,b)
- 2.37 (HPLC- k' correlation, Coates et al. 1985)
- 3.62, 3.60 (generator column-GC, calculated-activity coeff. γ , Schantz & Martire 1987)
- 3.45 (recommended, Sangster 1989, 1993)
- 3.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 2.05* (20.29°C, from GC-determined γ° in octanol, measured range 20.29 – 50.28°C, Gruber et al. 1997)
- 1.95 (calculated-measured γ° in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated *data at other temperatures see reference:

$k_{O(3P)} = 5.8 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(^3P)$ (Herron & Huie 1973)

$k_{OH} = (3.74 \pm 0.13) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)

$k_{OH} = 5.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1979)

$k_{OH} = 5.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{O(3P)} = 5.8 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ room temp. (abstraction mechanism, Gaffney & Levine 1979)

$k_{OH} = 4.13 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $299 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1982a)

$k_{NO_3} = (8.1 \pm 1.7) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (relative rate method, Atkinson et al. 1984a; Atkinson 1991)

$k_{OH} = (4.13 \pm 0.08) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 4.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (Atkinson 1986; quoted, Edney et al. 1986)

$k_{OH} = 4.29 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in Smog chamber (Nolting et al. 1988)

$k_{OH}^* = 3.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1991)

$k_{OH} = 4.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 8.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljic & Güsten 1990)

$k_{NO_3} = 8.1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = 3.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K with summer daylight atmospheric lifetime $\tau = 35 \text{ h}$ (Altshuller 1991)

$k_{OH}^* = 3.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{NO_3} = 9.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{NO_3}(\text{exptl}) = 8.2 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}(\text{calc}) = 7.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{OH}^* = 4.00 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 8.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

$k_{OH}^* = 3.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $3.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radical and an estimated atmospheric lifetime $\tau = 35 \text{ h}$ (Altshuller 1990).

TABLE 2.1.1.1.8.1**Reported aqueous solubilities of *n*-pentane at various temperatures**

1.

Nelson & De Ligny 1968		Pierotti & Liabastre 1972		Polak & Lu 1973		Price 1976	
shake flask-GC		shake flask-GC		shake flask-GC		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4.0	40.9	5.11	10.94	0	65.7	25	39.6
10	42.9	15.21	11.80	25	47.6	40.1	39.8
20	39.3	25.11	11.20			55.7	41.8
25	40.5	35.21	10.89			99.1	69.4
30	40.5					121.3	110
						137.3	210
						149.5	298

2.

Jonsson et al. 1982		Shaw 1989a		Mączyński et al. 2004	
vapor saturation-GC		IUPAC recommended		calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	42.9	0	66	0	56.12
20	41.4	10	43	4	52.11
25	40.6	20	40	10	48.1
30	40.3	25	42	15	48.1
40	40.6	30	41	20	44.09
		40	40	25	44.09
		50	41	30	44.09
		60	43	35.1	44.09
		70	46	40.1	44.09
		80	50	55.7	48.1
		90	58	99.1	88.18
		110	86	121.3	136.3
		130	150	137.3	192.4
		150	300	149.5	260.5

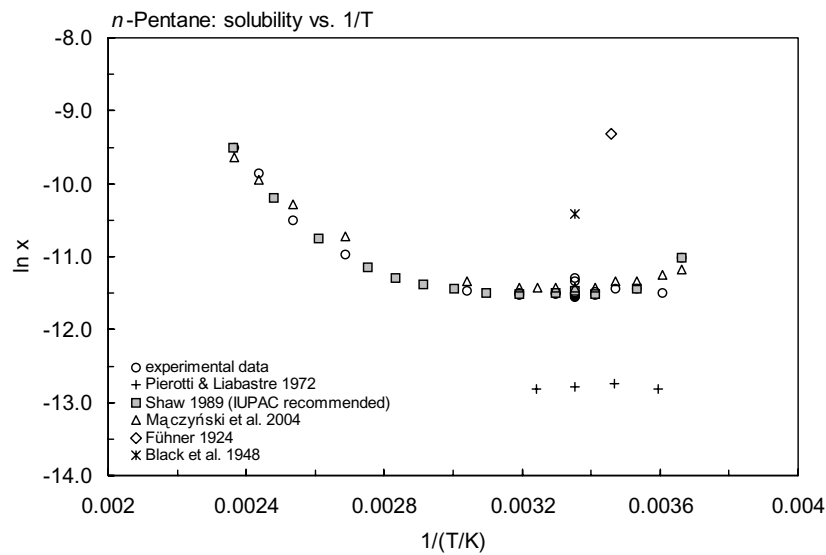


FIGURE 2.1.1.1.8.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *n*-pentane.

TABLE 2.1.1.1.8.2
Reported vapor pressures of *n*-pentane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log (P/P_{\phi}) = A[1 - \Phi/(T/K)]$	(5)	where $\log A = a + b(T/K) + c(T/K)^2$ - Cox eq. I	
$\ln [(P/kPa)/(P_{\phi}/kPa)] = [1 - (T_{\phi}/K)/(T/K)] \cdot \exp \{ A_0 - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2 \}$	(6)	- Cox eq. II	

1.

Messerly & Kennedy 1940		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static method-manometer		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-65.178	411	13.282	43322	-76.6	133.3	-50.14	1333
-48.811	1604	18.647	53657	-62.5	666.6	-40.25	2666
-39.537	2818	24.371	66756	-50.1	1333	-33.86	4000
-27.420	5951	30.592	83719	-40.1	2666	-29.24	5333
-17.476	10340	34.981	97604	-29.2	5333	-25.42	6666
-9.793	15341	35.453	99201	-22.2	7999	-22.19	7999
-2.359	21933	35.89	100694	-12.6	13332	-16.98	10666
3.618	28767	36.379	102393	1.9	26664	-12.59	13332
9.621	37303	36.818	103911	18.5	53329	-4.33	19998
14.653	45947			36.1	101325	1.92	26664
18.613	53773	bp/°C	36.073			7.01	33331
21.679	60539			mp/°C	-129.7	11.34	39997

(Continued)

TABLE 2.1.1.1.8.2 (Continued)

Messerly & Kennedy 1940		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static method-manometer		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.828	68213	eq. 2	P/mmHg			18.48	53329
		A	6.87372			24.322	66661
		B	1076.816			29.297	79993
		C	233.359			33.657	93326
						34.469	95992
						35.264	98659
						36.042	101325
						25.0	68368
						bp/°C	36.042
						eq. 2	P/mmHg
						A	6.87632
						B	1075.78
						C	233.205
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	26.43
						at bp	25.77

2.

Carruth & Kobayashi 1973		Osborn & Douslin 1974		Ruzicka & Majer 1994	
gas saturation		ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
−129.54	0.0809	−4.40	19933	144.82	0.1
−122.64	0.3893	0.512	25023	157.65	1
−115.87	0.7666	5.464	31177	173.73	10
−108.74	2.6	10.458	38656	193.17	100
−93.55	19.2	15.495	47375	219.13	1000
−83.75	56.93	20.572	57818	255.05	10000
−67.19	285.3	25.698	70121	309.21	101325
−54.18	926.6	30.86	84533	298.15	68350
−45.94	1733	36.068	101325		
−30.86	3400	41.32	120792	data calc from Cox eq.	
		46.613	143245	eq. 6	P/kPa
mp/°C	−129.7	51.951	169019	A ₀	2.73425
		57.331	198487	A ₁	1.966544×10^{-3}
eq. 1a	P/mmHg	62.755	232016	A ₂	2.408406×10^{-6}
A	19.7269	68.218	270022	with reference state at	
B	3899.67			P _o /kPa	101.325
		Cox eq.		T _o /K	309.21
		eq. 5	P/mmHg		
		Φ	309.218		
		a	0.81357		
		b	-7.73685×10^{-4}		
		c	9.06731×10^{-7}		
		P _Φ	760		
		temp range: 268–342 K			

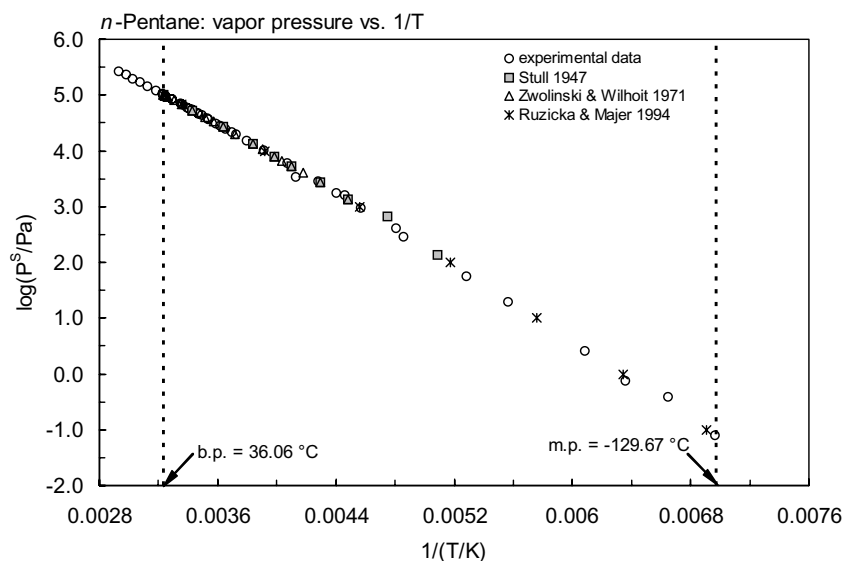


FIGURE 2.1.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-pentane.

TABLE 2.1.1.1.8.3

Reported Henry's law constants and octanol-air partition coefficients of *n*-pentane at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1)$$

$$\log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2)$$

$$\log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4)$$

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

Henry's law constant		log K_{OA}	
Jönsson et al. 1982		Gruber et al. 1997	
equilibrium cell-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OA}
15.0	78035#	20.29	2.053
15.1	77905	30.3	1.911
15.1	77905	40.4	1.781
20.0	98674	50.28	1.670
20	100713#		
20	97490		
25.0	121511		
25	125828		
25	127774		
30.0	146533#		
30	144022		
35.0	173105#		
35	175477		

interpolated from exptl data

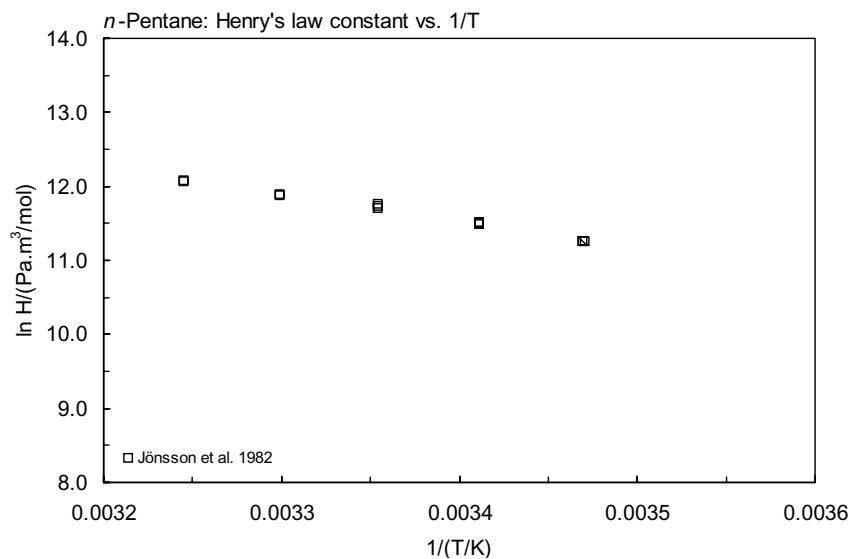


FIGURE 2.1.1.1.8.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-pentane.

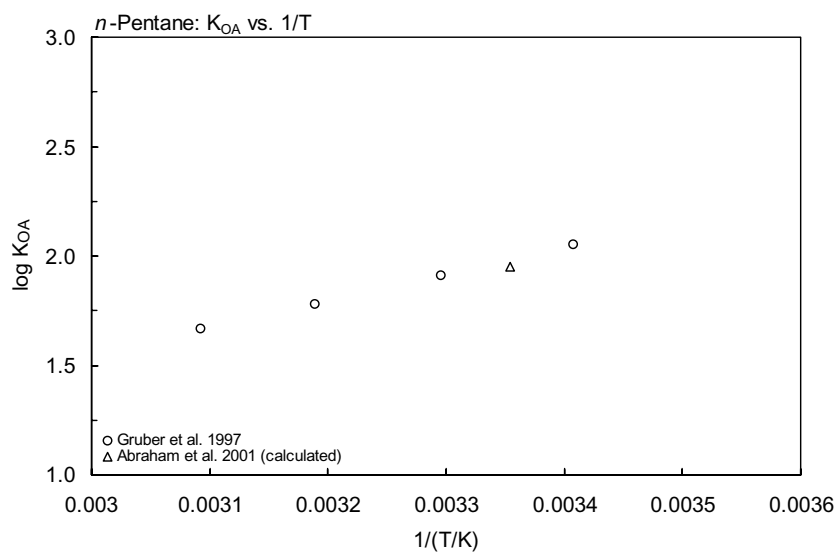
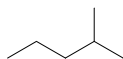


FIGURE 2.1.1.1.8.4 Logarithm of K_{OA} versus reciprocal temperature for *n*-pentane.

2.1.1.1.9 2-Methylpentane (Isohexane)



Common Name: 2-Methylpentane

Synonym: isohexane

Chemical Name: 2-methylpentane

CAS Registry No: 107-83-5

Molecular Formula: C_6H_{14} ; $CH_3CH(CH_3)CH_2CH_2CH_3$

Molecular Weight: 86.175

Melting Point ($^{\circ}C$):

-153.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

60.26 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.6322, 0.6485 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)Molar Volume (cm^3/mol):136.31, 132.88 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):29.87, 27.79 ($25^{\circ}C$, bp, Riddick et al. 1986)Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.203 (Dreisbach 1959)

6.268 (Riddick et al. 1986)

6.27 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

52.43, 50.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

13.8 (shake flask-GC, McAuliffe 1963, 1966)

16.21 (vapor saturation-GC, Barone et al. 1966)

19.45; 15.7, 15.6 (0, $25^{\circ}C$, shake flask-GC, calculated-group contribution, Polak & Lu 1973)

14.2 (shake flask-GC, Leinonen & Mackay 1973)

13.0* (shake flask-GC, measured range $25 - 149.5^{\circ}C$, Price 1976)13.7* (recommended best value, temp range $25 - 150^{\circ}C$, IUPAC Solubility Data Series, Shaw 1989a)13.88* (calculated-liquid-liquid equilibrium LLE data, temp range $273.2 - 422.7 K$, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

29040* ($25.64^{\circ}C$, ebulliometry, measured temp range $12.758 - 61.066^{\circ}C$, Willingham et al. 1945)log (P/mmHg) = $6.83910 - 1135.410/(226.572 + t/^{\circ}C)$; temp range $12.758 - 61.066^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)27820* (calculated-Antoine eq. regression, temp range -60 to $60.3^{\circ}C$, Stull 1947)

28240 (calculated from determined data, Dreisbach 1959)

log (P/mmHg) = $6.83910 - 1135.410/(226.572 + t/^{\circ}C)$; temp range -15 to $100^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

28238; 28200* (derived from compiled, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = $6.83910 - 1135.410/(226.572 + t/^{\circ}C)$; temp range -32.1 to $83.4^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

27780 (interpolated-Antoine eq., Weast 1972-73)

$\log (P/\text{mmHg}) = [-0.2185 \times 7676.6/(T/K)] + 7.944630$; temp range: -60.9 to 60.3°C (Antoine eq., Weast 1972-73)

28240 (interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.86839 - 1151.401/(228.477 + t/^\circ\text{C})$; temp range $12.78 - 61^\circ\text{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

28230 (interpolated-Antoine eq., temp range -32 to 83°C , Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.83910 - 1135.41/(226.57 + t/^\circ\text{C})$; temp range -32 to 83°C (Antoine eq., Dean 1985, 1992)

28300 (selected lit., Riddick et al. 1986)

$\log (P/\text{kPa}) = 5.98850 - 1148.74/(228.166 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

28250 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.97783 - 1142.922/(-45.657 + T/K)$; temp range $293-335$ K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 30.7477 - 2.4888 \times 10^3/(T/K) - 8.2295 \cdot \log (T/K) - 2.3723 \times 10^{-11} \cdot (T/K) + 3.2402 \times 10^{-6} \cdot (T/K)^2$; temp range $120-498$ K (vapor pressure eq., Yaws 1994)

72190 (50°C , vapor-liquid equilibria VLE data, Horstmann et al. 2004)

$\log (P/\text{kPa}) = 5.99313 - 1151.40/(T/K - 44.673)$; temp range not specified (Antoine eq., Horstmann et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

170000 (recommended; Mackay & Shiu 1981)

175490 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

196800, 49430 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

176160 (calculated-P/C, Eastcott et al. 1988)

83590* (EPICS-GC, measured range $10 - 30^\circ\text{C}$, Ashworth et al. 1988)

$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 2.959 - 957.2/(T/K)$; temp range $10 - 30^\circ\text{C}$ (EPICS measurements, Ashworth et al. 1988)

176280 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

746 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 2.470 - 288/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.80 (calculated- π constant, Hansch et al. 1968)

2.85 (calculated-MCI χ , Murray et al. 1975)

3.23 (calculated-molar volume V_M , Wang et al. 1992)

3.74 (calculated-fragment constant, Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{exptl}) = (3.2 \pm 0.6) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 305 ± 2 K (relative rate method, Lloyd et al. 1976, Darnall et al. 1976)

$k_{OH} = (5.68 \pm 0.24) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 5.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{NO_3} = 9.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{OH} = 5.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, estimated atmospheric lifetime was 25 h during summer daylight hours (Altshuller 1991)

$k_{NO_3}(\text{exptl}) = 1.71 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}(\text{calc}) = 1.83 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{OH} = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 1.8 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: half-life of 2.4–24 h based on photooxidation rate constant of $3.2 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with hydroxyl radical (Darnall et al. 1976);

atmospheric lifetime was estimated to be 25 h during summer daylight, based on photooxidation rate constant of $5.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in air (Altshuller 1991).

TABLE 2.1.1.1.9.1**Reported aqueous solubilities of 2-methylpentane at various temperatures**

Polak & Lu 1973		Price 1976		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC		shake flask-GC		IUPAC recommended		calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	19.45	25	13	25	13.7	0	18.19
25	15.7	40.1	13.8	30	13	25	13.88
		55.7	15.7	40	14	40	13.88
		99.1	27.1	50	15	55.7	15.32
		118	44.9	70	17	99.1	30.64
		137.3	86.8	90	23	118	46.92
		149.5	113	110	36	137.3	76.6
				130	68	145.9	110.12
				150	120		

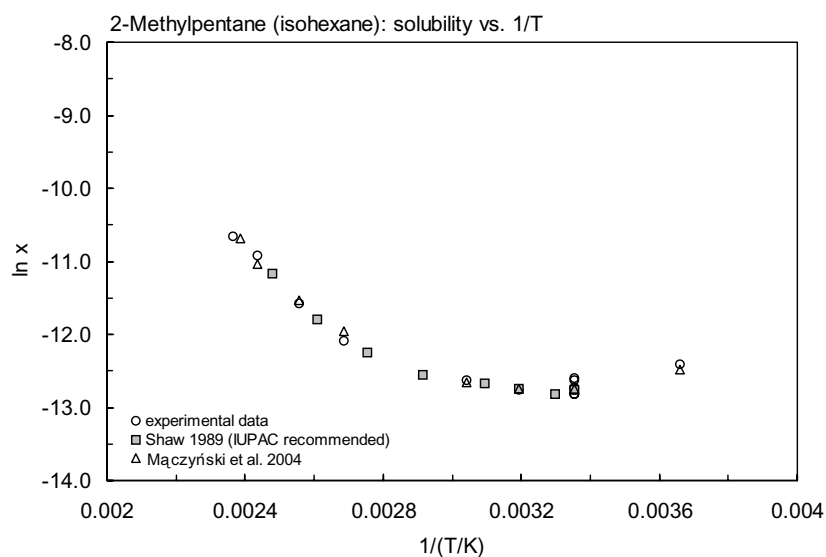
**FIGURE 2.1.1.1.9.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-methylpentane.

TABLE 2.1.1.1.9.2
Reported vapor pressures and Henry's law constants of 2-methylpentane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$	(5)						
Vapor pressure		Henry's law constant					
Willingham et al. 1945	Stull 1947	Zwolinski & Wilhoit 1971	Ashworth et al. 1988				
ebulliometry	summary of literature data	selected values	EPICS-GC				
t/°C	P/Pa	t/°C	H/(Pa m³/mol)				
12.758	16620	−60.9	133.3	−32.1	1333	10	70624
16.82	19921	−41.7	666.6	−21.6	2666	15	70320
20.584	23451	−32.1	1333	−14.8	4000	20	89470
25.617	29038	−214	2666	−9.8	5333	25	83593
30.237	34896	−9.7	5333	−5.7	6666	30	85924
35.810	43322	−1.9	7999	−2.2	7999		
41.507	53656	8.1	13332	3.45	10666	$\ln H = A - B/(T/K)$	
47.714	66757	24.1	26664	8.06	13332	$H/(\text{atm m}^3/\text{mol})$	
54.388	83718	41.5	53329	16.92	19998	A	2.959
59.099	97605	60.3	101325	23.624	26664	B	957.2
59.607	99204			29.084	33331		
60.074	100694	mp/°C	−154	33.724	39997		
60.602	102394			41.40	53329		
61.066	103913			47.672	66661		
				53.020	79993		
bp/°C	60.271			57.706	93326		
				58.579	95992		
eq. 2	P/mmHg			59.434	98659		
A	6.93910			60.271	101325		
B	1135.410			25.0	28238		
C	226.572						
				eq. 2	P/mmHg		
				A	6.83910		
				B	1135.410		
				C	226.572		
				bp/°C	60.271		
				$\Delta H_v/(\text{kJ mol}^{-1}) =$			
				at 25°C	29.76		
				at bp	27.79		

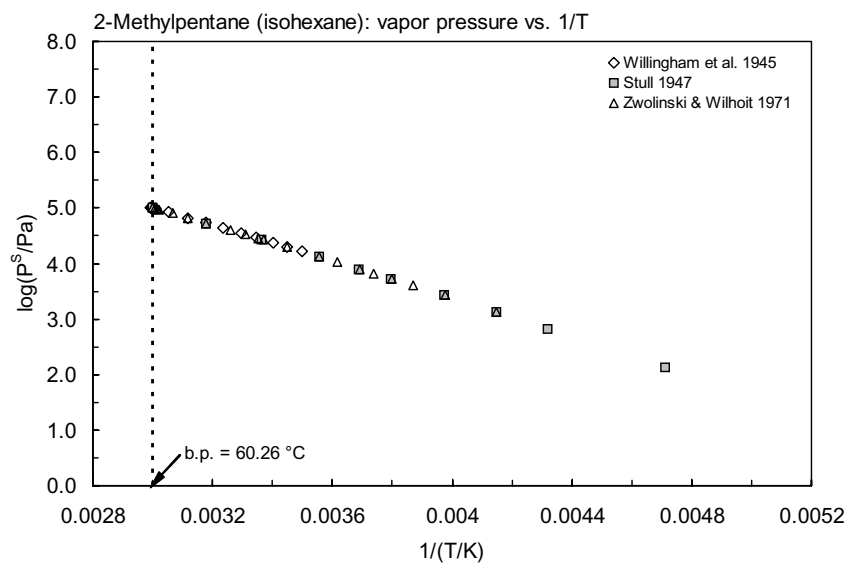


FIGURE 2.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpentane.

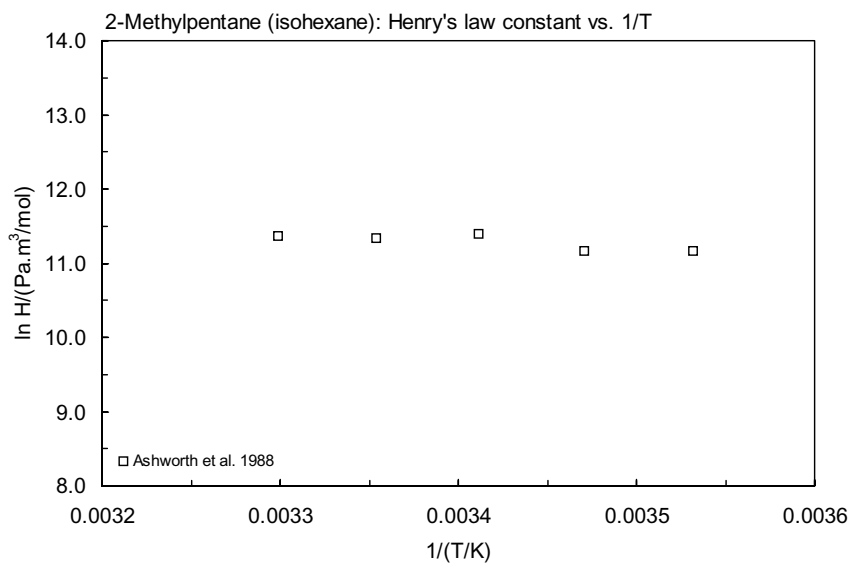
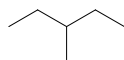


FIGURE 2.1.1.9.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-methylpentane.

2.1.1.1.10 3-Methylpentane



Common Name: 3-Methylpentane

Synonym: diethylmethylethane

Chemical Name: 3-methylpentane

CAS Registry No: 96-14-0

Molecular Formula: C_6H_{14} ; $CH_3CH_2(CH_3)CHCH_2CH_3$

Molecular Weight: 86.175

Melting Point ($^{\circ}C$):

-162.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

63.27 (Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

0.66431, 0.65976 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

129.7, 130.6 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

129.7 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

30.28, 28.08 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.035 (Riddick et al. 1986)

5.31 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

48.17, 50.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

12.8 (shake flask-GC, McAuliffe 1966)

21.5; 17.9, 17.2 (0; $25^{\circ}C$, shake flask-GC, calculated-group contribution, Polak & Lu 1973)

13.1 (shake flask-GC, Price 1976)

12.9 (partition coefficient-GC, Rudakov & Lutsyk 1979)

13.0 (selected, Riddick et al. 1986)

12.9 (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)

22.02, 16.76 (0, $25^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

29040 ($23.2^{\circ}C$, ebulliometry, measured range 15.29 – $64.083^{\circ}C$, Willingham et al. 1945)

$\log(P/mmHg) = 6.84887 - 1152.368/(227.129 + t/^{\circ}C)$; temp range 15.29 – $64.083^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

24970 (Antoine eq. regression, temp range -59 to $63.3^{\circ}C$, Stull 1947)

25300 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.84887 - 1152.368/(227.129 + t/^{\circ}C)$; temp range -15 to $105^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

25305, 25300 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.84887 - 1152.368/(227.129 + t/^{\circ}C)$; temp range -30.1 to $86.6^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

24940 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 7743.9/(T/K)] + 7.947042$; temp range -59 to $63.3^{\circ}C$ (Antoine eq., Weast 1972–73)

- 25310 (interpolated-Antoine eq, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.36895 - 1997.558/(202.608 + t/^{\circ}\text{C})$; temp range 69.2–271.1 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 25300 (interpolated-Antoine eq., temp range –30 to 87 $^{\circ}\text{C}$, Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.84887 - 1152.368/(227.13 + t/^{\circ}\text{C})$; temp range –30 to 87 $^{\circ}\text{C}$ (Antoine eq., Dean 1985, 1992)
- 25300 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.98356 - 11133.52/(224.944 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
- 25320 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.97897 - 1155.28/(-45.659 + T/\text{K})$; temp range 293–338 K (Antoine eq., Stephenson & Malanowski 1987)
- $\log(P/\text{mmHg}) = 35.2848 - 2.6773 \times 10^3/(T/\text{K}) - 9.8546 \cdot \log(T/\text{K}) + 2.2352 \times 10^{-11} \cdot (T/\text{K}) + 4.0277 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 110–504 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$):

- 172000 (recommended; Mackay & Shiu 1981)
171490 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
196800, 49430 (calculated-contribution, calculated-bond contribution, Hine & Mookerjee 1975)
170210 (calculated-P/C, Eastcott et al. 1988)
139390 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
113670 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.80 (calculated- π const., Hansch et al. 1968; Hansch & Leo 1979)
2.88 (calculated-MCI χ , Murray et al. 1975)
3.81 (calculated-intrinsic molar volume V_I and solvatochromic parameters, Leahy 1986)
 3.60 ± 0.20 (recommended, Sangster 1989)
3.18 (calculated-molar volume V_M , Wang et al. 1992)
3.74 (calculated-fragment constant, Müller & Klein 1992)
2.9168 (calculated-UNIFAC group contribution, Chen et al. 1993)
3.60 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

- Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH} = 1.28 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at 300 K (Greiner 1967; quoted, Altshuller & Bufalini 1971)
 $k_{OH} = (4.3 \pm 0.9) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Lloyd et al. 1976)
 $k_{OH} = 6.82 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at atmospheric pressure and 305 K (Darnall et al. 1978)
 $k_{OH} = (5.78 \pm 0.11) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
 $k_{OH} = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1991)
 $k_{OH} = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, estimated atmospheric lifetime 25 h, during summer daylight hours (Altshuller 1991)
 $k_{NO_3}(\text{exptl}) = 2.04 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}(\text{calc}) = 2.53 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)
 $k_{OH} = 5.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}^* = 2.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

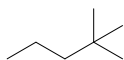
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $4.30 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ with hydroxyl radical with half-life of 2.4–24 h (Darnall et al. 1976; Lloyd et al. 1976);

rate constant of $5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ for the reaction with OH radical with an estimated atmospheric lifetime of 25 h during summer daylight (Altshuller 1991).

2.1.1.1.11 2,2-Dimethylpentane



Common Name: 2,2-Dimethylpentane

Synonym:

Chemical Name: 2,2-dimethylpentane

CAS Registry No: 590-35-2

Molecular Formula: C_7H_{16} ; $CH_3C(CH_3)_2CH_2CH_2CH_3$

Molecular Weight: 100.202

Melting Point ($^{\circ}C$):

-123.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

79.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6739 (Weast 1984)

0.6739, 0.6695 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)Molar Volume (cm^3/mol):148.69 ($20^{\circ}C$, calculated from density)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.812 (Dreisbach 1959)

5.86 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

39.55, 49.74 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.40 (shake flask-GC, Price 1976)

4.90 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):13824 ($24.67^{\circ}C$, manometer, measured range 15.325 – $80.05^{\circ}C$, Willingham et al. 1945) $\log(P/mmHg) = 6.81509 - 1190.298/(223.343 + t/^{\circ}C)$; temp range 15.325 – $80.05^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer measurements, Willingham et al. 1945)13850 ($24.708^{\circ}C$, ebulliometry, Forziati et al. 1949) $\log(P/mmHg) = 6.81479 - 1190.033/(223.303 + t/^{\circ}C)$; temp range 12.188 – $80.074^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

14030 (calculated from determined data, Dreisbach 1959)

 $\log(P/mmHg) = 6.81480 - 1190.033/(223.303 + t/^{\circ}C)$; temp range 0 – $115^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)14026 (interpolated-Antoine eq., temp range -18.6 to $103.75^{\circ}C$, Zwolinski & Wilhoit 1971) $\log(P/mmHg) = 6.81480 - 1190.033/(223.303 + t/^{\circ}C)$; temp range -18.6 to $103.75^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)13500 (interpolated-Antoine eq., temp range -69.3 to $49.7^{\circ}C$, Weast 1972–72) $\log(P/mmHg) = [-0.2185 \times 7271.0/(T/K)] + 7.841340$; temp range -69.3 to $49.7^{\circ}C$ (Antoine eq., Weast 1972–73)

14030 (interpolated-Antoine eq., Boublik et al. 1984)

 $\log(P/kPa) = 5.93788 - 1189.09/(223.198 + t/^{\circ}C)$; temp range 15.32 – $80.05^{\circ}C$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)14030 (interpolated-Antoine eq., temp range -18 to $103^{\circ}C$, Dean 1985, 1992) $\log(P/mmHg) = 6.84180 - 1190.033/(223.3 + t/^{\circ}C)$; temp range -18 to $103^{\circ}C$ (Antoine eq., Dean 1985, 1992)

14010 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.93117 - 1185.576/(-50.37 + T/\text{K})$; temp range 277–354 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.2280 - 1399.333/(-20.934 + T/\text{K})$; temp range 353–483 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 6.2875 - 2.1682 \times 10^3/(T/\text{K}) + 2.6936 \cdot \log (T/\text{K}) - 1.5525 \times 10^{-2} \cdot (T/\text{K}) + 1.0917 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 149–527 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

318000 (calculated-P/C, Mackay & Shiu 1981)

319200 (selected, Mills et al. 1982)

319420 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.10 (calculated- π substituent constant, Hansch et al. 1968)

3.62 (calculated- V_M , Wang et al. 1992)

4.14 (calculated-fragment constant, Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.66 \pm 0.08) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 3.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson 1989)

$k_{OH} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{OH} = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{NO_3} = 9.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{OH} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

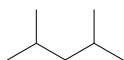
Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.1.1.12 2,4-Dimethylpentane



Common Name: 2,4-Dimethylpentane

Synonym: diisopropylmethane

Chemical Name: 2,4-dimethylpentane

CAS Registry No: 108-08-7

Molecular Formula: C_7H_{16} ; $CH_3CH(CH_3)CH_2CH(CH_3)CH_3$

Molecular Weight: 100.202

Melting Point ($^{\circ}C$):

-119.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

80.49 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6727, 0.6683 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

148.95, 149.9 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.89, 29.501 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.840 (Dreisbach 1959)

6.845 (Riddick et al. 1986)

6.85 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

44.46, 44.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

3.62 (shake flask-GC, McAuliffe 1963)

4.06 (shake flask-GC, McAuliffe 1966; quoted, Hermann 1972; Price 1976)

6.50; 5.50 (0; $25^{\circ}C$, shake flask-GC, Polak & Lu 1973)

4.41 (shake flask-GC, Price 1976)

4.20 (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)

6.12, 4.45 (0, $25^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

12635 (Antoine eq. regression, temp range -48 to $80.5^{\circ}C$, Stull 1947)

11730 ($22.54^{\circ}C$, ebulliometry, measured range 13.714 – $81.374^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 6.82621 - 1192.041/(221.634 + t/^{\circ}C)$; temp range 13.714 – $81.374^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Forziati et al. 1949)

13120 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.82621 - 1192.041/(221.634 + t/^{\circ}C)$; temp range 0 – $115^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

13119 (interpolated-Antoine eq, temp range -17.0 to $104.94^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.82621 - 1192.041/(221.634 + t/^{\circ}C)$; temp range -17.0 to $104.94^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

12620 (interpolated-Antoine eq., temp range -48.0 to $80.5^{\circ}C$, Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 8167.4/(T/K)] + 7.961374$; temp range -48.0 to $80.5^{\circ}C$ (Antoine eq., Weast 1972–73)

13120 (interpolated-Antoine eq., temp range 13.7 – $81.37^{\circ}C$, Boublik et al. 1984)

$\log(P/kPa) = 5.95675 - 1195.154/(221.992 + t/^{\circ}C)$; temp range 13.7 – $81.37^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

15450 (interpolated-Antoine eq., temp range -17 to 105°C, Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.82621 - 1192.04/(225.32 + t/^\circ\text{C})$; temp range -17 to 105°C (Antoine eq., Dean 1985, 1992)
 13000 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.94917 - 1191.06/(221.540 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 13125 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.95921 - 1196.516/(-50.993 + T/\text{K})$; temp range 284–355 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 35.9436 - 2.846 \times 10^3/(T/\text{K}) - 9.9938 \cdot \log(T/\text{K}) + 8.0613 \times 10^{-11} \cdot (T/\text{K}) + 3.6419 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 154–520 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

319300 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 326600, 73120 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 300000 (recommended; Mackay & Shiu 1981)
 297300 (calculated-P/C, Eastcott et al. 1988)
 160050 (calculated-molecular connectivity index MCI χ , Nirmalakhandan & Speece 1988)
 298050 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.10 (calculated- π constant, Hansch et al. 1968)
 3.17 (calculated-MCI χ , Murray et al. 1975)
 3.66 (calculated-molar volume V_M , Wang et al. 1992)
 4.14 (calculated-f constant, Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (5.26 \pm 0.11) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 5.10 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{NO_3}(\text{exptl}) = 1.44 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}(\text{calc}) = 2.89 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{OH} = 5.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}^* = 1.5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $5.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radicals and an estimated lifetime of 27 h during summer daylight (Altshuller 1991).

2.1.1.1.13 3,3-Dimethylpentane



Common Name: 3,3-Dimethylpentane

Synonym:

Chemical Name: 3,3-dimethylpentane

CAS Registry No: 562-49-2

Molecular Formula: C_7H_{16} ; $CH_3CH_2(CH_3)_2CH_2CH_3$

Molecular Weight: 100.202

Melting Point ($^{\circ}C$):

-134.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

86.06 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6933, 0.6891 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

144.5 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

33.02, 29.74 ($25^{\circ}C$, normal bp, Dreisbach 1959)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.067 (Dreisbach 1959)

7.07 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

51.16, 49.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$. Additional data at other temperatures designated * are compiled at the end of this section.):

5.94* (shake flask-GC, measured range 25 – $150.4^{\circ}C$, Price 1976)

6.68* (calculated-liquid-liquid equilibrium LLE data, temp range 298.2 – $423.2 K$, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

10600* (Antoine eq. regression, temp range -45.9 to $86.1^{\circ}C$ Stull 1947)

10316* ($23.521^{\circ}C$, ebulliometry, measured range -13.5 to $82^{\circ}C$ Forziati et al. 1949)

$\log(P/mmHg) = 6.82668 - 1228.063/(225.316 + t/^{\circ}C)$; temp range 13.484 – $80.962^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

11044 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.82667 - 1228.663/(225.316 + t/^{\circ}C)$; temp range 5 – $130^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

11039* (interpolated-Antoine eq., temp range -14.4 to $111.25^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.82667 - 1228.663/(225.316 + t/^{\circ}C)$; temp range -14.4 to $111.25^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

10600 (interpolated-Antoine eq., temp range -45.9 to $86.1^{\circ}C$, Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 8145.4/(T/K)] + 7.869254$; temp range -45.9 to $86.1^{\circ}C$ (Antoine eq., Weast 1972–73)

11045 (interpolated-Antoine eq., temp range 13.484 – $86.96^{\circ}C$, Boublik et al. 1984)

$\log(P/kPa) = 5.95327 - 1229.625/(225.427 + t/^{\circ}C)$; temp range 13.484 – $86.96^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

11045 (interpolated-Antoine eq., temp range -14 to $112^{\circ}C$, Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.82667 - 1228.663/(225.32 + t/^{\circ}\text{C})$; temp range -14 to 112°C (Antoine eq., Dean 1985, 1992)
 11150, 11040 (interpolated-Antoine eq.-I, III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.95139 - 1228.138/(-47.819 + T/\text{K})$; temp range 285–360 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.35011 - 1415.316/(-31.302 + T/\text{K})$; temp range 213–281 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.94685 - 1225.973/(-48.144 + T/\text{K})$; temp range 280–360 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 30.2570 - 2.6313 \times 10^3/(T/\text{K}) - 7.9839 \cdot \log (T/\text{K}) + 4.6848 \times 10^{-13} \cdot (T/\text{K}) + 2.717 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 139–536 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

186000 (calculated-P/C, Mackay & Shiu 1981)

186305 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 2.1.1.1.13.1
Reported aqueous solubilities of 3,3-dimethylpentane at various temperatures

Price 1976		Mączyński et al. 2004	
shake flask-GC		calc-recommended LLE data	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
25	5.92	25	6.68
40.1	6.78	40	6.68
55.7	8.17	56	7.79
69.7	10.3	70	8.91
99.1	15.8	99	16.14
118	27.3	118	26.17
140.4	67.3	150	66.81
150.4	86.1		

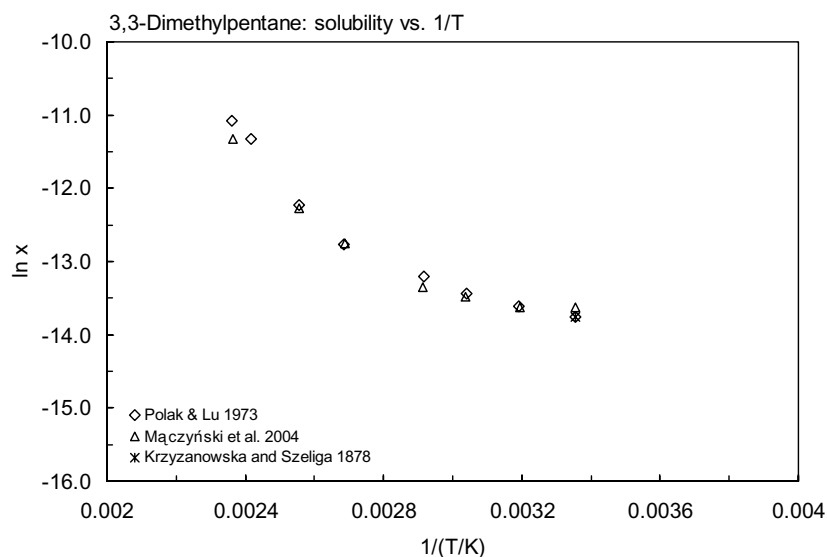


FIGURE 2.1.1.13.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3,3-dimethylpentane.

TABLE 2.1.1.13.2

Reported vapor pressures of 3,3-dimethylpentane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$	(5)						
Stull 1947	Forziati et al. 1949		Zwolinski & Wilhoit 1971				
summary of literature data	ebulliometry		selected values				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		set 1		set 2			
−45.9	133.3	13.443	6383	17.163	7658	−14.41	1333
−25.0	666.6	17.231	7677	20.484	8969	−2.96	2666
−14.4	1333	30.533	8985	34.355	16623	4.36	4000
−2.90	2666	23.521	10316	38.804	19926	9.852	5333
9.90	5333	26.318	11704	53.385	34902	14.297	6666
18.1	7999	30.086	13826	59.444	43327	18.055	7999
29.3	13332	34.406	16613	84.792	976–7	24.231	10666
46.2	26664	38.790	19917	85.344	99201	29.241	13332
65.5	53329	48.72	23438	85.854	100696	38.880	19998
86.1	101325	48.34	28954	86.429	102396	46.173	26664
		53.37	34893			52.114	33331
mp/°C	−135	59.44	43322			57.164	39997
		65.697	53645			65.519	53329
		72.384	66733			72.347	66661
		79.651	83682			78.168	79993
		84.78	97575	bp/°C	86.069	83.272	93326
		85.335	99206			84.222	95992

(Continued)

TABLE 2.1.1.13.2 (Continued)

Stull 1947		Forziati et al. 1949				Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry				selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		86.421	102377	eq. 2	P/mmHg	85.153	98659
		86.928	103895	A	6.81813	86.064	101325
				B	1223.543	25.0	11039
				C	224.687		
						eq. 2	P/mmHg
						A	6.82667
						B	1228.663
						C	225.316
						bp/°C	86.064
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	33.02
						at bp	29.65

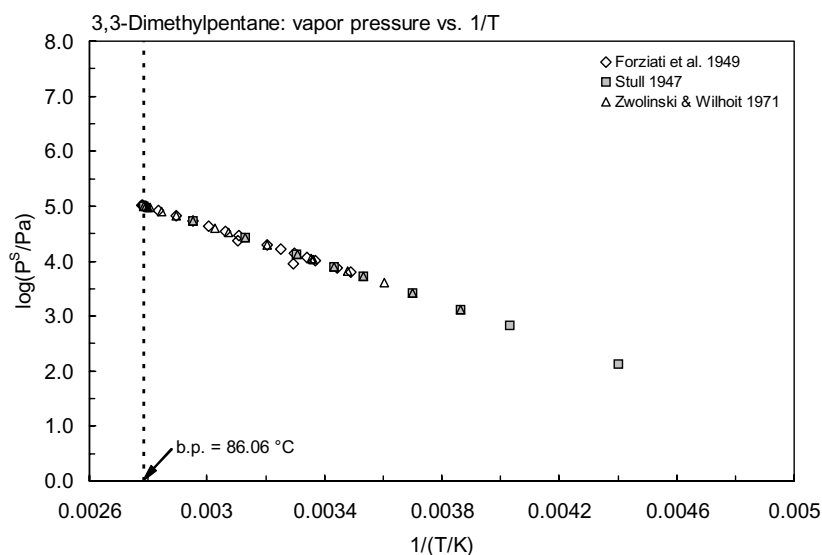
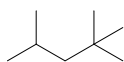


FIGURE 2.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for 3,3-dimethylpentane.

2.1.1.1.14 2,2,4-Trimethylpentane (Isooctane)



Common Name: 2,2,4-Trimethylpentane

Synonym: isooctane, isobutyltrimethylmethane

Chemical Name: 2,2,4-trimethylpentane

CAS Registry No: 504-84-1

Molecular Formula: C_8H_{18} ; $CH_3C(CH_3)_2CH_2CH(CH_3)CH_3$

Molecular Weight: 114.229

Melting Point ($^{\circ}C$):

-107.30 (Stull 1947; Lide 2003)

Boiling Point ($^{\circ}C$):

99.22 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6919, 0.6878 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

165.1 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

36.92, 32.01 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.196 (Riddick et al. 1986)

9.27 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

55.52, 43.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2.44 (shake flask-GC, McAuliffe 1963,1966)

2.46; 2.05 (0; $25^{\circ}C$, shake flask-GC, Polak & Lu 1973)

1.14 (shake flask-GC, Price 1976)

2.50, 2.0, 2.20 (0, 20, $25^{\circ}C$, IUPAC recommended values, Shaw 1989b)

2.30, 1.65, 1.65 (0, 20, $25^{\circ}C$, calculated-liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6371 ($24.4^{\circ}C$, ebulliometry, measured temp range 24.4 – $100.13^{\circ}C$, Willingham et al. 1945)

$\log(P/mmHg) = 6.81189 - 1257.840/(220.735 + t/^{\circ}C)$; temp range 24.4 – $100.13^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Willingham et al. 1945)

6250 (calculated-Antoine eq. regression, temp range -36.4 to $99^{\circ}C$, Stull 1947)

1739, 6573, 19528 (0, 25, $50^{\circ}C$, static method, vapor-liquid equilibrium VLE data, Kretschmer et al. 1948)

6580 (calculated from determined data, Dreisbach 1959; quoted, Hine & Mookerjee 1975)

$\log(P/mmHg) = 6.81189 - 1257.840/(220.735 + t/^{\circ}C)$; temp range 15 – $120^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

6573 (interpolated-Antoine eq., temp range -4.3 to $125.22^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.81189 - 1257.840/(220.735 + t/^{\circ}C)$; temp range -4.3 to $125.22^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

6570 (interpolated-Antoine eq., temp range 24.6 – $100.13^{\circ}C$, Boublik et al. 1973, 1984)

$\log(P/mmHg) = 6.80304 - 1252.59/(220.119 + t/^{\circ}C)$, temp range 24.6 – $100.13^{\circ}C$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

6240 (interpolated-Antoine eq., temp range -36.5 to $99.2^{\circ}C$, Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 8548.0/(T/K)] + 7.934852$; temp range -36.5 to $99.2^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/\text{kPa}) = 5.92751 - 1252.348/(220.09 + t/^\circ\text{C})$; temp range 69.2 – 271.1 $^\circ\text{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

6580 (interpolated-Antoine eq., temp range: 24 – 100 $^\circ\text{C}$, Dean 1985, 1992)

$\log(P/\text{mmHg}) = 6.81189 - 1257.84/(220.74 + t/^\circ\text{C})$, temp range: 24 – 100 $^\circ\text{C}$ (Antoine eq., Dean 1985, 1992)

6500 (quoted lit., Riddick et al. 1986)

$\log(P/\text{kPa}) = 5.92885 - 1153.36/(220.241 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

6580 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.93934 - 1254.146/(-52.831 + T/\text{K})$, temp range: 297–314 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.44016 - 1650.17/(T/\text{K})$; temp range 423–523 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.33252 - 1441.485/(-36.695 + T/\text{K})$; temp range 194–299 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.97534 - 1283/067/(-40.166 + T/\text{K})$; temp range 372–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.26002 - 1501.036/(-19.15 + T/\text{K})$; temp range 413–494 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 7.76427 - 3268.783/(206.659 + T/\text{K})$; temp range 490–544 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 35.954 - 3.0569 \times 10^3/(T/\text{K}) - 9.8896 \cdot \log(T/\text{K}) - 7.2916 \times 10^{-11} \cdot (T/\text{K}) + 3.1060 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 161–564 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25 $^\circ\text{C}$):

308030 (calculated-P/C, Mackay & Leinonen 1975)

330000; 308000, 365000 (recommended; calculated-P/C, Mackay & Shiu 1981)

304960 (calculated as $1/K_{AW} \cdot C_W/C_A$, reported as exptl., Hine & Mookerjee 1975)

472090, 110700 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

314110 (calculated-P/C, Lyman et al. 1982)

350140 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

327200 (calculated-P/C, Eastcott et al. 1988)

338270 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.83 (estimated-HPLC/MS, Burkhard et al. 1985)

4.54 (calculated-fragment const., Burkhard et al. 1985)

5.02 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

4.06 (calculated-molar volume V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} = 5.5$ h from a water column 1 m^2 in cross section of depth 1 m (Mackay & Leinonen 1975);

$t_{1/2} \sim 3.1$ h at 20 $^\circ\text{C}$ in a river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^*(\text{exptl}) = 2.83 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 2.35 \times 10^{12} \text{ cm}^3 \text{ mole}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–493 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{OH} = 3.73 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Darnall et al. 1978)

$k_{\text{O}(3\text{P})} = 9.10 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom at room temp. (Herron & Huie 1973)
 $k_{\text{OH}} = 3.7 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979)
 $k_{\text{O}_3}^* = 2.0 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–323 K (Atkinson & Carter 1984)
 $k_{\text{OH}} = (3.66 \pm 0.16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
 $k_{\text{OH}} = 3.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and $3.56 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (Atkinson 1985)
 $k_{\text{OH}} = 3.68 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
 $k_{\text{NO}_3}(\text{exptl}) = 7.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{calc}) = 1.65 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)
 $k_{\text{OH}}^* = 3.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 9.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

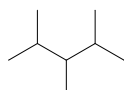
Half-Lives in the Environment:

Air: atmospheric lifetime was estimated to be 16 h, based on the photooxidation reaction rate constant of $3.68 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radical in air during summer daylight (Altshuller 1991).

Surface water: volatilization $t_{1/2} = 5.5 \text{ h}$ from a water column 1 m^2 in cross section of depth 1-m (Mackay & Leinonen 1975);

estimated $t_{1/2} = 3.1 \text{ h}$ at 20°C in a river 1 m deep flowing at 1 m/s with a wind velocity of 3 m s^{-1} (Lyman et al. 1982).

2.1.1.1.15 2,3,4-Trimethylpentane



Common Name: 2,3,4-Trimethylpentane

Synonym:

Chemical Name: 2,3,4-trimethylpentane

CAS Registry No: 565-75-3

Molecular Formula: C_8H_{18} ; $CH_3CH(CH_3)CH(CH_3)CH(CH_3)CH_3$

Molecular Weight: 114.229

Melting Point ($^{\circ}C$):

-109.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

113.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7191 (Weast 1984)

0.7191, 0.7191 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

158.9 (calculated-density, Stephenson & Malanowski 1987)

185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

38.0, 32.67 ($25^{\circ}C$, at normal bp, Dreisbach 1959)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.27 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.65, 38.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2.34, 2.30 (0; $25^{\circ}C$, shake flask-GC, Polak & Lu 1973)

1.36 (shake flask-GC, Price 1976)

2.30, 1.36 (quoted lit., IUPAC Solubility Data Series, Shaw 1989)

2.86, 2.03 (0, $25^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log(P/mmHg) = 6.85396 - 1315.034/(217.526 + t/^{\circ}C)$; temp range 36.568 – $114.381^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

3431 (Antoine eq. regression, temp range -26 to $113.5^{\circ}C$ Stull 1947)

3600 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.85396 - 1315.084/(217.526 + t/^{\circ}C)$; temp range 25 – $150^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

3600 (interpolated-Antoine eq., temp range 7.1 – $140.0^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.85396 - 1315.084/(217.526 + t/^{\circ}C)$; temp range 7.1 – $140.0^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

3430 (interpolated-Antoine eq., temp range -26.3 to $113.5^{\circ}C$, Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 8988.2/(T/K)] + 7.997094$; temp range -26.3 to $113.5^{\circ}C$ (Antoine eq., Weast 1972–73)

1179 ($4.912^{\circ}C$, static method-inclined piston manometer, measured range -50.325 to $4.912^{\circ}C$, Osborn & Douslin 1974)

3600 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.98137 - 1316.608/(217.70 + t/^{\circ}\text{C})$; temp range 69.2–271.1 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

3600 (extrapolated-Antoine eq., temp range 36–114 $^{\circ}\text{C}$, Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.85396 - 1315.08/(217.53 + t/^{\circ}\text{C})$; temp range 36–114 $^{\circ}\text{C}$ (Antoine eq., Dean 1985, 1992)

3610 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.00347 - 1330.047/(-53.921 + T/\text{K})$; temp range 288–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.37038 - 1511.86/(-38.054 + T/\text{K})$; temp range 223–289 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 35.1565 - 3.0232 \times 10^3/(T/\text{K}) - 9.2267 \cdot \log (T/\text{K}) + 2.7691 \times 10^{-11} \cdot (T/\text{K}) + 2.7828 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 164–566 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$):

190000; 302000, 179000 (recommended; calculated-P/C, Mackay & Shiu 1981)

178700 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^* = 6.99 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 243–313 K (relative rate method with reference to *n*-hexane, Harris & Kerr 1988; Atkinson 1989)

$k_{OH} = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1990)

$k_{OH} = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and the atmospheric lifetime was estimated to be 20 h during summer daylight hours (Altshuller 1991)

$k_{OH} = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

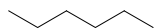
Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric lifetime was estimated to be 20 h, based on the photooxidation reaction rate constant of $7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radicals in air during summer daylight (Altshuller 1991).

2.1.1.1.16 *n*-HexaneCommon Name: *n*-Hexane

Synonym: hexane

Chemical Name: *n*-hexane

CAS Registry No: 110-54-3

Molecular Formula: C₆H₁₄; CH₃(CH₂)₄CH₃

Molecular Weight: 86.175

Melting Point (°C):

-95.35 (Lide 2003)

Boiling Point (°C):

68.73 (Lide 2003)

Density (g/cm³ at 20°C):

0.6593, 0.6548 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

130.7; 131.6(20°C, 25°C, calculated-density)

140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.552, 28.853 (25°C, bp, Riddick et al. 1986)

31.52 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

13.028 (Dreisbach 1959)

13.079 (Riddick et al. 1986)

13.08 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

73.22, 72.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

140 (15.5°C, shake flask-cloud point, Fühner 1924)

< 262 (shake flask-residue volume, Booth & Everson 1948)

36.0 (shake flask-cloud point, Durand 1948)

120 (shake flask-cloud point, McBain & Lissant 1951)

9.50 (shake flask-GC, McAuliffe 1963, 1966;)

16.2 (vapor saturation-GC, Barone et al. 1966)

18.3* (shake flask-GC, measured range 4–55°C, Nelson & De Ligny 1968)

12.3 (shake flask-GC, Leinonen & Mackay 1973)

12.4* (shake flask-GC, Polak & Lu 1973)

13.0 (shake flask-GC, Krasnoshchekova & Gubertritis 1973)

16.2 (shake flask-GC, Mackay et al. 1975)

9.47* (shake flask-GC, measured range 25–151.8°C, Price 1976)

12.3 (shake flask-GC, Aquan-Yuen et al. 1979)

10.09* (vapor saturation-GC, measured range 15.5–40°C, Jönsson et al. 1982)

12.24 (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982; Miller et al. 1985)

14.1 (calculated-activity coeff. γ and K_{ow}, Tewari et al. 1982b)

11.4* (37.78°C, shake flask-GC, measured 37.78–200°C, Tsonopoulos & Wilson 1983)

9.55 (shake flask-GC, Coates et al. 1985)

14.0 (shake flask-purge and trap-GC, Coutant & Keigley 1988)

9.8* (recommended best value, IUPAC Solubility Data Series, temp range 0–140°C, Shaw 1989)

$\ln x = -374.90804 + 16327.128/(T/K) + 53.89582 \cdot \ln(T/K)$; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

11.5* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–425 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 24811* (30°C, static-manometer, measured range 30–60°C, Smyth & Engel 1929)
 19920* (24.7°C, ebulliometry, measured range 13.033–69.541°C Willingham et al. 1945)
 $\log(P/\text{mmHg}) = 6.87776 - 1171.530/(224.366 + t/^\circ\text{C})$; temp range 13.033–69.541°C (Antoine eq. from exptl. data, ebulliometry, Willingham et al. 1945)
 19700* (calculated-Antoine eq. regression, temp range –53.9 to 68.7°C, Stull 1947)
 20170 (calculated from determined data, Dreisbach 1959)
 $\log(P/\text{mmHg}) = 6.87776 - 1171.53/(224.366 + t/^\circ\text{C})$; temp range –10 to 110°C (Antoine eq. for liquid state, Dreisbach 1959)
 20198* (interpolated-Antoine eq., temp range –25.1 to 92.1°C, Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = 6.87776 - 1171.530/(224.366 + t/^\circ\text{C})$; temp range –25.1 to 92.1°C (Antoine eq., Zwolinski & Wilhoit 1971)
 3120* (–0.51°C, gas saturation, measured range –95.44 to –0.51°C, Carruth & Kobayashi 1973)
 20130 (Campbell et al. 1968)
 20124, 20141 (static method-differential pressure gauge, Bissell & Williamson 1975)
 22090* (27.1°C, Letcher & Marsicano 1974)
 21809, 57929, 130189 (26.85, 51.85, 76.85°C, vapor-liquid equilibrium VLE data, Gutsche & Knapp 1982)
 20160 (interpolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.01098 - 1176.102/(224.899 + t/^\circ\text{C})$; temp range 13.033–69.54°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.72763 - 1031.938/(208.304 + t/^\circ\text{C})$; temp range 27.11–45.11°C (Antoine eq. from reported exptl. data of Letcher & Marsicano 1974, Boublik et al. 1984)
 20190 (interpolated-Antoine eq., temp range –25 to 92°C, Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.87601 - 1171.17/(224.41 + t/^\circ\text{C})$; temp range –25 to 92°C (Antoine eq., Dean 1985, 1992)
 20700, 20180, 20160(headspace-GC, correlated, Antoine eq., Hussam & Carr 1985)
 20170 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.00091 - 1171.91/(224.408 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 20180, 20300, 20165 (interpolated-Antoine equations I, II and IV, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.00431 - 1172.04/(-48.747 + T/\text{K})$; temp range 293–343 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.15142 - 1224.492/(-45.358 + T/\text{K})$; temp range 238–298 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 8.47892 - 1800.89/(-4.115 + T/\text{K})$; temp range 189–259 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.99521 - 1167.388/(-49.272 + T/\text{K})$; temp range 298–341 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.91942 - 1123.687/(-54.776 + T/\text{K})$; temp range 341–377 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.4106 - 1469.286/(-7.702 + T/\text{K})$; temp range 374–451 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.30814 - 2367.155/(111.016 + T/\text{K})$; temp range 445–508 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 10854 (calculated-UNIFAC activity coeff., Banerjee et al. 1990)
 20136* (24.96°C, Hg manometer, measured range 9.95–49.97°C, Gracia et al. 1992)
 20180* (recommended, Ruzicka & Majer 1994)
 $\ln[(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/K)/(T/K)] \cdot \exp\{2.79797 - 2.022083 \times 10^{-3} \cdot (T/K) + 2.287564 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_o = 101.325 \text{ kPa}$, $T_o = 341.863 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log(P/\text{mmHg}) = 69.7378 - 3.6278 \times 10^3/(T/\text{K}) - 23.927 \cdot \log(T/\text{K}) + 1.281 \times 10^{-2} \cdot (T/\text{K}) - 1.6844 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 178–507 K (vapor pressure eq., Yaws 1994)
 24938, 53982 (30, 50°C, VLE equilibrium data, Carmona et al. 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 183690 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

- 160000, 50590 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 190000 (calculated-P/C, Mackay & Shiu 1975,1981; Bobra et al. 1979)
 177060 (equilibrium cell-concn ratio-GC, Vejrosta et al. 1982)
 173340* (equilibrium cell-concentration ratio-GC, measured range 14.52–34.9°C Jönsson et al. 1982)
 103262, 135400, 172140, 215420, 261420 (15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)
 $\ln (1/K_{AW}) = 21493.1/(T/K) + 59.299 \cdot \ln (T/K) - 414.193$; temp range 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)
 77820* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 25.25 - 7530/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 130790 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 18600* (40°C, equilibrium headspace-GC, measured range 40–70°C, Kolb et al. 1992)
 $\ln (1/K_{AW}) = -28.60 + 8375/(T/K)$; temp range 40–70°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
 163812 (EPICS-GC, Ryu & Park 1999)
 65318 (20°C, selected from reported experimental values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 12.150 - 3143/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.00 (calculated- π constant, Hansch et al. 1968; Hansch & Leo 1979)
 3.90 (shake flask-concn. ratio-GC, Platford 1979; Platford 1983)
 4.20 (calculated-activity coeff. γ , Wasik et al. 1981, 1982)
 4.11 (generator column-GC, Tewari et al. 1982a,b)
 2.90 (HPLC- k' correlation, Coates et al. 1985)
 4.25 (calculated-activity coeff., Berti et al. 1986)
 4.16 (generator column-GC, Schantz & Martire 1987)
 4.00 (recommended, Sangster 1989, 1993)
 4.29 (calculated-activity coeff., Tse & Sandler 1994)
 3.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 2.55* (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.29–50.28°C Gruber et al. 1997)
 2.44 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated *data at other temperatures and/or the Arrhenius expression see reference:

$$k_{O(3P)} = 9.30 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with O(}^3\text{P) atoms (Herron & Huie 1973)}$$

$$k_{OH} = (3.8 \pm 0.8) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ at 305 K (relative rate method, Llyod et al. 1976)}$$

$$k_{OH} = 5.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson et al. 1979)}$$

$$k_{OH} = (6.1 - 6.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ 292–303 K, } k_{OH} \text{ (calc)} = 6.96 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 300 K (Darnall et al. 1978)}$$

$$k_{OH} = 5.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{O(3P)} = 9.3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with O(}^3\text{P) atoms, at room temp. (abstraction mechanism, Gaffney & Levine 1979)}$$

$$k_{OH} = (5.71 \pm 0.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \pm 2 \text{ K (relative rate method, Atkinson et al. 1982a)}$$

$$k_{NO_3} = (1.05 \pm 0.2) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 K (Atkinson et al. 1984a, Atkinson 1991)}$$

$$k_{OH} = (5.70 \pm 0.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (relative rate, Atkinson et al. 1984c)}$$

$k_{\text{OH}} = 5.21 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson & Aschmann 1984)

$k_{\text{OH}} = 6.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)

$k_{\text{OH}}^* = 5.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1991, Altshuller 1991)

$k_{\text{OH}} = 5.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.05 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljić & Güsten 1990)

$k_{\text{OH}} = 5.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 10.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{\text{NO}_3} = 1.05 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson 1991)

$k_{\text{NO}_3}(\text{exptl}) = 1.06 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{calc}) = 1.11 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{\text{OH}}^* = 5.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 11 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

$k_{\text{OH}}^* = 5.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction $t_{1/2} = 2.4\text{--}24 \text{ h}$ in air, based on reaction rate constant of $3.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical (Darnall et al. 1976);

atmospheric lifetime $\sim 25 \text{ h}$, based on a rate constant of $5.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radicals in summer daylight (Altshuller 1991).

TABLE 2.1.1.1.16.1

Reported aqueous solubilities of *n*-hexane at various temperatures

1.

Nelson & De Ligny 1968		Polak & Lu 1973		Price 1976		Jönsson et al. 1982	
shake flask-GC		shake flask-GC		shake flask-GC		vapor saturation-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4.0	16.4	0	16.5	25.0	9.47	15	10.72
14.0	15.2	25	12.4	40.1	10.1	20	10.32
25.0	18.3			55.7	13.2	25	10.09
35.0	12.9			69.7	15.4	30	10.02
45.0	22.2			69.7	15.2	35	10.10
55.0	21.2			99.1	22.4		
				114.4	29.2		
				121.3	37.6		
				137.3	56.9		
				151.8	106.0		

(Continued)

TABLE 2.1.1.1.16.1 (Continued)

2.

Tsonopoulos & Wilson 1983		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC		IUPAC recommended		calc-recommended LLE	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
37.78	11.4	0	17	0	15.8
93.33	27.4	20	12	4	14.36
94.4	25.6	24	11	13	12.45
100	29.7	30	9.9	15	12.45
148.09	130	40	11	20	12.0
150	162	50	12	25	11.5
200	885	60	13.6	30	11.5
		70	15.7	35	11.5
		80	18.5	40.1	11.5
		100	27	55.7	12.93
		120	45	69.7	15.32
		140	80	99.1	26.33
				113.8	37.34
				121.3	44.52
				137.2	67.02
				151.8	105.3

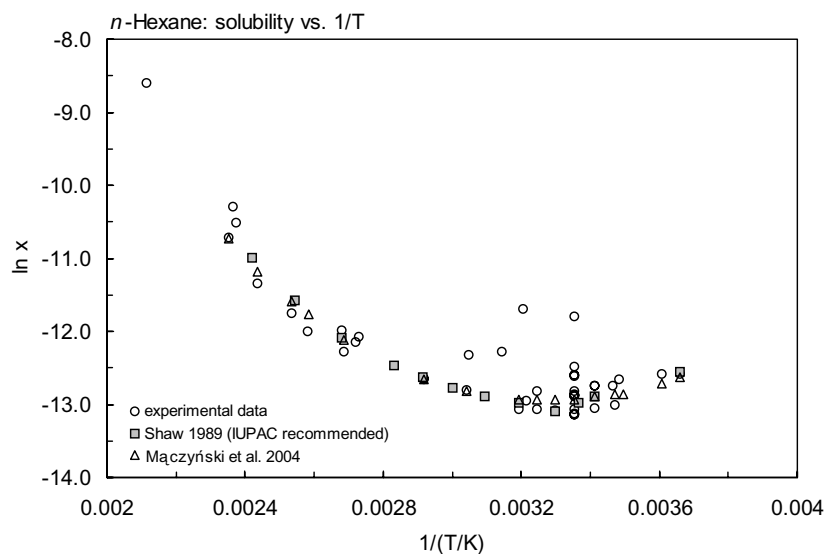
FIGURE 2.1.1.1.16.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *n*-hexane.

TABLE 2.1.1.1.16.2

Reported vapor pressures of *n*-hexane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \quad \ln P = A - B/\{(T/K) - C\} & (3a) \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & & \\ \ln [(P/\text{kPa})/(P_o/\text{kPa})] &= [1 - (T_o/K)/(T/K)] \cdot \exp\{A_o - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2\} & & (5) - \text{Cox eq.}\end{aligned}$$

1.

Smyth & Engel 1929		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static-manometer		ebulliometry		summary of literature data		selected values	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
30	24811	13.033	11698	-53.9	133.3	-25.19	1333
40	36757	16.576	13819	-34.5	666.6	-14.36	2666
50	53409	20.618	16620	-25.0	1333	-7.50	4000
60	75727	24.717	19920	-14.1	2666	-2.36	5333
		28.528	23451	-2.30	5333	1.79	6666
bp/ $^{\circ}\text{C}$	68.8	33.631	28956	5.40	7999	5.31	7999
		38.311	34896	15.8	13332	11.08	10666
		43.967	43322	31.6	26664	15.762	13332
		49.803	53655	49.8	53329	24.764	19998
		56.030	66757	68.7	101325	31.572	26664
		62.785	83719			37.114	33331
		67.554	97605	mp/ $^{\circ}\text{C}$	-95.3	41.824	39997
		68.067	99201			49.612	53329
		68.540	100694			55.973	66661
		69.081	102394			61.394	79993
		69.541	103913			66.145	93326
						67.030	95992
		bp/ $^{\circ}\text{C}$	68.740			67.896	98659
						68.744	101325
		eq. 2	P/mmHg			eq. 2	P/mmHg
		A	6.87776			A	6.87024
		B	1171.530			B	118.72
		C	224.366			C	224.210
		temp range: 13–69.5 $^{\circ}\text{C}$				bp/ $^{\circ}\text{C}$	68.744
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25 $^{\circ}\text{C}$	31.55
						at bp	28.85

(Continued)

TABLE 2.1.1.1.16.2 (Continued)

2.

Carruth & Kobayashi 1973		Letcher & Marsicano 1974		Gracia et al. 1992		Ruzicka & Majer 1994	
gas saturation		static method-manometer		Hg manometer		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
−95.44	1.360	27.11	22091	9.95	10081	162.54	0.1
−95.13	1.373	29.31	24151	14.98	12818	176.70	1.0
−91.70	2.266	33.81	29197	19.97	16136	193.88	10
−88.93	3.213	36.44	32437	24.96	20136	215.51	100
−83.99	5.973	39.88	37117	29.96	24949	243.81	1000
−75.94	13.60	42.45	40996	34.95	30577	282.95	10000
−61.25	64.13	45.15	45289	39.93	37185	341.863	101325
−53.29	128	48.11	50476	44.96	45000	298.15	20180
−34.84	656			49.97	54028		
−24.91	1264	Antoine eq.				data calc. from Cox eq.	
−14.39	2560	eq. 3	P/mmHg			eq. 5	P/kPa
−0.51	3120	A	6.6298	Antoine eq.		A ₀	2.73425
		B	1050.38	eq. 3a	P/kPa	A ₁	2.02283 × 10 ^{−3}
mp/°C	−95.36	C	210.477	A	13.74029	A ₂	2.287564 × 10 ^{−6}
				B	2654.670	with reference state at	
eq. 1a	P/mmHg	$\Delta H_v/(\text{kJ mol}^{-1}) = 30.84$		C	50.869	P ₀ /kPa	101.325
A	19.5553					T ₀ /K	341.863
B	4292.8						

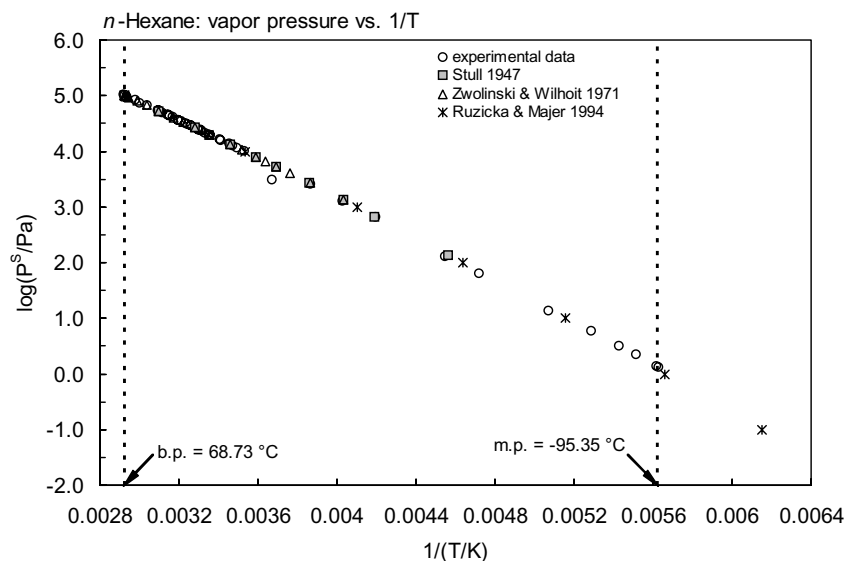


FIGURE 2.1.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-hexane.

TABLE 2.1.1.1.16.3
Reported Henry's law constants and octanol-air partition coefficients of *n*-hexane at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$
$$\ln (1/K_{AW}) = A - B/(T/K)$$
$$\ln (k_H/atm) = A - B/(T/K)$$
$$\ln [H/(Pa\ m^3/mol)] = A - B/(T/K)$$
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$
$$\log (1/K_{AW}) = A - B/(T/K)$$
$$\log [H/(atm \cdot m^3/mol)] = A - B/(T/K)$$

$$(1)$$
$$(2)$$
$$(3)$$
$$(4)$$
$$(5)$$

$$(1a)$$
$$(2a)$$
$$(4a)$$

Henry's law constant						log K _{OA}	
Jönsson et al. 1982		Ashworth et al. 1988		Kolb et al. 1992		Gruber et al. 1997	
equilibrium cell-GC		EPICS-GC		equilibrium headspace-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
14.52	103536	10	24115	40	18600	20.29	2.548
14.52	103090	15	41847	60	64410	30.3	2.386
15.0	103262	20	89470	70	237750	40.4	2.216
20.05	135426	25	77818			50.28	2.090
20.05	136182	30	158067	eq. 2	1/K _{AW}		
20.0	135403			A	−28.60		
25	174565	eq. 4	H/(atm m ³ /mol)	B	−8375		
25	172140	A	25.25				
25	172140	B	7530				
30.2	215560						
30.2	211937						
30.0	215418						
34.9	264034						
34.9	256113						
35.0	261424						

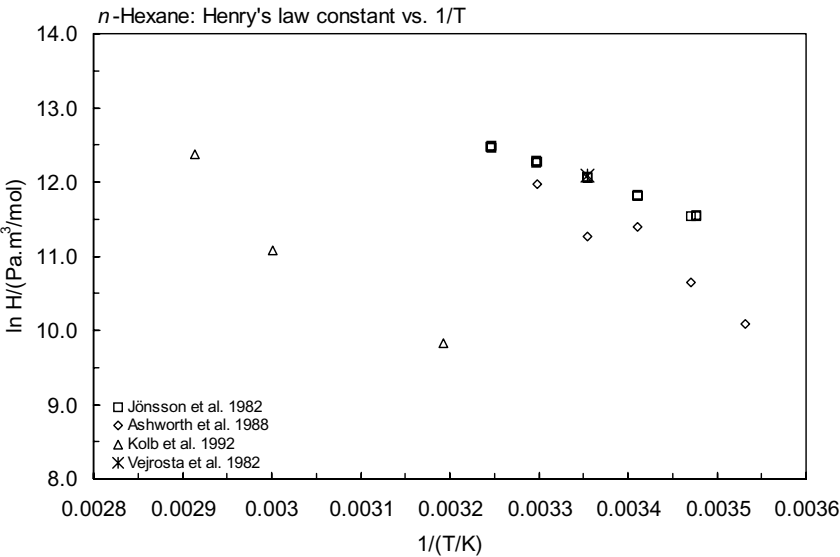


FIGURE 2.1.1.1.16.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-hexane.

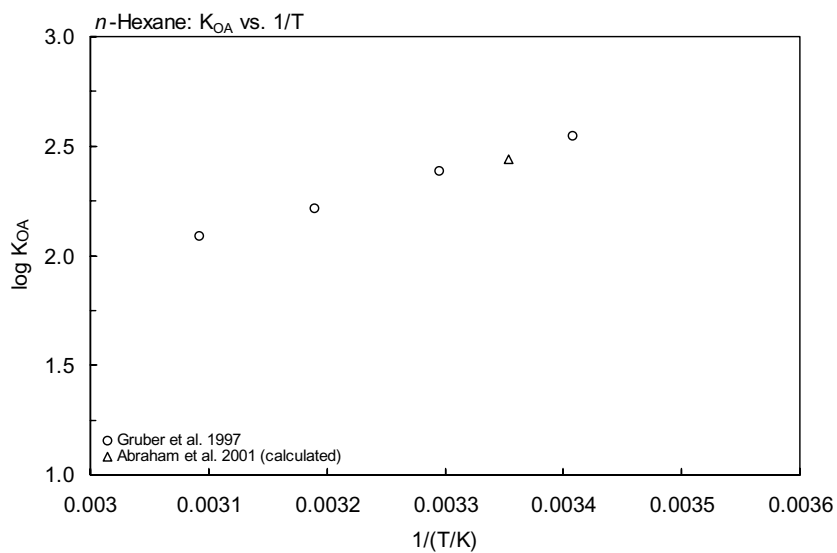
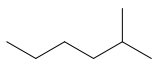


FIGURE 2.1.1.16.4 Logarithm of K_{OA} versus reciprocal temperature for *n*-hexane.

2.1.1.1.17 2-Methylhexane (Isoheptane)



Common Name: 2-Methylhexane

Synonym: isoheptane, ethylisobutylmethane

Chemical Name: 2-methylhexane

CAS Registry No: 591-76-4

Molecular Formula: C_7H_{16} ; $CH_3CH(CH_3)CH_2(CH_2)_2CH_3$

Molecular Weight: 100.202

Melting Point ($^{\circ}C$):

-118.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

90.04 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6786, 0.6744 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

0.6786, 0.6548 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

147.66, 148.58 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

34.807, 30.669 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.184 (Dreisbach 1959; Riddick et al. 1986)

9.18 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

59.29, 57.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.54 (shake flask-GC, Price 1976)

3.51 (calculated-recommended liquid-liquid equilibrium LLE data, Męczyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

8380 (calculated-Antoine eq. regression, temp range -40.4 to $90^{\circ}C$, Stull 1947)

9000 ($25.518^{\circ}C$, ebulliometry, measured range 18.5 – $90.9^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 6.87319 - 1236.026/(219.545 + t/^{\circ}C)$; temp range (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

8780 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.87318 - 1236.026/(219.545 + t/^{\circ}C)$; temp range 10 – $110^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

8780 (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 5.87318 - 1236.026/(219.545 + t/^{\circ}C)$; temp range -9.10 to $114.78^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

8370 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 8538.7/(T/K)] + 8.055523$; temp range -40.4 to $90^{\circ}C$ (Antoine eq., Weast 1972–73)

87778, 8785 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.0031 - 1238.614/(219.867 + t/^{\circ}C)$; temp range 18.5 – $90.9^{\circ}C$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

$\log(P/kPa) = 6.06712 - 1270.535/(222.971 + t/^{\circ}C)$; temp range 0 – $45^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

8790 (interpolated-Antoine eq., temp range -9 to $115^{\circ}C$, Dean 1985, 1992)

$\log(P/mmHg) = 6.87318 - 1236.026/(219.55 + t/^{\circ}C)$; temp range -9 to $115^{\circ}C$ (Antoine eq., Dean 1985, 1992)

8800 (lit. average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 5.99612 - 1235.10/(219.469 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

8790 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.00513 - 1240.11/(-53.123 + T/\text{K})$; temp range 296–365 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 54.1075 - 3.785 \times 10^3/(T/\text{K}) - 17.547 \cdot \log (T/\text{K}) + 8.2594 \times 10^{-3} \cdot (T/\text{K}) - 3.4967 \times 10^{-14} \cdot (T/\text{K})^2$; temp range 155–530 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

346000 (calculated-P/C, Mackay & Shiu 1981, Eastcott et al. 1988)

346500 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

51878* (26.9°C , EPICS-GC, measured range 26.9 – 45°C , Hansen et al. 1993)

$\ln [H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = 3608/(T/\text{K}) - 8.0$; temp range 26.9 – 45°C (EPICS-GC, Hansen et al. 1993)

63856 (20°C , selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = -4.274 + 1669/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 6.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1990, 1991)

$k_{\text{OH}} = 6.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetime of 25 h in summer daylight (Altshuller 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $6.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radicals and an estimated lifetime of 25 h in summer daylight (Altshuller 1990).

TABLE 2.1.1.1.17.1

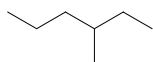
Reported Henry's law constants of 2-methylhexane at various temperatures

Hansen et al. 1993

EPICS-GC

$t/^{\circ}\text{C}$	$H/(\text{kPa m}^3/\text{mol})$
26.9	51.878
35.0	31.512
45.0	25.939
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/\text{K})$	
eq. 4	$H/(\text{kPa m}^3/\text{mol})$
A	-8 ± 3.53
B	-3608 ± 1088

2.1.1.1.18 3-Methylhexane



Common Name: 3-Methylhexane

Synonym: ethylmethylpropylmethane

Chemical Name: 3-methylhexane

CAS Registry No: 589-34-4

Molecular Formula: C_7H_{16} ; $CH_3CH_2CH(CH_3)(CH_2)_2CH_3$

Molecular Weight: 100.202

Melting Point ($^{\circ}C$):

-119.4 (Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

92 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6860 (Weast 1984)

0.6871, 0.6830 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

145.83, 146.71 (calculated-density)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.087, 30.79 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.95 (shake flask-GC, Polak & Lu 1973)

2.64 (shake flask-GC, Price 1976)

3.80 (suggested IUPAC tentative value, Shaw 1989)

6.12, 4.29 ($0.25^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

7782 (Antoine eq. regression, temp range -39 to $91.9^{\circ}C$ Stull 1947)

7702 ($23.662^{\circ}C$, ebulliometry, measured range 19.915 – $92.737^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 6.86754 - 1240.196/(219.223 + t/^{\circ}C)$; temp range 19.9 – $92.7^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

8210 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.86764 - 1240.196/(219.223 + t/^{\circ}C)$; temp range 10 – $130^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

8213 (interpolated-Antoine eq., temp range -7.90 to $116.73^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.86764 - 1240.196/(219.223 + t/^{\circ}C)$; temp range -7.90 to $116.73^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

7772 (interpolated-Antoine eq., temp range -39.0 to $91.9^{\circ}C$, Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 8596.3/(T/K)] + 8.065472$; temp range -39.0 to $91.9^{\circ}C$ (Antoine eq., Weast 1972–73)

8212 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.99489 - 1241.528/(219.375 + t/^{\circ}C)$; temp range 20 – $92.74^{\circ}C$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

8210 (interpolated-Antoine eq., temp range -8 to $117^{\circ}C$ Dean 1985, 1992)

$\log(P/mmHg) = 6.86764 - 1240.196/(219.22 + t/^{\circ}C)$; temp range -8 to $117^{\circ}C$ (Antoine eq., Dean 1985, 1992)

8300 (lit. average, Riddick et al. 1986)

$\log(P/kPa) = 5.98993 - 1238.88/(219.10 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

8215 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.9926 - 1239.57/(-53.979 + T/\text{K})$; temp range 289–366 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 35.2535 - 2.931 \times 10^3/(T/\text{K}) - 9.667 \cdot \log (T/\text{K}) - 5.2026 \times 10^{-11} \cdot (T/\text{K}) + 3.2107 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 154–535 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

172000 (recommended, Mackay & Shiu 1981)

312170 (calculated-P/C, Eastcott et al. 1988)

311620 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 7.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990,1991)

$k_{OH} = 7.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime of 20 h during summer daylight (Altshuller 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

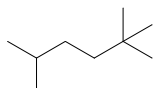
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24$ h for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction rate constant of $7.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radical and an estimated lifetime of 20 h during summer daylight (Altshuller 1991).

2.1.1.1.19 2,2,5-Trimethylhexane



Common Name: 2,2,5-Trimethylhexane

Synonym:

Chemical Name: 2,2,5-trimethylhexane

CAS Registry No: 3522-94-9

Molecular Formula: C_9H_{20} , $(CH_3)_3CCH_2CH_2CH(CH_3)_2$

Molecular Weight: 128.255

Melting Point ($^{\circ}C$):

−105.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

124.09 (Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

0.7072 (Weast 1984)

0.7072, 0.7032 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

181.3, 182.4 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

207.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.175, 33.76 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.192 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.15 (shake flask-GC, McAuliffe 1966)

0.79; 0.54, 0.54 (0; $25^{\circ}C$, shake flask-GC, calculated-group contribution, Polak & Lu 1973)

0.80, 0.80 (0, $25^{\circ}C$, IUPAC recommended best value, Shaw 1989b)

0.613 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log (P/mmHg) = 6.83532 - 1324.049/(210.737 + t/^{\circ}C)$; temp range $46.1-125.0^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

2212 (extrapolated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.83531 - 1324.059/(210.737 + t/^{\circ}C)$; temp range $35-145^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

2210 (interpolated-Antoine eq., temp range $16.17-151.1^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.83531 - 1324.049/(210.737C + t/^{\circ}C)$; temp range $16.17-151.1^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

2216 (static method-inclined piston manometer, measured range -35 to $30^{\circ}C$, Osborn & Douslin 1964)

2207 (interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.96385 - 1326.27/(212.991 + t/^{\circ}C)$; temp range $46.14-126.05^{\circ}C$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

2207 (extrapolated-Antoine eq., temp range 46 to $125^{\circ}C$ Dean 1985, 1992)

$\log (P/mmHg) = 6.83775 - 1325.54/(210.91 + t/^{\circ}C)$; temp range $46-125^{\circ}C$ (Antoine eq., Dean 1985, 1992)

2216 (lit. average, Riddick et al. 1986)

$\log (P/kPa) = 5.96021 - 1324.049/(210.737 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

2218 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.99253 - 1243.85/(-60.158 + T/K)$; temp range $288-399$ K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.25179 - 1471.621/(-48.901 + T/\text{K})$; temp range 238–293 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 7.8816 - 2.6422 \times 10^3/(T/\text{K}) + 23.902 \cdot \log (T/\text{K}) - 1.5376 \times 10^{-2} \cdot (T/\text{K}) + 7.7931 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 167–568 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

350000 (recommended, Mackay & Shiu 1981)

523760 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.63 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

4.46 (calculated-molar volume V_M , Wang et al. 1992)

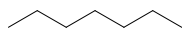
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants and Half-Lives:

Half-Lives in the Environment:

2.1.1.1.20 *n*-HeptaneCommon Name: *n*-Heptane

Synonym: heptane

Chemical Name: *n*-heptane

CAS Registry No: 142-82-5

Molecular Formula: C_7H_{16} , $CH_3(CH_2)_5CH_3$

Molecular Weight: 100.202

Melting Point ($^{\circ}C$):

-90.55 (Lide 2003)

Boiling Point ($^{\circ}C$):

98.4 (Dreisbach 1959; Weast 1972–73; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6837 (Weast 1972–73)

0.6837, 0.6795 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)Molar Volume (cm^3/mol):146.6, 147.5 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):36.55, 31.7 ($25^{\circ}C$, bp, Riddick et al. 1986)

36.57 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.037 (Riddick et al. 1986)

14.04 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

76.9, 81.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

50.0 (15.5 $^{\circ}C$, shake flask-cloud point, Fühner 1924)

150 (radiotracer method, Black et al. 1948)

15.0 (16 $^{\circ}C$, shake flask-cloud point, Durand 1948)

2.93 (shake flask-GC, McAuliffe 1963, 1966)

11.0* (22 $^{\circ}C$, cloud point, measured range 295–355 K at 17–55 MPa, Connolly 1966)2.66* (shake flask-GC, measured range 4.3–45 $^{\circ}C$, Nelson & De Ligny 1968)4.39; 3.37* (0, 25 $^{\circ}C$, shake flask-GC, Polak & Lu 1973)

2.57 (shake flask-GC, Krasnoshchekova & Gubertritis 1975)

2.24* (shake flask-GC, measured range 25–150.4 $^{\circ}C$, Price 1976)

3.70 (shake flask-GC, Bittrich et al. 1979)

2.90 (partition coefficient-GC, Rudakov & Lutsyk 1979)

3.58 (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982)

4.62 (calculated-activity coeff. γ and K_{ow} , Tewari et al. 1982b)2.51* (vapor saturation-GC, measured range 15–40 $^{\circ}C$, Jönsson et al. 1982)

2.95 (shake flask-GC, Coates et al. 1985)

3.57 (lit. average, Riddick et al. 1986)

2.90 (shake flask-purge and trap-GC, Coutant & Keigley 1988)

2.40* (recommended best value, IUPAC Solubility Data Series, temp range 0–140 $^{\circ}C$, Shaw 1989)

$\ln x = -396.93979 + 17232.298/(T/K) + 56.95927 \cdot \ln (T/K)$, temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

2.95* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–423.6 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 5520* (22.7°C, static-manometer, measured range 22.7–98.4°C, Smyth & Engel 1929)
 6370* (25.9°C, ebulliometry, measured range 25.9–99.3°C, Willingham et al. 1945)
 $\log(P/\text{mmHg}) = 6.90342 - 1268.636/(216.951 + t/^\circ\text{C})$; temp range 25.9–99.3°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
 5795* (calculated-Antoine eq. regression, temp range –34 to 98.4°C Stull 1947)
 6425* (26.039°C, ebulliometry, measured range 26–99.3°C Forziati et al. 1949)
 $\log(P/\text{mmHg}) = 6.90027 - 1296.871/(216.757 + t/^\circ\text{C})$; temp range 26.0–99.3°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
 6110 (calculated from determined data, Dreisbach 1959)
 $\log(P/\text{mmHg}) = 6.90240 - 1268.115/(216.90 + t/^\circ\text{C})$; temp range 15–155°C (Antoine eq. for liquid state, Dreisbach 1959)
 6105 (Harris & Dunlop 1970)
 6113* (interpolated-Antoine eq., temp range –2.10 to 123.41°C, Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = 6.90240 - 1268.115/(216.900 + t/^\circ\text{C})$; temp range –2.10 to 123.41°C (Antoine eq., Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = [-0.2185 \times 8409.6/(T/K)] + 7.786586$; temp range –34.0 to 247.5°C (Antoine eq., Weast 1972–73)
 5080* (22.46°C, gas saturation, measured range –87.85 to 22.46°C, Carruth & Kobayashi 1973)
 6037, 6057 (static method-differential pressure gauge, Bissell & Williamson 1975)
 7826, 18929, 40469, 57059(30, 50, 70, 80°C, vapor-liquid equilibrium VLE data, Gutsche & Knapp 1982)
 6090 (interpolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.02701 - 1167.592/(216.796 + t/^\circ\text{C})$; temp range 25.92–99.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 4.38001 - 668.768/(159.522 + t/^\circ\text{C})$; temp range –87.85 to 22.4°C (Antoine eq. from reported exptl. data of Carruth & Kobayashi 1973, Boublik et al. 1984)
 6110, 5958, 6090 (headspace-GC, correlated, Antoine eq., Hussam & Carr 1985)
 6090 (interpolated-Antoine eq., temp range –2 to 124°C Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.98677 - 1264.90/(216.54 + t/^\circ\text{C})$; temp range –2 to 124°C (Antoine eq., Dean 1985, 1992)
 6090 (literature average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.02167 - 1264.90/(216.544 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 6110 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.02633 - 1268.583/(-56.054 + T/K)$; temp range 297–375 K (Antoine eq., Stephenson & Malanowski 1987)
 6102* (recommended, Ruzicka & Majer 1994)
 $\ln[(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/K)/(T/K)] \cdot \exp\{2.86470 - 2.113204 \times 10^{-3} \cdot (T/K) + 2.250991 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_o = 101.325 \text{ kPa}$, $T_o = 371.552 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log(P/\text{mmHg}) = 65.0257 - 3.8188 \times 10^3/(T/K) - 21.684 \cdot \log(T/K) + 1.0387 \times 10^{-2} \cdot (T/K) + 1.0206 \times 10^{-14} \cdot (T/K)^2$; temp range 183–540 K (vapor pressure eq., Yaws 1994)
 12309 (40°C, average value, vapor-liquid equilibrium VLE data, Rhodes et al. 1997)
 7811, 18869(30, 50°C, VLE equilibrium data, Carmona et al. 2000)
 62503* (355.899 K, ebulliometry, measured range 355.899–503.406 K, Weber 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 206200 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 226000, 73120 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 230000 (recommended, Mackay & Shiu 1981)
 250420* (25.04°C, equilibrium cell-concentration ratio-GC, measured range 15.3–35.05°C Jönsson et al. 1982)
 136120, 184640, 243020, 315050, 394150(15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)

$\ln 1/K_{AW} = 23748.4/(T/K) + 64.927 \cdot \ln (T/K) - 454.172$; temp range 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)

273400 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

91294* (26°C, EPICS-GC, measured range 26–45°C, Hansen et al. 1993)

$\ln [H/(kPa \cdot m^3/mol)] = -3730/(T/K) + 17.0$; temp range 26–45°C (EPICS-GC, Hansen et al. 1993)

220825 (EPICS-GC, Ryu & Park 1999)

68000 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.532 - 1491/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.50 (calculated- π constant, Hansch et al. 1968, Hansch & Leo 1979)

4.76 (calculated-activity coeff. γ , Wasik et al. 1981, 1982)

4.66 (generator column-GC, Tewari et al. 1982a,b)

3.44 (HPLC- k' correlation, Coates et al. 1985)

4.48 (Berti et al. 1986)

4.66, 4.72 (generator column-GC, calculated-activity coeff. γ , Schantz & Martire 1987)

4.50 ± 0.25 (recommended, Sangster 1989)

4.66 (recommended, Sangster 1993)

4.99 (calculated-activity coefficients, Tse & Sandler 1994)

4.66 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

3.05* (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.29–50.28°C Gruber et al. 1997)

2.95 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = (7.30 \pm 0.17) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $299 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1982a, 1984c)

$k_{NO_3} = 1.36 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1988, 1990)

$k_{OH} = 7.52 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)

$k_{OH}^* = 7.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1991)

$k_{OH} = 7.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{NO_3} = 1.36 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{OH} = 7.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 1.36 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljic & Güsten 1990)

$k_{OH} = 7.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, with a calculated atmospheric lifetime of 19 h during summer daylight hours (Altshuller 1991)

$k_{NO_3} = (1.34 - 1.37) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1991)

$k_{NO_3}(\text{exptl}) = (1.36, 1.38) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}(\text{recommended}) = 1.37 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}(\text{calc}) = 1.45 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{OH}^* = 7.02 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 15 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $7.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radicals with an estimated lifetime of 19 h in summer daylight (Altshuller 1991).

TABLE 2.1.1.1.20.1

Reported aqueous solubilities of *n*-heptane at various temperatures

1.

Connolly 1966		Nelson & De Ligny 1968		Polak & Lu 1973	
shake flask-cloud point		shake flask-GC		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
22	1.1	4.3	1.95	0	4.39
57	3.3	13.5	2.02	25	3.37
77	3.7	25.0	2.66		
82	10.3	35.0	2.27		

2.

Price 1976		Jonsson et al. 1982		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC		vapor saturation-GC		IUPAC "tentative" best values		calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
25.0	2.24	15	2.67	0	3.0	0	4.18
40.1	2.63	20	2.57	10	2.0	15	3.23
55.7	3.11	25	2.51	20	2.4	20	3.06
99.1	5.60	30	2.49	25	2.4	25	2.95
118.0	11.4	35	2.52	30	2.40	30	2.90
136.6	27.3			40	2.5	35	2.90
150.4	43.7			50	2.9	40.1	2.95
				60	3.3	45	3.01
				90	3.9	55.7	3.34
				100	5.8	99.1	7.79
				120	13	118	12.8
				140	31	136.6	22.8
						150.4	36.7

$$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = -2.43$$

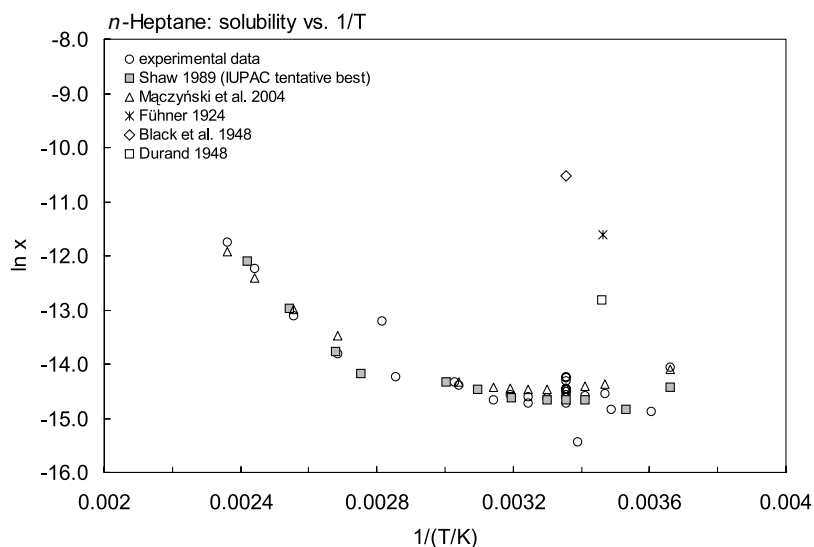


FIGURE 2.1.1.1.20.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *n*-heptane.

TABLE 2.1.1.1.20.2

Reported vapor pressures of *n*-heptane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \log (T/K) & (4) & \\ \ln [(P/\text{kPa})/(P_o/\text{kPa})] &= [1 - (T_o/K)/(T/K)] \cdot \exp\{A_o - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2\} & (5) & \text{- Cox eq.} \end{aligned}$$

1.

Smyth & Engel 1929		Willingham et al. 1945		Stull 1947		Forziati et al. 1949	
static method-manometer		ebulliometry		summary of literature data		ebulliometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
22.7	5520	25.925	6370	-34.0	133.3	26.030	6425
30.0	7759	29.699	7665	-12.7	666.6	29.813	7717
30.3	7839	33.024	8977	-2.1	1333	33.108	9013
38.4	11466	36.017	10311	9.5	2666	36.105	10352
50.0	18812	38.822	11700	22.3	5333	38.901	11740
51.2	19998	42.599	13821	30.6	7999	42.680	13866
61.2	29331	46.929	16604	41.8	13332	46.987	16659
69.5	39703	51.320	19920	58.7	26664	51.373	19966
70.0	40183	55.394	23443	78.0	53329	55.442	23499
79.5	55955	60.862	28950	98.4	101325	60.902	29003
98.4	101325	65.882	34897			65.916	34948
		71.930	43326	mp/ $^{\circ}\text{C}$	-90.6	71.966	43386
mp/ $^{\circ}\text{C}$	-90.5	78.160	53647			78.202	53270
bp/ $^{\circ}\text{C}$	98.4	84.823	66749			84.856	66815
		92.053	83706			92.678	83769
		97.154	97590			97.180	97663
		97.702	99186			97.728	99257
		98.207	100689			98.237	100758

(Continued)

TABLE 2.1.1.1.20.2 (Continued)

Smyth & Engel 1929		Willingham et al. 1945		Stull 1947		Forziati et al. 1949	
static method-manometer		ebulliometry		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		98.773	102393			98.813	102476
		99.285	103907			99.322	104018
		bp/°C	98.426			bp/°C	98.427
		eq. 2	P/mmHg			eq. 2	P/mmHg
		A	6.90342			A	6.90027
		B	1268.636			B	1266.871
		C	216.951			C	216.757
		temp range: 25.9–99.3°C				temp range: 26.0–99.3°C	

2.

Zwolinski & Wilhoit 1971		Carruth & Kobayashi 1973		Ruzicka & Majer 1994		Weber 2000	
selected values		gas saturation		recommended		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–2.22	1333	–87.85	0.288	–40	76.3	355.899	62503
9.43	2666	–80.41	0.867	–20	393	359.210	69482
16.78	4000	–68.21	4.240	0	1520	363.492	79475
22.29	5333	–55.70	16.40	20	4730	367.925	89500
26.75	6666	–42.11	57.46	25	6102	370.925	99446
30.519	7999	–27.95	196	40	12300	374.219	109546
36.706	10666	–14.0	595	60	28100	377.268	119434
41.723	13332	1.01	1667	80	57100	380.130	129452
51.366	19998	11.92	2986	100	106000	382.836	139321
58.656	26664	22.46	5080			386.617	154371
64.591	33331			OR		390.085	169321
69.632	39997	mp/°C	–90.60	T/K	P/Pa	394.397	189252
77.966	53329			179.40	0.1	335.188	30303
84.772	66661	eq. 1a	P/mmHg	194.52	1.0	339.317	35308
90.571	79993	A	20.1590	212.98	10	342.996	40310
95.650	93326	B	4852.65	236.18	100	349.358	50269
96.597	95992			266.53	1000	352.183	55286
97.523	98659			308.48	10000	354.804	60285
98.429	101325			371.55	101325	357.252	65269
				298.15	6102	359.559	70277
eq. 2	P/mmHg					363.894	60452
A	6.89385			data calc. from Cox eq.		367.733	90423
B	1264.37			eq. 5	P/kPa	371.255	100423
C	216.636			A ₀	2.86470	374.510	110415
bp/°C	98.429			A ₁	2.113204 × 10 ^{–3}	377.544	120394
ΔH _V /(kJ mol ^{–1}) =				A ₂	2.250991 × 10 ^{–6}	380.390	130382
at 25°C	36.55			with reference state at		383.069	140381
at bp	31.70			P _o /kPa	101.325	386.826	155364
				T _o /K	371.552	390.313	170377
						394.609	190385
						to	
						503.406	1597746

see [ref.](#) for complete set of data

see [ref.](#) for complete set of data

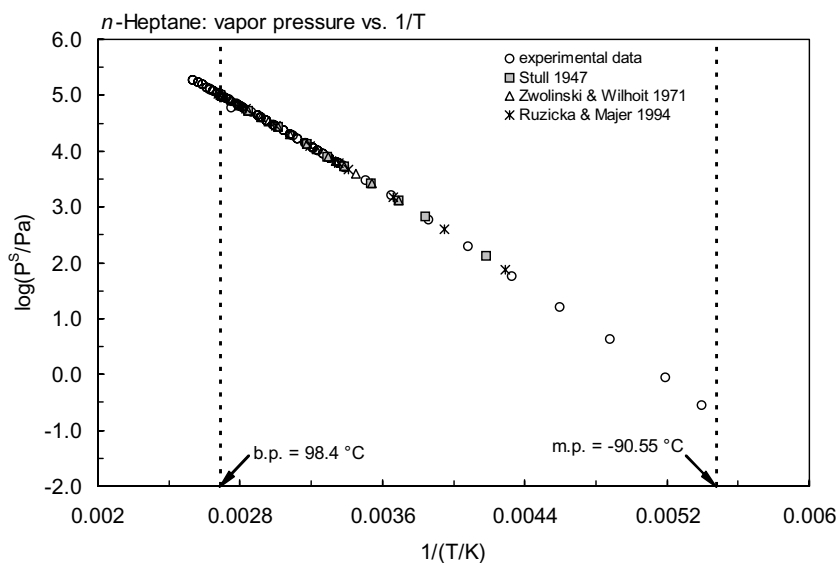


FIGURE 2.1.1.1.20.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-heptane.

TABLE 2.1.1.1.20.3

Reported Henry's law constants and octanol-air water partition coefficients of *n*-heptane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Henry's law constant				log K_{OA}	
Jönsson et al. 1982		Hansen et al. 1993		Gruber et al. 1997	
equilibrium cell-GC		EPICS-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OA}
15.0	136118*	26.0	91294	20.29	3.047
15.3	140244	35.8	121083	30.3	2.839
15.3	136260	45.0	193024	40.4	2.654
20.0	184640*			50.28	2.510
20.05	190443	eq. 4	H/(kPa m ³ /mol)		
20.05	187513	A	17 ± 2.22		
25.0	243021*	B	3730 ± 686		
25.05	193690				
25.05	190710				
25.04	250419				
29.8	302857				
29.8	316821				
30.0	315049*				
35.05	389419				
34.83	405792				
34.83	379903				
35.0	394148*				

* interpolated data

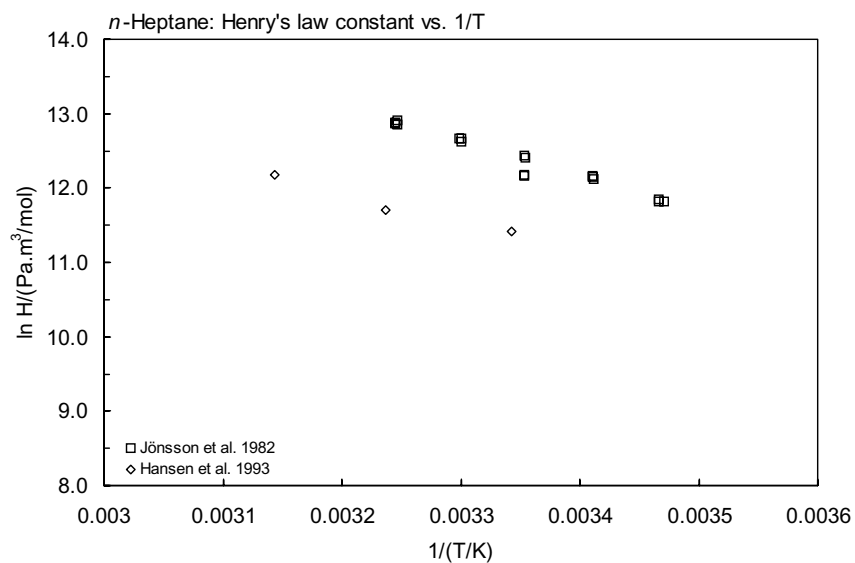


FIGURE 2.1.1.1.20.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-heptane.

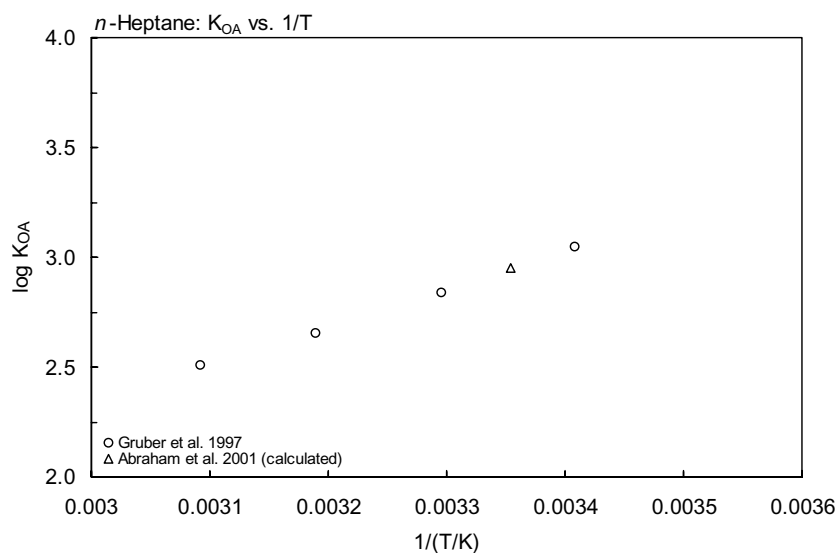
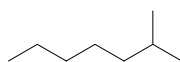


FIGURE 2.1.1.1.20.4 Logarithm of K_{OA} versus reciprocal temperature for *n*-heptane.

2.1.1.1.21 2-Methylheptane



Common Name: 2-Methylheptane

Synonym:

Chemical Name: 2-methylheptane

CAS Registry No: 592-27-8

Molecular Formula: C_8H_{18} ; $CH_3CH(CH_3)(CH_2)_4CH_3$

Molecular Weight: 114.229

Melting Point ($^{\circ}C$):

-109.02 (Lide 2003)

Boiling Point ($^{\circ}C$):

117.66 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.698 (Lide 2003)

Molar Volume (cm^3/mol):

163.7 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.68, 33.60 ($25^{\circ}C$, normal bp, Dreisbach 1959)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.92 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

72.62, 64.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.95, 4.55 (quoted, calculated-molar volume V_M , Wang et al. 1992)

2.84; 5.94 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

0.95; 1.61, 1.61 (quoted exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 6.91737 - 1337.468/(213.693 + t/^{\circ}C)$; temp range 41.7 – $118.5^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

2620 (calculated-Antoine eq. regression, temp range -21 to $117.6^{\circ}C$ Stull 1947)

6386 ($23.4^{\circ}C$, Nicolini & Laffitte 1949)

2748 (extrapolated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.91735 - 1337.468/(213.693 + t/^{\circ}C)$; temp range 35 – $150^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

2748 (interpolated-Antoine eq., temp range 12.3 – $143.8^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.91735 - 1337.468/(213.693 + t/^{\circ}C)$; temp range 12.3 – $143.8^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

2620 (interpolated-Antoine eq., temp range -21 – $117.6^{\circ}C$, Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 9362.0/(T/K)] + 8.154424$; temp range -21 – $117.6^{\circ}C$ (Antoine eq., Weast 1972–73)

2732, 6850 (calculated-Antoine eq., Boublik et al. 1973, 1984)

$\log(P/mmHg) = 6.88814 - 1319.539/(211.625 + t/^{\circ}C)$; temp range 41 – $118.5^{\circ}C$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1973)

$\log(P/mmHg) = 6.85999 - 1313.125/(230.02 + t/^{\circ}C)$; temp range 23.4 – $75^{\circ}C$ (Antoine eq. from reported exptl. data of Nicolini & Laffitte 1949, Boublik et al. 1973)

1161 ($10^{\circ}C$, static method-inclined piston manometer, measured range -40 to $10^{\circ}C$, Osborn & Douslin 1974)

2750 (extrapolated-Antoine eq., temp range 42–119°C, Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.91735 - 1337.47/(213.69 + t/^{\circ}\text{C})$; temp range 42–119°C (Antoine eq., Dean 1985, 1992)

2750 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.05858 - 1346.996/(-30.648 + T/\text{K})$; temp range 285–392 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.81199 - 1703.6/(-30.648 + T/\text{K})$; temp range 233–286 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 37.693 - 3.2611 \times 10^3/(T/\text{K}) - 10.391 \cdot \log (T/\text{K}) - 1.0524 \times 10^{-12} \cdot (T/\text{K}) + 3.056 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 164–560 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

369880 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.91 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

4.04 (calculated- V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 8.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (SAR structure reactivity relationship, Atkinson 1987)

$k_{OH} = 8.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime $\tau = 17 \text{ h}$ during summer daylight hours (Altshuller 1991).

Hydrolysis:

Biodegradation:

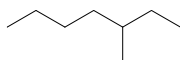
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $8.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radical and an estimated lifetime of 17 h during summer daylight (Altshuller 1991).

2.1.1.1.22 3-Methylheptane



Common Name: 3-Methylheptane

Synonym:

Chemical Name: 3-methylheptane

CAS Registry No: 589-81-1

Molecular Formula: C_8H_{18} ; $CH_3CH_2CH(CH_3)(CH_2)_3CH_3$

Molecular Weight: 114.229

Melting Point ($^{\circ}C$):

−120.48 (Lide 2003)

Boiling Point ($^{\circ}C$):

118.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7075 (Weast 1984)

0.7058, 0.7018 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

161.4 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.83, 34.08 ($25^{\circ}C$, normal bp, Dreisbach 1959)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.38 (Dreisbach 1959)

11.7 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

76.6, 64.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.792 (shake flask-GC, Price 1976; quoted, Mackay & Shiu 1981; Shaw 1989; Myrdal et al. 1992)

0.850 (estimated-nomograph, Brookman et al. 1985)

1.015 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log (P/mmHg) = 6.89945 - 1331.530/(212.414 + t/^{\circ}C)$; temp range 42.7 – $119.8^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry, manometer, Willingham et al. 1945)

2610 (calculated from determined data, Dreisbach 1959)

$\log (P/mmHg) = 6.89944 - 1331.530/(212.414 + t/^{\circ}C)$; temp range 30 – $150^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

2600 (interpolated-Antoine eq., temp range 13.3 – $145.2^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.89944 - 1331.530/(212.414 + t/^{\circ}C)$; temp range 13.3 – $145.2^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

2466 (interpolated-Antoine eq., temp range -19.8 to $118.9^{\circ}C$, Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 9432.0/(T/K)] + 8.179407$; temp range -19.8 to $118.9^{\circ}C$ (Antoine eq., Weast 1972–73)

1486 ($15^{\circ}C$, static method-inclined piston manometer, measured range -35 to $15^{\circ}C$, Osborn & Douslin 1974)

2600, 3232 (quoted, calculated-bp, Mackay et al. 1982)

2600 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.01647 - 1326.329/(211.776 + t/^{\circ}C)$; temp range 42.67 – $119.8^{\circ}C$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

2605 (extrapolated, Antoine eq., temp range 43 – $120^{\circ}C$ Dean 1985, 1992)

$\log (P/mmHg) = 6.89944 - 1331.53/(212.41 + t/^{\circ}C)$; temp range 43 – $120^{\circ}C$ (Antoine eq., Dean 1985, 1992)

2630 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.02047 - 1329.42/(-60.945 + T/\text{K})$; temp range 286–393 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.50909 - 1567.45/(-40.786 + T/\text{K})$; temp range 238–286 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 52.8828 - 3.6231 \times 10^3/(T/\text{K}) - 16.804 \cdot \log (T/\text{K}) + 7.1828 \times 10^{-3} \cdot (T/\text{K}) + 7.4077 \times 10^{-14} \cdot (T/\text{K})^2$; temp range 153–564 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$):

376000 (calculated-P/C, Mackay & Shiu 1981)

375900 (selected, Mills et al. 1982)

375800 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 8.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{OH} = 8.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime $\tau = 16 \text{ h}$ during summer daylight hours (Altshuller 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $8.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radical with an estimated lifetime of 16 h during summer daylight (Altshuller 1991).

2.1.1.1.23 *n*-OctaneCommon Name: *n*-Octane

Synonym: octane

Chemical Name: *n*-octane

CAS Registry No: 111-65-9

Molecular Formula: C_8H_{18} ; $CH_3(CH_2)_6CH_3$

Molecular Weight: 114.229

Melting Point ($^{\circ}C$):

-56.82 (Lide 2003)

Boiling Point ($^{\circ}C$):

125.67 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.7027, 0.6886 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)0.70256 ($20^{\circ}C$, digital precision densimeter, Dejoz et al. 1996)Molar Volume (cm^3/mol):162.6, 165.8 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):41.49, 34.431 ($25^{\circ}C$, bp, Riddick et al. 1986)

41.56 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.74 (Dreisbach 1959; Riddick et al. 1986; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

95.86, 91.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

14.0 (cloud point, Fühner 1924, quoted, Deno & Berkheimer 1960)

0.66 (shake flask-GC, McAuliffe 1963, 1966)

0.493 (radiotracer method, Baker 1967)

0.880* (shake flask-GC, measured range 5 – $25^{\circ}C$, Nelson & De Ligny 1968)

0.700 (shake flask-GC, Krzsnoshchekova & Gubergits 1973)

1.35; 0.85 (0 , $25^{\circ}C$, shake flask-GC, Polak & Lu 1973)0.431* (shake flask-GC, measured range 25 – $149.5^{\circ}C$, Price 1976)0.615* (vapor saturation-GC, measured range 15 – $35^{\circ}C$, Jönsson et al. 1982)

1.103 (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982)

1.56 (calculated-activity coeff. and K_{ow} , Tewari et al. 1982b)

0.615 (vapor saturation-partition coefficient-GC, Jönsson et al. 1982)

0.660 (shake flask-GC, Coates et al. 1985)

0.762* ($37.75^{\circ}C$, shake flask-GC, measured range 37.75 – $280^{\circ}C$, pressure range 0.0103 – 8.86 MPa, Heidmen et al. 1985)
 $\ln x = -343.1497 + 13862.49/(T/K) + 49.24600 \cdot \ln (T/K)$; temp range 37.75 – $280^{\circ}C$ (shake flask-GC, Heidman et al. 1985)
0.884, 0.949 ($20^{\circ}C$, shake flask-GC, Burris & MacIntyre 1986)

1.250 (shake flask-purge and trap-GC, Coutant & Keigley 1988)

0.71* (recommended, temp range 0 – $100^{\circ}C$, IUPAC Solubility Data Series, Shaw 1989)
 $\ln x = -415.7563 + 17975.386/(T/K) + 59.55451 \cdot \ln (T/K)$; temp range 290 – 400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)
0.774* ($29.9^{\circ}C$, shake flask-solid extraction-GC/FID, measured range 29.9 – $183^{\circ}C$, Marche et al. 2003)
 $\ln x = -362.618 + 14904.474/(T/K) + 52.067 \cdot \ln (T/K)$; temp range 29.9 – $183^{\circ}C$ (shake flask-solid extraction-GC/FID measurements, Marche et al. 2003)

- 0.635* (calculated-liquid-liquid equilibrium LLE data, temp range 288.2–36.1 K, Mączyński et al. 2004)
 0.807 (24.9°C, generator column-GC/FID, measured range 10–45°C, Sarraute et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 486.6* (3.7°C, static-McLeod gauge, measured range –9.31 to 3.7°C, Linder 1931)
 7670* (52.972°C, ebulliometry, measured range 52.972–126.570°C, Willingham et al. 1945)
 $\log(P/\text{mmHg}) = 6.92377 - 1355.126/(209.517 + t/^\circ\text{C})$; temp range 52.9–126.6°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
 1777* (calculated-Antoine eq. regression, temp range –14 to 125.6°C, Stull 1947)
 1870 (calculated from determined data, Dreisbach 1959)
 $\log(P/\text{mmHg}) = 6.92377 - 1355.126/(209.517 + t/^\circ\text{C})$; temp range 40–155°C (Antoine eq. for liquid state, Dreisbach 1959)
 1885* (interpolated-Antoine eq., temp range 19.2–152.1°C, Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = 6.92377 - 11355.126/(209.517 + t/^\circ\text{C})$; temp range 19.2–152.1°C (Antoine eq., Zwolinski & Wilhoit 1971)
 1825 (interpolated-Antoine eq., temp range –14 to 281.4°C, Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 9221.0/(T/\text{K})] + 7.894018$; temp range –14 to 281.4°C (Antoine eq., Weast 1972–73)
 1573* (23.96°C, gas saturation, measured range –56.35 to 23.96°C, Carruth & Kobayashi 1973)
 1885, 2060 (quoted, calculated-bp, Mackay et al. 1982)
 1860 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.04394 - 1351.938/(209.12 + t/^\circ\text{C})$; temp range 52.93–126.57°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 1860 (interpolated-Antoine eq., temp range 19–152°C, Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.91868 - 1351.99/(209.15 + t/^\circ\text{C})$; temp range 19–152°C (Antoine eq., Dean 1985, 1992)
 1870 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.04358 - 1351.99/(209.155 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 1854, 1814, 1854 (headspace-GC, correlated, Antoine eq., Hussam & Carr 1985)
 1862 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.04231 - 1351.491/(-64.014 + T/\text{K})$; temp range 297–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.90115 - 2238.9/(-4.53 + T/\text{K})$; temp range 216–278 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.16936 - 1440.32/(-52.894 + T/\text{K})$; temp range 396–432 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.23406 - 1492.068/(-45.851 + T/\text{K})$; temp range 428–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.66614 - 7.66614/(159.091 + T/\text{K})$; temp range 506–569 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 1872* (recommended, Ruzicka & Majer 1994)
 $\ln[(P/\text{kPa})/(P_0/\text{kPa})] = [1 - (T_0/\text{K})/(T/\text{K})] \cdot \exp\{2.90150 - 2.046204 \times 10^{-3} \cdot (T/\text{K}) + 2.010759 \times 10^{-6} \cdot (T/\text{K})^2\}$; reference state at $P_0 = 101.325$ kPa, $T_0 = 398.793$ K (Cox equation, Ruzicka & Majer 1994)
 $\log(P/\text{mmHg}) = 29.0948 - 3.0114 \times 10^3/(T/\text{K}) - 7.2653 \cdot \log(T/\text{K}) - 2.2696 \times 10^{-11} \cdot (T/\text{K}) + 1.468 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 216–569 K (vapor pressure eq., Yaws 1994)
 1820* (24.6°C, ebulliometry, measured range 291.25–409.95 K, Dejoz et al. 1996)
 $\ln(P/\text{Pa}) = 13.9183 - 3114.43/[(T/\text{K}) - 63.9225]$; temp range 291–409 K (ebulliometry, Dejoz et al. 1996)
 6727* (50.43°C, comparative ebulliometry, measured range 323–563 K, data fitted to Wagner eq., Ewing & Ochoa 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 326800 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee)
 311900, 110670 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 325300 (calculated-P/C, Mackay & Leinonen 1975; Mackay & Shiu 1990)
 323200 (calculated-P/C, Bobra et al. 1979; Mackay et al. 1979; Mackay 1981)

- 325000 (calculated-P/C, Mackay & Shiu 1981)
 355500* (25.1°C, equilibrium cell-concentration ratio-GC, measured range 14.8–34.92°C, Jönsson et al. 1982)
 180130, 253880, 344280, 458250, 595800 (15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl. data, Jönsson et al. 1982)
 $\ln (1/K_{AW}) = 26003.7/(T/K) + 70.571 \cdot \ln (T/K) - 494.151$; temp range: 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)
 324200 (calculated-P/C, Lyman et al. 1982)
 $\ln (k_H/\text{MPa}) = 357.733 - 19363.1/(T/K) - 9.04865 \cdot (T/K)^2 - 49.5296 \cdot \ln (T/K)$; maximum $k_H = 7.836 \times 10^4$ MPa at 372.1 K (Heidman et al. 1985)
 314700 (calculated-P/C, Eastcott et al. 1988)
 326200 (Valsaraj 1988)
 201500 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 499500 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 39213* (27.9°C, EPICS-GC, measured range 27.9–45°C, Hansen et al. 1993)
 $\ln [H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -8014/(T/K) + 30.0$; temp range: 27.9–45°C (EPICS-GC, Hansen et al. 1993)
 297951 (EPICS-GC, Ryu & Park 1999)
 21838 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 12.08 - 3263/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)
 257797 (24.9°C, calculated-P/C, Sarraute et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.0 (calculated- π substituent const., Hansch et al. 1968; Hansch & Leo 1979)
 5.29 (calculated-activity coefficient γ , Wasik et al. 1981, 1982)
 5.18 (generator column-GC, Tewari et al. 1982a,b)
 4.0 (HPLC- k' correlation, Coates et al. 1985)
 5.24 (generator column-GC, calculated-activity coefficient γ , Schantz & Martire 1987)
 5.15 \pm 0.45 (recommended, Sangster 1989; 1993)
 5.61 (calculated-activity coefficients, Tse & Sandler 1994)
 5.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.55* (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
 3.30 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 5.55$ h for a water column of 1 m² minimum cross section of depth 1 m (Mackay & Leinonen 1975)

estimated $t_{1/2} \sim 3.1$ h at 20°C in a river 1 m deep flowing at 1 m s⁻¹ and with a wind velocity of 3 m s⁻¹ (Lyman et al. 1982).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^*(\text{exptl}) = 6.03 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 2.35 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 296 K, measured range 296–497 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{O(3P)} = 1.70 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with O(³P) atom at room temp. (Herron & Huie 1973)

$k_{OH}(\text{exptl}) = 8.42 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, $k_{OH}(\text{calc}) = 7.35 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Darnall et al. 1978)

$k_{\text{OH}} = (9.01 \pm 0.19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $299 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1982a, 1984c)

$k_{\text{OH}} = 8.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)

$k_{\text{OH}}^* = 8.68 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 8.68 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.81 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{\text{OH}} = 8.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.81 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljic & Güsten 1990)

$k_{\text{OH}} = 8.68 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, estimated atmospheric lifetime of 16 h (Altshuller 1991)

$k_{\text{NO}_3} = 1.82 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson 1991)

$k_{\text{OH}} = 8.68 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Paulson & Seinfeld 1992)

$k_{\text{NO}_3}(\text{exptl}) = 1.84 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{calc}) = 1.79 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{\text{OH}}^* = 8.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}^* = 1.9 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ for C_4H_{10} and higher paraffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction $k = 8.68 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radicals with an estimated lifetime of 16 h in air during summer daylight (Altshuller 1991).

Surface water: volatilization $t_{1/2} = 5.55 \text{ h}$ for a water column of 1 m^2 minimum cross section of depth 1 m (Mackay & Leinonen 1975); estimated volatilization $t_{1/2} = 3.1 \text{ h}$ at 20°C in a river 1 m deep flowing at 1 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982).

Ground water:

Sediment:

Soil:

Biota:

TABLE 2.1.1.1.23.1

Reported aqueous solubilities of *n*-octane at various temperatures

1.

Nelson & De Ligny 1968		Polak & Lu 1973		Price 1976		Jonsson et al. 1982	
shake flask-GC		shake flask-GC/FID		shake flask-GC		vapor saturation-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
5	1.65	0	1.35	25.0	0.431	15	0.653
15	0.89	25	0.85	40.1	0.524	20	0.628
25	1.84			69.7	0.907	25	0.615
				99.1	1.12	30	0.612
				121.3	4.62	35	0.620
				136.6	8.52		
				149.5	11.80		

TABLE 2.1.1.1.23.1 (Continued)

2.

Heidman et al. 1985		Shaw 1989a		Marche et al. 2003		Mączyński et al. 2004	
shake flask-GC		IUPAC "tentative" best values		shake flask-GC		calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
37.75	0.76	0	0.14	29.9	0.774	15	0.698
93.35	3	20	0.63	30.3	0.762	20	0.698
148.85	24	25	0.71	69.2	1.517	25	0.635
206.35	25	30	0.61	70	2.234	30	0.635
262.35	220	40	0.8	99.9	3.046	35	0.635
279.65	380	50	1	101.1	3.414	37.7	0.635
		60	1.2	124	7.806	40.1	0.952
		70	1.5	124	9.011	69.7	4.00
pressures range from		80	2	131	11.23	121.3	6.98
0.0103 to 8.86 MPa		90	2.7	131	12.25	136.6	12.06
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 13.3$		100	3.7	151.2	24.88	149.5	22.21
25°C		120	7.2	165.1	43.79	262.9	50.77
		140	15	165.4	43.28		
		160	22	183	84.85		

$\ln x = A + B/T + C \cdot \ln T$
T in K
A -362.618
B 14904.474
C 52.067

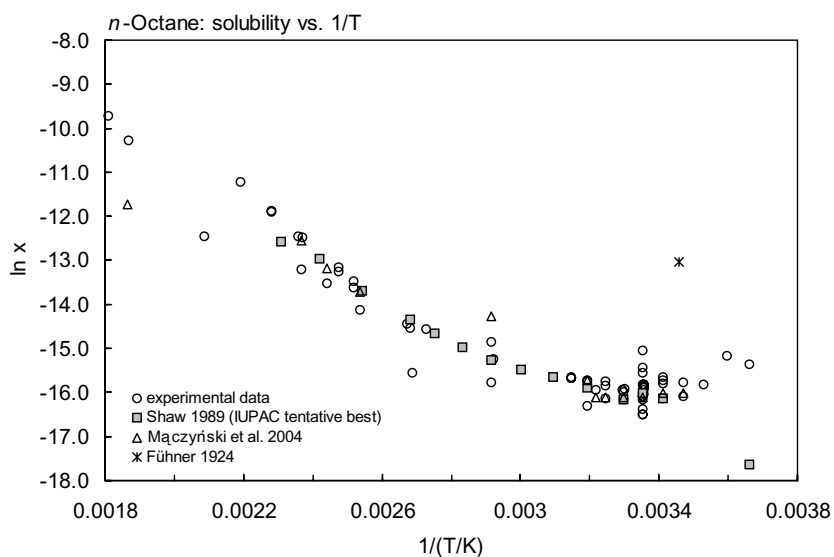
FIGURE 2.1.1.1.23.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *n*-octane.

TABLE 2.1.1.1.23.2

Reported vapor pressures of *n*-octane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(C + T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \quad \ln P = A - B/(C + T/K) & (3a) \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & & (4a) \\ \ln [(P/\text{kPa})/(P_o/\text{kPa})] &= [1 - (T_o/K)/(T/K)] \cdot \exp\{A_0 - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2\} & & & (5) - \text{Cox eq.} \end{aligned}$$

1.

Linder 1931		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
McLeod gauge		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-9.31	196.0	52.972	7670	-14.0	133.3	19.03	1333
-3.0	309.3	56.456	8979	8.30	666.6	39.06	2666
3.7	486.6	59.615	10314	10.2	1333	39.10	4000
		62.592	11702	31.5	2666	44.95	5333
		66.587	13823	45.1	5333	49.68	6666
		71.163	16600	53.8	7999	53.67	7999
		75.820	19918	65.7	13332	60.24	10666
		80.134	23441	83.6	26664	65.56	13332
		85.916	28952	104.0	53329	75.79	19998
		91.230	34894	125.6	101325	83.52	26664
		97.635	43326			89.813	33331
		104.233	53646	mp/°C	-56.8	95.158	39997
		111.277	66742			103.991	53329
		118.924	83695			111.204	66661
		124.319	97584			117.349	79993
		124.809	99161			122.731	93326
		125.433	100662			123.734	95992
		126.035	102386			124.715	98659
		126.570	103900			125.675	101325
		bp/°C	123.665				
		eq. 2	P/mmHg			eq. 2	P/mmHg
		A	6.92377			A	6.90940
		B	1355.126			B	1349.82
		C	209.517			C	209.385
		temp range: 52.9–126.6°C				bp/°C	125.675
						$\Delta H_v/(\text{kJ mol}^{-1})$	
						at 25°C	41.49
						at bp	34.41

TABLE 2.1.1.1.23.2 (Continued)

2.

Carruth & Kobayashi 1973		Ruzicka & Majer 1994		Dejoz et al. 1996		Ewing & Ochoa 2003	
gas saturation		recommended		vapor-liquid equilibrium		comparative ebulliometry	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−56.35	2.40	194.67	0.1	18.1	1250	50.03	6727
−54.64	2.746	210.84	1.0	20.7	1450	51.811	7640
−49.92	4.40	230.53	10	24.69	1820	60.642	10766
−42.73	9.706	255.25	100	27.4	2130	67.754	14507
−35.08	20.13	287.52	1000	29.6	2410	73.195	18016
−23.06	59.33	332.03	10000	31.2	2630	79.794	23174
−13.75	127.7	398.79	101325	33.8	3020	88.950	32265
5.26	532.0	298.15	1872	36.8	3520	93.009	37123
16.41	1047			42.4	4670	99.293	45789
23.96	1573	data calc. from Cox eq. eq. 5		48.6	6290	104.234	53686
			P/kPa	51.4	7150	110.649	65523
mp/°C	−56.81	A ₀	2.90150	55.7	8690	115.266	75253
		A ₁	2.046204×10^{-3}	58.9	10000	118.867	83613
eq. 1a	P/mmHg	A ₂	2.010759×10^{-6}	61.4	11130	121.958	91358
A	20.3621	with reference state at		64.0	12410	125.705	101486
B	5294.36	P ₀ /kPa	101.325	66.7	13890	128.458	109480
		T ₀ /K	398.793	68.3	14820	131.853	130296
				71.8	17050	134.957	138.490
				74.9	19240		
				77.6	21330	Antoine eq. for P < 145 kPa in the following form $\ln P/\text{kPa} = (A-B)/(T-C)$ with	
				80.7	23900		
				85.3	28330		
				90.05	34030		
				96.1	41180		
				100.5	47680	A	13.91204
				102.2	50300	B	3110.704
						C	64.086
				eq. 3(a)	kPa	for temp 323–563 K or pressure 6.7–2301 kPa data fitted to Wagner eq.	
				A	13.9183		
				B	3114.43		
				C	−63.925		
				for temp 291–409 K			

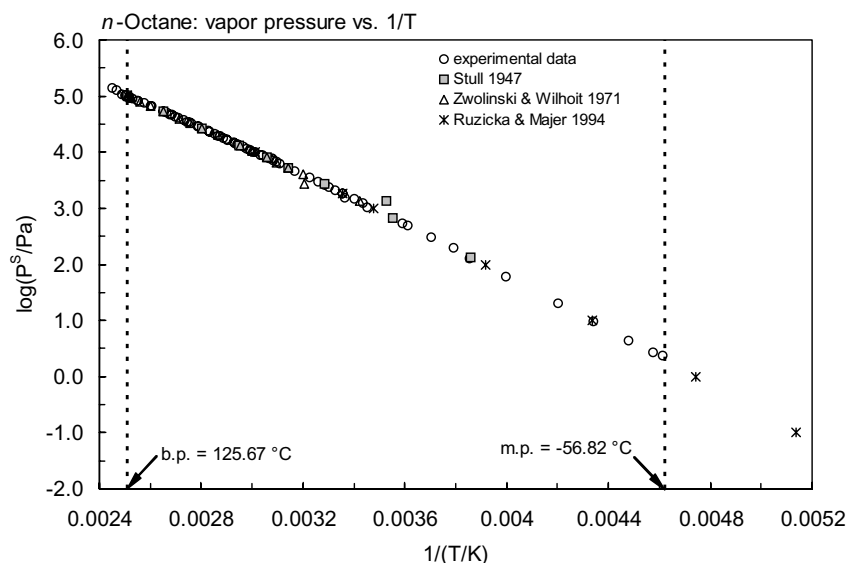


FIGURE 2.1.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-octane.

TABLE 2.1.1.1.23.3

Reported Henry's law constants and octanol-air partition coefficients of *n*-octane at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$

$$\ln (1/K_{AW}) = A - B/(T/K)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$

$$\log (1/K_{AW}) = A - B/(T/K)$$

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

(1)

(2)

(3)

(4)

(5)

(1a)

(2a)

(4a)

Henry's law constant				log K _{OA}	
Jönsson et al. 1982		Hansen et al. 1993		Gruber et al. 1997	
equilibrium cell-GC		EPICS-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
14.8	171001	27.9	39213	20.29	3.554
14.8	176031	35.0	93827	30.3	3.302
15.0	180126*	45.0	167693	40.4	3.089
20.0	253880*			50.28	2.927
20.05	259326	eq. 4	H/(kPa m ³ /mol)		
20.05	256596	A	30 ± 5.25		
25.0	344280*	B	8014 ± 1617		
25.1	357298				
25.1	353730				
30.0	458253*				
30.1	452643				
34.92	587452				
35.0	595804*				

* interpolated data

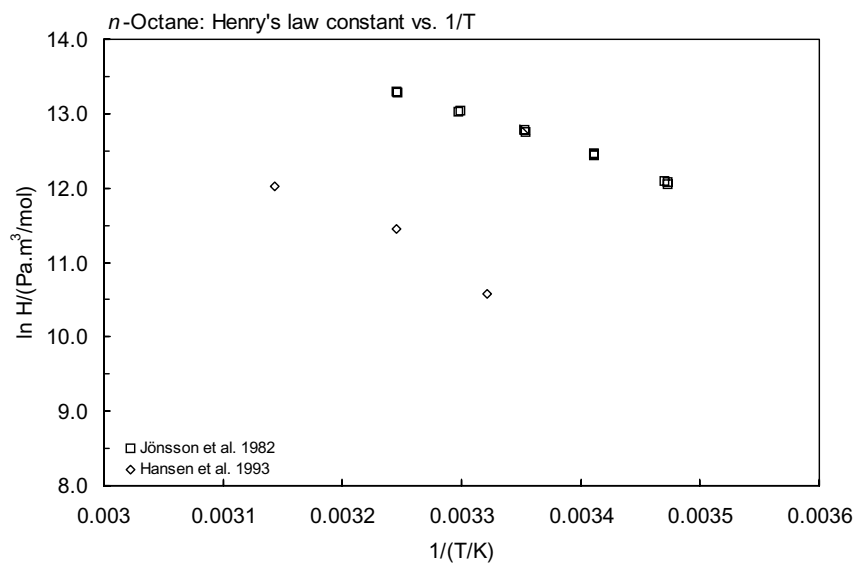


FIGURE 2.1.1.1.23.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-octane.

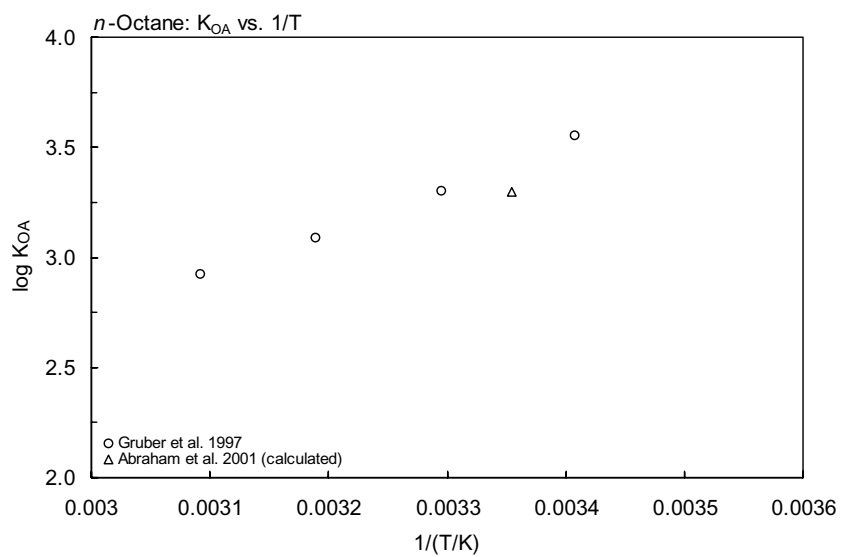
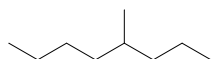


FIGURE 2.1.1.1.23.4 Logarithm of K_{OA} versus reciprocal temperature for *n*-octane.

2.1.1.1.24 4-Methyloctane



Common Name: 4-Methyloctane

Synonym:

Chemical Name: 4-methyloctane

CAS Registry No: 2216-34-4

Molecular Formula: C_9H_{20} ; $CH_3(CH_2)_2CH(CH_3)(CH_2)_3CH_3$

Molecular Weight: 128.255

Melting Point ($^{\circ}C$):

-113.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

142.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7199, 0.7169 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

178.2 ($20^{\circ}C$, calculated-density)

207.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

44.75, 36.60 ($25^{\circ}C$, normal bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.115 (shake flask-GC, Price 1976; quoted, Shaw 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

901 (extrapolated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.9155 - 1406.0/(206.0 + t/^{\circ}C)$; temp range $50-165^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

933 (extrapolated-Antoine eq., temp range $32-170^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.90318 - 1399.12/(205.41 + t/^{\circ}C)$; temp range $32-170^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 11.2012 - 2.9467 \times 10^3/(T/K) + 1.2133 \cdot \log(T/K) - 1.4423 \times 10^{-2} \cdot (T/K) + 9.177 \times 10^{-6} \cdot (T/K)^2$; temp range 160–588 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1010000; 1000000 (calculated-P/C, recommended, Mackay & Shiu 1981)

1007000 (selected, Mills et al. 1982)

1007000 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 9.72 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson 1989)

$k_{\text{OH}} = 9.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

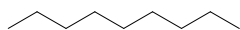
Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.1.1.25 *n*-NonaneCommon Name: *n*-Nonane

Synonym: nonane

Chemical Name: *n*-nonane

CAS Registry No: 111-84-2

Molecular Formula: C₉H₂₀; CH₃(CH₂)₇CH₃

Molecular Weight: 128.255

Melting Point (°C):

-53.46 (Lide 2003)

Boiling Point (°C):

150.82 (Lide 2003)

Density (g/cm³ at 20°C):

0.7176, 0.7138 (20°C, 25°C, Dreisbach 1959)

0.7177, 0.7138 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

178.7, 179.7 (20°C, 25°C, calculated-density)

207.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

44.442, 36.915 (25°C, bp, Riddick et al. 1986)

46.55 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.468 (Dreisbach 1959; Riddick et al. 1986)

6.28, 15.38 (-55.95, -53.45°C, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

99.2, 100.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

0.220 (shake flask-GC, McAuliffe 1969;)

0.098 (Baker 1967)

0.071 (shake flask-GC, Krasnoshchekova & Gubertritis 1973)

0.122* (shake flask-GC, measured range 25–136.6°C, Price 1976)

0.289, 0.272 (15, 20°C, vapor saturation-GC, Jönsson et al. 1982)

0.219 (shake flask-GC, Coates et al. 1985)

1.70* (tentative best value, temp range 20–130°C, IUPAC Solubility Data Series, Shaw 1989)

$\ln x = -433.434 + 18767.82/(T/K) + 61.940 \cdot \ln (T/K)$; temp range 290–400 K (eq. derived from lit. calorimetric and solubility data, Tsionopoulos 1999)

0.135, 0.477 (25, 100.1°C, calculated-liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6349* (70.127°C, ebulliometry, measured range 70.127–151.764°C, Willingham et al. 1945)

$\log (P/\text{mmHg}) = 6.94495 - 1435.158/(202.331 + t/^\circ\text{C})$; temp range 70.1–151.8°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

623* (calculated-Antoine eq. regression, temp range 1.4–149.5°C, Stull 1947)

6405* (70.343°C, ebulliometry-manometer, measured range 70.343–151.786°C, Forziati et al. 1949)

$\log (P/\text{mmHg}) = 6.93513 - 1428.811/(201.619 + t/^\circ\text{C})$; temp range 70.343–151.786°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

580 (extrapolated-Antoine eq., Dreisbach 1959)

$\log (P/\text{mmHg}) = 6.93513 - 1428.811/(201.619 + t/^\circ\text{C})$; temp range 60–185°C (Antoine eq. for liquid state, Dreisbach 1959)

- 571* (extrapolated-Antoine eq., temp range 39.32–178.48°C, Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = 6.93513 - 1428.811/(201.619 + t/^\circ\text{C})$; temp range 39.32–178.48°C (Antoine eq., Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = [-0.2185 \times 10456.9/(T/\text{K})] + 8.332532$; temp range 2.4–149.5°C (Antoine eq., Weast 1972–73)
 404.0* (20.99°C, gas saturation, measured range –53.49 to 34.59°C, Carruth & Kobayashi 1973)
 570, 713 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.0628 - 1430.638/(201.827 + t/^\circ\text{C})$, temp range: 70.434–151.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.0847 - 1439.2/(205.962 + t/^\circ\text{C})$, temp range: 66.61–147.86°C (Antoine eq. from reported exptl. data Forziati et al. 1949, Boublik et al. 1984)
 571 (extrapolated-Antoine eq., temp range 39–179°C, Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.93893 - 1431.82/(202.01 + t/^\circ\text{C})$; temp range 39–179°C (Antoine eq., Dean 1985, 1992)
 570 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.06383 - 1431.82/(202.011 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 517; 571 (extrapolated-Antoine eq.-I; interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.0593 - 1429.46/(-71.33 + T/\text{K})$; temp range 344–426 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 8.17855 - 2523.8/(T/\text{K})$; temp range 219–308 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 580.7* (recommended, Ruzicka & Majer 1994)
 $\ln[(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/\text{K})/(T/\text{K})] \cdot \exp\{2.94690 - 2.061933 \times 10^{-3} \cdot (T/\text{K}) + 1.903683 \times 10^{-6} \cdot (T/\text{K})^2\}$; reference state at $P_o = 101.325 \text{ kPa}$, $T_o = 423.932 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log(P/\text{mmHg}) = 8.8817 - 2.8042 \times 10^3/(T/\text{K}) + 1.5262 \cdot \log(T/\text{K}) - 1.0464 \times 10^{-2} \cdot (T/\text{K}) + 5.7972 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 220–596 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 601000, 748000, 333000; 500000 (calculated-P/C values, recommended, Mackay & Shiu 1981)
 147400*, 372820 (14.8, 20.05°C, equilibrium cell-concentration ratio-GC, Jönsson et al. 1982)
 173520, 348200 (15, 20°C, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)
 $\ln(1/K_{AW}) = 28259/(T/\text{K}) + 76.183 \cdot \ln(T/\text{K}) - 524.13$; temp range 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)
 41950* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln[H/(\text{atm m}^3/\text{mol})] = -0.1847 + 202.1/(T/\text{K})$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 599600 (calculated-P/C, Eastcott et al. 1988)
 601000 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 459668 (EPICS-GC, Ryu & Park 1999)
 42164 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 1.104 + 39/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.51 (estimated-HPLC- k' correlation, Coates et al. 1985)
 5.65 ± 0.60 (recommended, Sangster 1989)
 5.42 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor,

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (10.7 \pm 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $299 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1982a, 1984c)
 $k_{\text{OH}} = 10.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)
 $k_{\text{OH}} = 1.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)
 $k_{\text{OH}} = 1.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , $k_{\text{NO}_3} = 2.39 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)
 $k_{\text{OH}} = 1.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated atmospheric lifetime of 14 h (Altshuller 1991)
 $k_{\text{OH}} = 1.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , $k_{\text{NO}_3} = 2.30 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljic & Güsten 1990)
 $k_{\text{NO}_3} = 2.41 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson 1991)
 $k_{\text{NO}_3}(\text{exptl}) = (1.92, 2.59) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{calc}) = 2.47 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)
 $k_{\text{OH}}^* = 10.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 2.3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ for C_4H_{10} and higher paraffins for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976); photooxidation reaction rate constant of $1.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radical with an estimated lifetime $\tau = 14 \text{ h}$ during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.25.1

Reported aqueous solubilities of *n*-nonane at various temperatures

Price 1976		Jonsson et al. 1982		Shaw 1989a	
shake flask-GC		vapor saturation-GC		IUPAC "tentative" best	
<i>t</i> /°C	S/g·m ⁻³	<i>t</i> /°C	S/g·m ⁻³	<i>t</i> /°C	S/g·m ⁻³
25.0	0.122	15	0.289	20	0.29
69.7	0.309	20	0.272	25	0.17
99.1	0.420			30	0.14
121.3	1.70			40	0.17
136.6	5.07			50	0.22
				60	0.26
				70	0.31
				80	0.34
				90	0.37
				100	0.42
				110	0.80
				120	1.60
				130	3.20

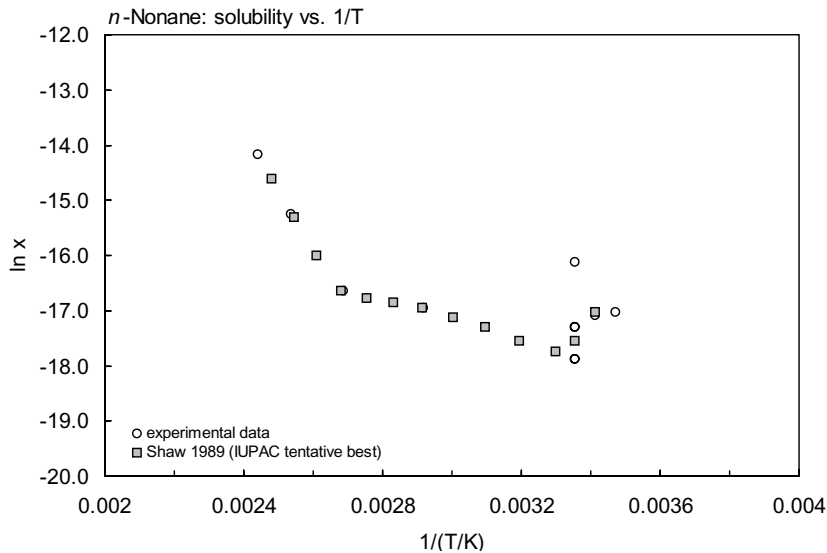


FIGURE 2.1.1.1.25.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for n-nonane.

TABLE 2.1.1.1.25.2
Reported vapor pressures of n-nonane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K)$$
$$\log P = A - B/(C + t/^{\circ}\text{C})$$
$$\log P = A - B/(C + T/K)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K)$$
$$\ln [(P/\text{kPa})/(P_0/\text{kPa})] = [1 - (T_0/K)/(T/K)] \cdot \exp\{A_0 - A_1 \cdot (T/K) + A_2 \cdot (T/K)^2\}$$

(1)

(2)

(3)

(4)

$$\ln P = A - B/(T/K)$$
$$\ln P = A - B/(C + t/^{\circ}\text{C})$$

(1a)

(2a)

1.

Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
ebulliometry-manometer		summary of literature data		ebulliometry-manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70.127	6349	2.4	133.3	70.343	6405	39.06	1333
74.388	7650	26.3	666.6	74.546	7697	51.93	2666
78.097	8955	38.0	1333	78.219	8995	60.12	4000
81.458	10294	51.0	2666	81.548	10335	66.25	5333
84.582	11687	65.6	5333	84.658	11724	71.216	6666
88.801	13822	74.1	7999	88.864	13847	75.409	7999
93.610	16611	86.0	13332	93.601	16639	82.293	10666
98.491	19913	104.7	26664	98.545	19949	87.873	13332
103.047	23451	126.8	53329	103.072	23479	98.593	19998
109.115	28952	149.5	101325	109.136	28984	106.694	26664
114.684	34892			114.712	34.930	113.284	33331
121.399	43319	mp/°C	−53.7	121.433	43366	118.882	39997
128.329	53653			128.357	53703	128.131	53329
136.721	66757			135.741	66801	135.680	66661
143.738	83721			143.751	83755	142.110	79993
149.394	97609			149.409	97652	147.741	93326

(Continued)

TABLE 2.1.1.1.25.2 (Continued)

Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
ebulliometry-manometer		summary of literature data		ebulliometry-manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
150.002	99207			150.017	99241	148.790	95992
150.565	100833			150.579	100734	149.816	98659
151.195	102401			151.222	102467	150.321	101325
151.764	103921			151.786	104006		
						eq. 2	P/mmHg
bp/°C	150.796			bp/°C	150.798	A	6.93440
						B	1508.75
eq. 2	P/mmHg			eq. 2	P/mmHg	C	195.374
A	6.94445			A	6.93513	bp/°C	150.821
B	1435.158			B	1428.811	$\Delta H_v/(\text{kJ mol}^{-1})$	
C	202.331			C	201.619	at 25°C	36.92
temp range: 70.1–151.8°C				temp range: 70.3–151.8°C		at bp	46.44

2.

Carruth & Kobayashi 1973		Ruzicka & Majer 1994	
gas saturation		recommended	
t/°C	P/Pa	T/K	P/Pa
–53.49	0.7586	209.23	0.1
–49.4	0.825	226.30	1.0
–48.26	0.925	247.08	10
–36.32	3.240	273.13	100
–27.45	7.866	307.09	1000
–9.97	37.33	353.86	10000
2.60	100.4	423.392	101325
20.99	404.0	298.15	580.7
26.9	602.6		
34.59	722.6	data calc. from Cox eq.	
		eq. 5	P/kPa
mp/°C	–53.7	A ₀	2.94690
		A ₁	2.051933×10^{-3}
eq. 1a	P/mmHg	A ₂	1.903683×10^{-6}
A	20.8468	with reference state at	
B	–5811.26	P ₀ /kPa	101.325
		T ₀ /K	423.392

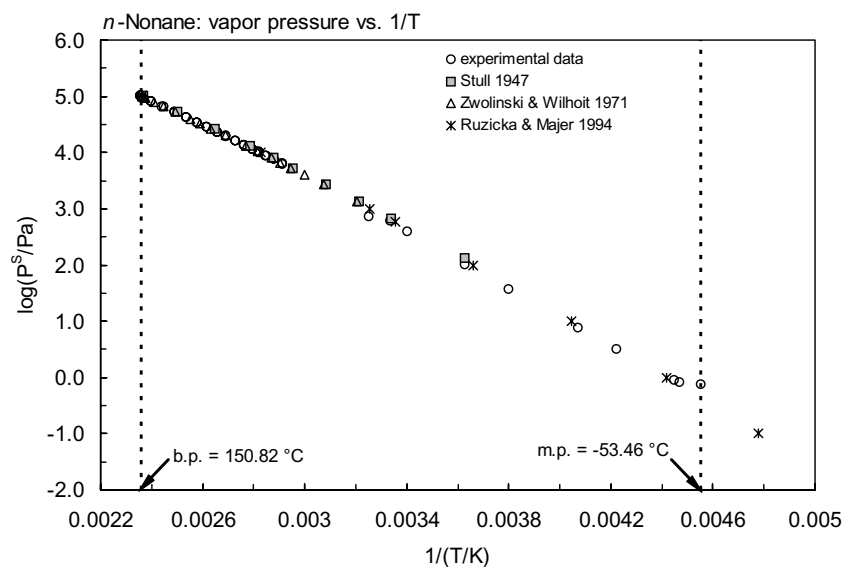


FIGURE 2.1.1.1.25.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-nonane.

TABLE 2.1.1.1.25.3

Reported Henry's law constants of *n*-nonane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$\ln [H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4)		
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Jönsson et al. 1982		Ashworth et al. 1988	
equilibrium cell-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
14.8	244287	10	40530
14.8	221668	15	50257
15.0	237196	20	33640
20.0	348179	25	41949
20.05	369343	30	47116
20.05	363831		
		eq. 4a	H/(atm m ³ /mol)
		A	-0.1847
		B	202.1

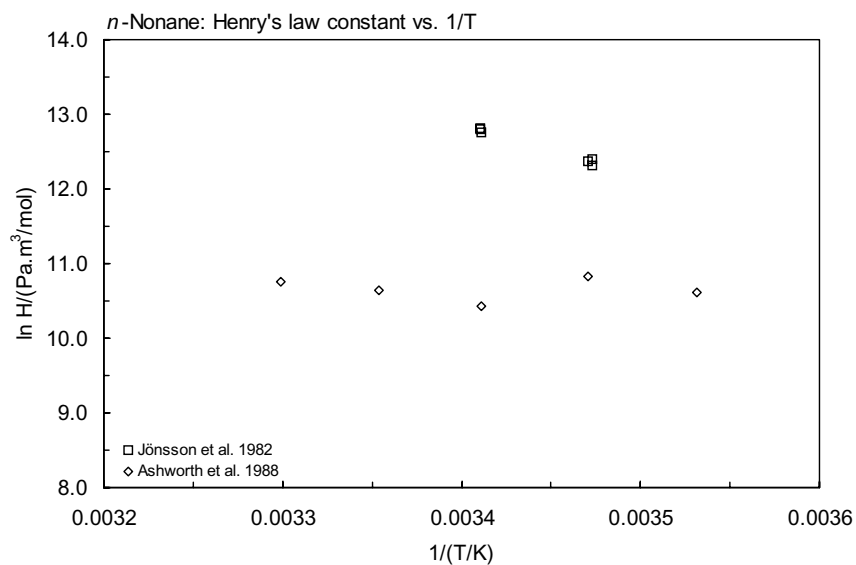
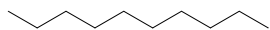


FIGURE 2.1.1.1.25.3 Logarithm of Henry's law constant versus reciprocal temperature for *n*-nonane.

2.1.1.1.26 *n*-DecaneCommon Name: *n*-Decane

Synonym: decane

Chemical Name: *n*-decane

CAS Registry No: 124-18-5

Molecular Formula: $C_{10}H_{22}$; $CH_3(CH_2)_8CH_3$

Molecular Weight: 142.282

Melting Point ($^{\circ}C$):

-29.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

174.15 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.7301, 0.7273 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)0.7301, 0.7264 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)Molar Volume (cm^3/mol):194.9, 195.9 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

229.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):51.367, 31.279 ($25^{\circ}C$, bp, Riddick et al. 1986)

51.42 (209.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.72 (Dreisbach 1959)

28.677 (Riddick et al. 1986)

28.7 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

117.99, 109.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.016 (radiotracer, Baker 1958, 1959)

0.0198 (shake flask-GC, Franks 1966)

0.022 (Baker 1967)

0.052 (shake flask-GC, McAuliffe 1969)

0.0087 (shake flask-GC, Krasnoshchekova & Gubertritis 1973)

0.182, 1.220 (shake flask-headspace-GC, Mackay et al. 1975)

0.0029 (shake flask-refractometer, Becke & Quitzsch 1977)

0.0524 (shake flask-GC, Coates et al. 1985)

0.02, 0.015 ($20^{\circ}C$, $25^{\circ}C$, tentative best values, IUPAC Solubility Data Series, Shaw 1989)0.0277, 0.0261 ($20^{\circ}C$, $25^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, temp range 273.2–422.7 K, Mączyński et al. 2004)Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):62.66* ($8.50^{\circ}C$, static-McLeod gauge, measured range -3.80 to $8.50^{\circ}C$, Linder 1931)7649* ($94.481^{\circ}C$, ebulliometry, measured range 94.481 – $175.121^{\circ}C$, Willingham et al. 1945) $\log(P/mmHg) = 6.95367 - 1501.268/(194.480 + t/^{\circ}C)$; temp range 94.6 – $175.1^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)238* (calculated-Antoine eq. regression, temp range 17.1 – $173^{\circ}C$, Stull 1947)

182 (extrapolated-Antoine eq., Dreisbach 1959)

 $\log(P/mmHg) = 6.95367 - 1501.268/(194.480 + t/^{\circ}C)$; temp range 75 – $210^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)180* (extrapolated-Antoine eq., temp range 57.7 – $202.9^{\circ}C$, Zwolinski & Wilhoit 1971)

- $\log (P/\text{mmHg}) = 6.95367 - 1501.268/(194.480 + t/^{\circ}\text{C})$; temp range 57.7–202.9°C (Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = [-0.2185 \times 10912.0/(T/\text{K})] + 8.248089$; temp range 17.1–173°C (Antoine eq., Weast 1972–73)
 86.53* (16.74°C, gas saturation, measured range –29.65 to 37.45°C, Carruth & Kobayashi 1973)
 174 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.08321 - 1504.405/(194.831 + t/^{\circ}\text{C})$; temp range 94.48–175.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 173 (extrapolated-Antoine eq., temp range 58–203°C, Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 6.94365 - 1495.17/(193.86 + t/^{\circ}\text{C})$; temp range 58–203°C (Antoine eq., Dean 1985, 1992)
 180* (24.941°C, gas saturation, measured temp range 298.091–347.887 K, Allemand et al. 1986)
 170 (lit. average, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 5.55216 - 1594.49/(126.36 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 171 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.80914 - 1900.343/(-47.319 + T/\text{K})$; temp range 252–383 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.09206 - 1510.415/(-77.646 + T/\text{K})$; temp range 373–443 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.04899 - 1482.502/(-80.635 + T/\text{K})$; temp range 447–526 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 9.71412 - 6858.314/(454.63 + T/\text{K})$; temp range 524–617 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 874.1* (50.64°C, static-quartz pressure gauge, measured range 50.64–314.982°C, Morgan & Kobayashi 1994)
 182* (recommended, Ruzicka & Majer 1994)
 $\ln [(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/\text{K})/(T/\text{K})] \cdot \exp\{2.96690 - 1.932579 \times 10^{-3} \cdot (T/\text{K}) + 1.644626 \times 10^{-6} \cdot (T/\text{K})^2\}$; reference state at $P_o = 101.325 \text{ kPa}$, $T_o = 447.269 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log (P/\text{mmHg}) = 26.5125 - 3.3584 \times 10^3/(T/\text{K}) - 6.1174 \cdot \log (T/\text{K}) - 3.3225 \times 10^{-10} \cdot (T/\text{K}) + 4.8554 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 243–618 K (vapor pressure eq., Yaws 1994)
 127.6* (20°C, ebulliometer and inclined piston gauge, measured temp range 268–490 K. Chirico et al. 1989)
 324 (liquid P_L , GC-RT correlation; Donovan 1996)
 520* (41.6°C, ebulliometry, measured range 314.75–458.45 K, Dejoz et al. 1996)
 $\ln (P/\text{kPa}) = 13.9735 - 3441.40/[(T/\text{K}) - 79.434]$; temp range 314.75–458.45 K (ebulliometry, Dejoz et al. 1996)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 326300 (calculated-P/C, Mackay & Shiu 1975)
 499500 (calculated-P/C, Bobra et al. 1979; Mackay et al. 1979; selected, Mills et al. 1982)
 489400 (calculated-P/C, Mackay 1981)
 700000; 500000, 108000 (recommended; calculated-P/C, Mackay & Shiu 1981)
 431100 (calculated-P/C, Eastcott et al. 1988)
 477870 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.67 (estimated-fragment const., Lyman 1982)
 6.69, 5.98 (estimated-HPLC/MS, calculated-fragment const., Burkhard et al. 1985)
 5.01 (estimated, Coates et al. 1985)
 6.25 \pm 0.70 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (11.4 \pm 0.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $299 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1982a, 1984c)

$k_{OH} = 11.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)

$k_{OH} = 1.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1991)

$k_{OH} = 11.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , atmospheric lifetime of 12 h during summer daylight (Altshuller 1991)

$k_{NO_3}(\text{exptl}) = 2.59 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}(\text{calc}) = 2.47 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm \text{K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{OH}^* = 11.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 2.8 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ for C_4H_{10} and higher paraffins for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction rate constant $k = 1.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radical with an estimated lifetime of 12 h during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.26.1

Reported vapor pressures of *n*-decane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log(T/K) & (4) \\ \ln(P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2) & (5) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \ln P = A - B/(C + T/K) & (3a) \end{array}$$

1.

Linder 1931		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static-McLeod gauge		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-3.80	22.0	94.481	7649	17.1	133.3	57.6	1333
0.20	28.0	98.352	8954	42.5	666.6	71.06	2666
0.50	30.66	101.859	10292	55.4	1333	79.61	4000
8.50	62.66	105.118	11686	69.1	2666	86.02	5333
		109.526	13812	84.6	5333	91.20	6666
		114.540	16609	94.6	7999	95.576	7999
		119.640	19913	108.0	13332	102.759	10666
		124.372	23451	127.8	26664	108.579	13332
		130.690	28951	149.9	53329	119.759	19998
		136.490	34892	173.0	101325	128.203	26664

(Continued)

TABLE 2.1.1.1.26.1 (Continued)

Linder 1931		Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
static-McLeod gauge		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		143.495	43318	mp/°C	−29.7	135.071	33331
		150.718	53654			140.903	39997
		158.419	66757			150.535	53329
		166.772	83722			158.39	66661
		172.661	97609			165.088	79993
		173.295	99206			170.947	93326
		173.882	100701			172.039	95992
		174.538	102401			173.106	98659
		175.121	103921			174.152	101325
		bp/°C	174.123			eq. 2	P/mmHg
						A	6.95375
		eq. 2	P/mmHg			B	1508.75
		A	6.95367			C	193.374
		B	1501.268			bp/°C	174.152
		C	194.480			ΔH_v /(kJ mol ^{−1})	
		temp range: 94.5–175.1°C				at 25°C	51.37
						at bp	39.28

2.

Carruth & Kobayashi 1973		Allemand et al. 1986		Chirico et al. 1989			
gas saturation		gas saturation		ebulliometry		inclined piston gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−29.65	1.72	24.941	180.0	100.086	9596	−5.002	17.0
−21.84	3.20	30.022	253.3	103.317	10897	−0.002	26.4
−18.68	4.586	35.019	352.0	106.561	12348	9.994	59.9
−9.54	10.60	40.005	481.3	109.82	13961	19.999	127.6
4.35	33.20	45.002	650.6	113.09	15752	30.001	256.1
16.74	86.53	50.006	874.6	116.373	17737	34.999	355.0
31.45	186.7	55.001	1161	119.67	19933	40.0	486.3
37.45	205.3	59.996	1520	126.299	25023	44.0	657.8
		64.916	1969	132.983	31177	50.0	879.9
mp/°C	−29.71	70.049	2545	139.716	39565	60.006	1523.8
		74.737	3190	146.502	47375	80.002	2536.1
eq. 1a	P/mmHg			153.399	57817	75.001	3227.1
A	20.8865			160.227	70120		
B	6170.32			167.167	84533		
				174.157	101325	Cox eq.	
				181.199	120790	eq. 5a	P/kPa
				188.291	143250	P _{ref} /kPa	101.325
				195.43	169920	T _{ref} /K	447.307
				202.622	198490	a	2.96081
				209.859	232020	10 ³ b/K ^{−1}	−1.90111
				217.142	270020	10 ⁶ c/K ^{−2}	1.60359
						temp range: 268–490 K	

TABLE 2.1.1.1.26.1 (Continued)

3.

Morgan & Kobayashi 1994		Ruzicka & Majer 1994		Dejor et al. 1996			
static-quartz pressure gauge		recommended		vapor-liquid equilibrium			
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	P/Pa
50.64	874.1	222.67	0.1	41.6	520	144.1	44090
59.933	1509	240.65	1.0	45.2	650	146.7	47640
79.938	4050	262.50	10	49.5	840	149.3	51420
99.970	9562	289.84	100	55.2	1170	151.2	54380
119.981	20150	325.64	1000	60.1	1520	153.4	57920
119.971	20154	374.25	10000	69.1	2410	156.5	63220
139.972	38892	447.27	101325	75.8	3330	159.3	69330
159.973	69695	298.15	182.0	84.2	4900	162.3	74190
179.974	117250			93.1	7200	165.5	80890
199.976	187250	Cox eq.		97.9	8760	168.4	87350
219.976	285770	eq. 5	P/kPa	100.7	9820	174.6	102460
239.979	420380	P _{ref} /kPa	101.325	103.5	10970	178.9	114160
259.979	598790	T _{ref} /K	447.27	105.9	12020	182.7	125370
279.98	830150	a	2.96690	108.3	13180	185.3	133470
299.98	1125900	10 ³ b/K ⁻¹	-1.932579	110.	14250		
314.982	1395000	10 ⁶ c/K ⁻²	1.644626	113.3	15870	eq. 3(a)	P/kPa
				117.1	18200	A	13.9735
				121.8	21470	B	3441.40
				126.6	25280	C	-79.434
				129.4	27750	temp range 315–458 K	
				133.4	31600		
				137.2	35660		
				141.9	41250		

data fitted to Wagner eq.

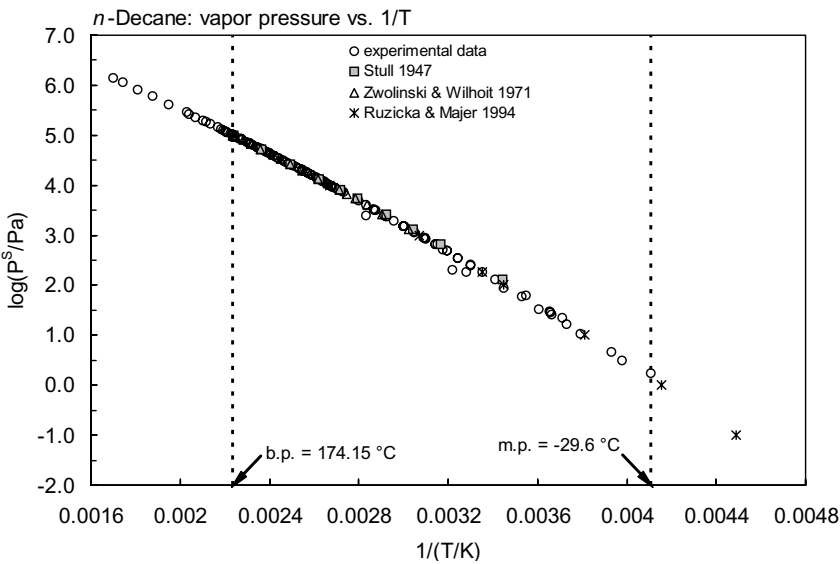
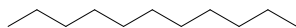


FIGURE 2.1.1.1.26.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-decane.

2.1.1.1.27 *n*-UndecaneCommon Name: *n*-Undecane

Synonym: undecane

Chemical Name: *n*-undecane

CAS Registry No: 1120-21-4

Molecular Formula: $C_{11}H_{24}$; $CH_3(CH_2)_9CH_3$

Molecular Weight: 156.309

Melting Point ($^{\circ}C$):

-25.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

195.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.74024, 0.73652 ($20^{\circ}C$, $25^{\circ}C$, Camin & Rossini 1955)0.7402, 0.7366 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)Molar Volume (cm^3/mol):211.2 ($20^{\circ}C$, calculated-density)

251.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):56.5, 41.524 ($25^{\circ}C$, bp, Dreisbach 1959)

56.58 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):6.86, 22.18, 29.03 (-36.55 , $-25.55^{\circ}C$, total phase change enthalpy, Chickos et al. 1999)Entropy of Fusion, ΔS_{fus} (J/mol K):

118.6, 119.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0044 (shake flask-GC, McAuliffe 1969)

0.0036 (shake flask-GC, Krashoshchekova & Gubertritis 1973)

0.0040 ("best" value, IUPAC Solubility Data Series, Shaw 1989)

0.0042 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($31.4^{\circ}C$, summary of literature data, temp range 31.4 – $194.5^{\circ}C$, Stull 1947)
 $\log(P/mmHg) = 6.97674 - 1572.477/(188.022 + t/^{\circ}C)$; temp range 105.4 – $197.3^{\circ}C$ (Antoine eq., ebulliometry-manometer measurement, Camin & Rossini 1955)

57.18 (extrapolated-Antoine eq., Dreisbach 1959)

 $\log(P/mmHg) = 6.97674 - 1572.477/(188.022 + t/^{\circ}C)$; temp range 98 – $258^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)
52.20* (extrapolated-Antoine eq., temp range 75.1 – $225.8^{\circ}C$, Zwolinski & Wilhoit 1971)
 $\log(P/mmHg) = 6.97220 - 1569.57/(187.700 + t/^{\circ}C)$; temp range 75.1 – $225.8^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

 $\log(P/mmHg) = [-0.2185 \times 11481.7/(T/K)] + 8.260477$; temp range 31.4 – $194.5^{\circ}C$ (Antoine eq., Weast 1972–73)

52.5 (extrapolated-Antoine eq., Boublik et al. 1984)

 $\log(P/kPa) = 6.12013 - 1572.031/(188.062 + t/^{\circ}C)$; temp range 104.5 – $197.3^{\circ}C$ (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)

 $\log(P/mmHg) = 6.97220 - 1569.57/(187.70 + t/^{\circ}C)$; temp range 75 – $226^{\circ}C$ (Antoine eq., Dean 1985, 1992)

54.8 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

 $\log(P_L/kPa) = 6.10154 - 1572.411/(-85.128 + T/K)$; temp range 278 – 470 K (Antoine eq., Stephenson & Malanowski 1987)

56.89* (recommended, Ruzicka & Majer 1994)

$\ln [(P/\text{kPa})/(P_0/\text{kPa})] = [1 - (T_0/K)/(T/K)] \cdot \exp\{3.02771 - 2.045579 \times 10^{-3} \cdot (T/K) + 1.712658 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_0 = 101.325 \text{ kPa}$, $T_0 = 469.042 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)

$\log (P/\text{mmHg}) = 82.9230 - 5.6085 \times 10^3/(T/K) - 23.7327 \cdot \log (T/K) + 1.0469 \times 10^{-2} \cdot (T/K) + 7.087 \times 10^{-13} \cdot (T/K)^2$; temp range 248–639 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

185000 (calculated-P/C, Mackay & Shiu 1981)

185390 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

6.94 (estimated-HPLC/MS, Burkhard et al. 1985)

6.51 (calculated-fragment const., Burkhard et al. 1985)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 13.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)

$k_{\text{OH}} = 1.32 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}} = 1.29 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 2.1.1.1.27.1

Reported vapor pressures of *n*-undecane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$	(5) - Cox eq.						
Stull 1947	Camin & Rossini 1955	Zwolinski & Wilhoit 1971	Ruzicka & Majer 1994				
summary of literature data	ebulliometry	selected values	recommended				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
31.4	133.3	104.58	5540	75.1	1333	236.04	0.1
58.4	666.6	110.952	8287	89.06	2666	254.71	1.0
72.2	1333	115.522	8337	97.93	4000	277.39	10
86.3	2666	118.963	9358	104.58	5333	305.75	100
103.1	5333	122.607	10954	109.95	6666	342.64	1000
113.9	7999	127.467	13104	114.486	7999	393.33	10000
126.8	13332	132.757	15837	121.934	10666	469.04	101325

(Continued)

TABLE 2.1.1.1.27.1 (Continued)

Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Ruzicka & Majer 1994	
summary of literature data		ebulliometry		selected values		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
148.0	26664	138.713	19448	127.969	13332	298.15	56.89
170.6	53329	143.585	22889	139.559	19998		
194.5	101325	150.437	28550	148.312	26664	Cox eq.	
mp/°C		156.841	34826	155.431	33331	eq. 5	P/kPa
		164.039	43031	161.475	39997	P _{ref} /kPa	101.325
		171.724	53780	171.458	53329	T _{ref} /K	469.64
		179.802	67077	179.603	66661	a	3.02711
		188.431	84053	186.537	79993	10 ³ b/K ⁻¹	-2.045579
		194.595	98132	192.608	93326	10 ⁶ c/K ⁻²	1.712658
		195.242	101081	193.739	95992		
		196.511	102882	194.845	98659		
		197.272	104822	195.928	101325		
		bp/°C	195.890	bp/°C	195.928		
		eq. 2	P/mmHg	eq. 2	P/mmHg		
		A	6.97674	A	6.97220		
		B	1572.477	B	1569.57		
		C	188.022	C	187.700		
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	
						at bp	

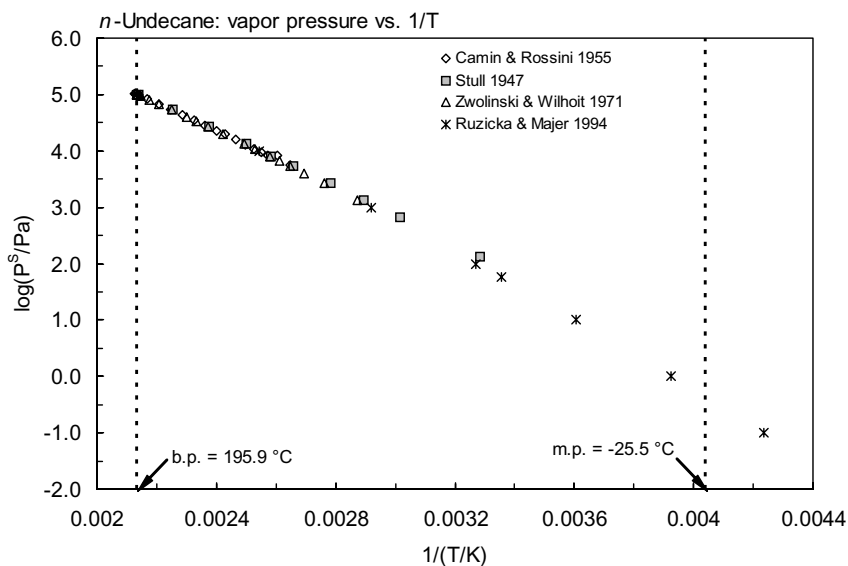


FIGURE 2.1.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-undecane.

2.1.1.1.28 *n*-DodecaneCommon Name: *n*-Dodecane

Synonym: dodecane

Chemical Name: *n*-dodecane

CAS Registry No: 112-40-3

Molecular Formula: $C_{12}H_{26}$; $CH_3(CH_2)_{10}CH_3$

Molecular Weight: 170.334

Melting Point ($^{\circ}C$):

-9.57 (Lide 2003)

Boiling Point ($^{\circ}C$):

216.32 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.7487, 0.7452 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)0.74941 ($20^{\circ}C$, densimeter, Dejoz et al. 1996)Molar Volume (cm^3/mol):227.5 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

273.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):61.287, 43.64 (25° , bp, Riddick et al. 1986)

61.52 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.84 (Dreisbach 1959)

35.86 (Riddick et al. 1986)

36.82 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

139.75, 128.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0084 (shake flask-GC, Franks 1966)

0.0034 (shake flask-GC, McAuliffe 1969)

0.0037 (shake flask-GC, Sutton & Calder 1974)

0.0037 (recommended, IUPAC Solubility Data Series, Shaw 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6365* ($126.31^{\circ}C$, ebulliometry, measured range 126.31 – $217.345^{\circ}C$, Willingham et al. 1945)
 $\log(P/mmHg) = 6.98059 - 1625.928/(180.311 + t/^{\circ}C)$; temp range 126.4 – $217.3^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
133.3* ($47.7^{\circ}C$, summary of literature data, temp range 47.7 – $214.5^{\circ}C$, Stull 1947)

17.60 (extrapolated-Antoine eq., Dreisbach 1959)

 $\log(P/mmHg) = 6.98059 - 1625.928/(180.311 + t/^{\circ}C)$; temp range 150 – $280^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)
15.70* (extrapolated-Antoine eq., temp range 91.47 – $247.08^{\circ}C$, Zwolinski & Wilhoit 1971)

7.60 (derived from compiled data, Zwolinski & Wilhoit 1971)

 $\log(P/mmHg) = 6.99795 - 1639.27/(181.835 + t/^{\circ}C)$; temp range 91.47 – $247.08^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

 $\log(P/mmHg) = [-0.2185 \times 11857.7/(T/K)] + 8.150997$; temp range 47.7 – $345.8^{\circ}C$ (Antoine eq., Weast 1972–73)

15.5 (Antoine eq., Boublik et al. 1973, 1984)

 $\log(P/mmHg) = 6.9829 - 1627.714/(180.521 + t/^{\circ}C)$; temp range 104.5 – $197.3^{\circ}C$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1973)

32.53 (calculated-bp, Mackay et al. 1982)

$\log (P/\text{kPa}) = 6.1074 - 1627.417/(180.489 + t/^{\circ}\text{C})$; temp range 104.5–197.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 6.99795 - 1639.27/(181.84 + t/^{\circ}\text{C})$; temp range 91–247°C (Antoine eq., Dean 1985, 1992)
 17.3* (24.931°C, gas saturation, measured temp range 298.081–389.66 K, Allemand et al. 1986)
 16.0 (lit. average, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.12285 - 1639.27/(181.835 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 18.6 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.62064 - 1942.122/(-65.587 + T/\text{K})$; temp range 278–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.12285 - 1639.27/(-91.315 + T/\text{K})$; temp range 400–492 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 18.40, 18.67* (25.30, 25.35°C, electronic manometry, measured range –9.27 to 98.10°C, Sasse et al. 1988)
 733.8* (79.969°C, static-differential pressure, measured range 79.969–314.982°C, Morgan & Kobayashi 1994)
 18.02 (recommended, Ruzicka & Majer 1994)
 $\ln [(P/\text{kPa})/(P_0/\text{kPa})] = [1 - (T_0/\text{K})/(T/\text{K})] \cdot \exp\{3.05854 - 2.018454 \times 10^{-3} \cdot (T/\text{K}) + 1.606849 \times 10^{-6} \cdot (T/\text{K})^2\}$;
 reference state at $P_0 = 101.325 \text{ kPa}$, $T_0 = 489.438 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log (P/\text{mmHg}) = -5.6532 - 3.4698 \times 10^3/(T/\text{K}) + 9.0272 \cdot \log (T/\text{K}) - 2.3185 \times 10^{-2} \cdot (T/\text{K}) + 1.1235 \times 10^{-5} \cdot (T/\text{K})^2$;
 temp range 264–658 K (vapor pressure eq., Yaws 1994)
 14.1; 17.8 (liquid P_L , GC-RT correlation; quoted lit., Donovan 1996)
 440* (71.6°C, ebulliometry, measured range 344.25–501.55 K, Dejoz et al. 1996)
 $\ln (P/\text{kPa}) = 14.1090 - 3781.84/[(T/\text{K}) - 90.975]$; temp range 344.25–501.55 K (ebulliometry, Dejoz et al. 1996)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

723000 (calculated-P/C, Bobra et al. 1979)
 723000, 786000, 317000; 750000 (calculated-P/C values; recommended, Mackay & Shiu 1981)
 721400 (selected, Mills et al. 1982)
 726900 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.24, 7.04 (estimated-HPLC/MS, calculated-fragment const., Burkhard et al. 1985)
 6.10 (Coates et al. 1985)
 6.80 \pm 1.00 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization: rate constants: $k = 0.60 \text{ d}^{-1}$, $t_{1/2} = 1.1 \text{ d}$ in spring at 8–16°C, $k = 0.97 \text{ d}^{-1}$, $t_{1/2} = 0.7 \text{ d}$ in summer at 20–22°C, $k = 0.20 \text{ d}^{-1}$, $t_{1/2} = 3.6 \text{ d}$ in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.377 \text{ d}^{-1}$, $t_{1/2} = 1.8 \text{ d}$ with HgCl_2 , and $k = 1.085 \text{ d}^{-1}$, $t_{1/2} = 0.64 \text{ d}$ without HgCl_2 in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 15.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)

$k_{OH} = 14.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = 13.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: Surface water: estimated $t_{1/2} = 0.5$ d for surface waters in case of first order reduction process (Zoeteman et al. 1980)

marine mesocosm $t_{1/2} = 1.1$ d at 8–16°C in spring, $t_{1/2} = 0.7$ d at 20–22°C in summer and $t_{1/2} = 3.6$ h at 3–7°C in winter when volatilization dominates, and $t_{1/2} = 1.8$ d with HgCl_2 as poison, and $k = 1.085 \text{ d}^{-1}$, $t_{1/2} = 0.64$ d without poison in mid-September (Wakeham et al. 1983)

TABLE 2.1.1.1.28.1

Reported vapor pressures of *n*-dodecane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)	$\ln P = A - B/(T/K)$	(1a)
$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$	(5) - Cox eq.		

1.

Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971		Allemand et al. 1986	
ebulliometry		summary of literature data		selected values		gas saturation	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
126.31	6365	47.7	133.3	91.47	1333	24.931	17.33
131.108	7663	75.7	666.6	105.91	2666	28.95	24.66
135.223	8971	89.9	1333	115.09	4000	29.966	26.66
138.962	10306	104.3	2666	121.96	5333	35.043	40.00
142.444	11696	121.4	5333	127.521	6666	40.023	58.13
147.152	13816	131.7	7999	132.213	7999	40.29	60.26
152.529	16611	145.5	13332	139.915	10666	45.023	84.79
157.986	19917	165.8	26664	146.153	13332	49.978	120.5
163.030	23443	188.4	53329	158.131	19998	50.0	118.8
169.814	28948	214.5	101325	167.175	26664	55.32	170.7
176.039	34896			174.527	33331	59.936	232.0
183.537	43331	mp/ $^{\circ}\text{C}$	−9.6	180.769	39997	64.936	310.6
191.255	53654			191.075	53329	69.23	409.3
199.488	66750			199.481	66661	70.093	422.6
208.417	83701			206.636	79993	74.947	558.6
214.709	97594			212.898	93326	78.83	691.9
215.303	99189			214.065	95992	80.174	745.3
216.006	100671			215.206	98659	99.87	2013
216.712	102385			216.323	101325	116.5	4258
217.345	103910						
bp/ $^{\circ}\text{C}$	216.278			bp/ $^{\circ}\text{C}$	216.323		
eq. 2	P/mmHg			eq. 2	P/mmHg		
A	6.98059			A	6.97220		
B	1625.928			B	1639.27		
C	180.311			C	181.835		
				$\Delta H_v/(\text{kJ mol}^{-1}) =$			
				at 25 $^{\circ}\text{C}$	61.59		
				at bp	43.64		

(Continued)

TABLE 2.1.1.1.28.1 (Continued)

2.

Sasse et al. 1988				Dejoz et al. 1996		Ruzicka & Majer 1994	
electronic manometry				vapor-liquid equilibrium		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
-9.27	0.587	92.17	1380	71.2	440	248.34	0.1
-3.94	1.069	95.15	1599	75.6	570	267.74	1.0
0.49	1.720	98.10	1847	81.6	800	291.28	10
5.48	2.986			86.7	1040	320.68	100
5.53	2.920	eq. 2	P/mmHg	91.1	1310	358.87	1000
10.47	4.800	A	1.17283	98.2	1860	411.27	10000
15.41	6.906	B	1766.802	102	2230	489.44	101325
15.46	7.706	C	194.662	106.8	2780	298.15	18.02
20.35	12.36			111.2	3380		
20.38	12.05			118.5	4430	Cox eq.	
25.30	18.40	Morgan & Kobayashi 1994 static-differential pressure gauge		122.9	5540	eq. 5	P/kPa
25.35	18.67			126.5	6380	P _{ref} /kPa	101.325
30.27	27.60			130.6	7520	T _{ref} /K	489.438
30.30	28.13	t/°C	P/Pa	135.2	8960	a	3.05854
35.27	40.80	79.969	733.8	143	11930	10 ³ b/K ⁻¹	-2.018454
35.30	41.33	99.970	2031	149.5	14980	10 ⁶ c/K ⁻²	1.606849
40.25	59.33	119.921	4912	154.8	17930		
40.30	60.13	139.927	10690	160.8	21810		
45.15	84.93	159.973	21248	166.1	25800		
45.22	85.86	179.974	39125	171.0	29990		
50.04	119.3	199.975	67572	175.7	34530		
50.18	121.2	219.976	110500	180.8	40060		
55.02	164.9	239.976	172410	183.3	42990		
55.12	167.3	259.979	258710	186.0	46390		
60.08	227.0	279.980	375270	189.8	51530		
60.12	230.4	299.981	528820	193.2	56510		
65.11	313.2	314.982	671130	197.6	63480		
70.09	420.2			200.0	67570		
75.08	558.4	data fitted to Wagner eq.					
76.68	612.2		see ref.	eq. 3(a)	P/kPa		
80.12	735.8			A	14.1090		
82.10	820.0			B	3781.84		
85.11	949.1			C	-90.975		
87.26	1069			temp range 345–502 K			

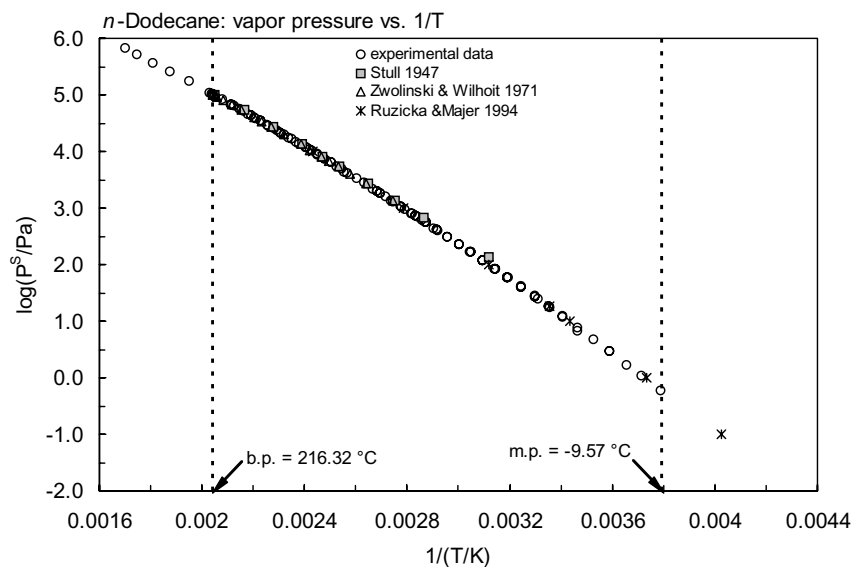


FIGURE 2.1.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-dodecane.

2.1.1.1.29 *n*-Tridecane

Common Name: Tridecane

Synonym:

Chemical Name: *n*-tridecane

CAS Registry No: 629-50-5

Molecular Formula: $C_{13}H_{28}$; $CH_3(CH_2)_{11}CH_3$

Molecular Weight: 184.361

Melting Point ($^{\circ}C$):

-5.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

235.47 (Lide 2003)

Density (g/cm^3):0.76522, 0.75270 (20 $^{\circ}C$, 25 $^{\circ}C$, Camin & Rossini 1955)0.7564, 0.7528 (20 $^{\circ}C$, 25 $^{\circ}C$, Dreisbach 1959)Molar Volume (cm^3/mol):

296.0 (calculated-Le Bas method at normal boiling point)

243.7 (20 $^{\circ}C$, Stephenson & Malanowski 1987)Enthalpy of Vaporization, ΔH_v (kJ/mol):66.23, 45.65 (25 $^{\circ}C$, bp, Riddick et al. 1986)

66.68 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.501 (Riddick et al. 1986)

7.66, 28.49; 36.15 (-18.15, -5.35 $^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)Entropy of Fusion, ΔS_{fus} (J/mol K):

136.31, 137.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25 $^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

0.00104 (extrapolated from data of McAuliffe 1966, Coates et al. 1985)

0.0047–0.0217 (estimated, Coates et al. 1985)

0.06 (Riddick et al. 1986)

0.33; 0.198 (measured; calculated molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):133.3* (59.4 $^{\circ}C$, summary of literature data, temp range 59.4–234.0 $^{\circ}C$, Stull 1947)5530* (139.3 $^{\circ}C$, ebulliometry, measured range 139.3–236.065 $^{\circ}C$, Camin & Rossini 1955) $\log(P/mmHg) = 7.00339 - 1689.093/(174.284 + t/^{\circ}C)$; temp range 145.1–236.1 $^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Camin & Rossini 1955)

5.30 (extrapolated-Antoine eq., Dreisbach 1959; quoted, Riddick et al. 1986)

 $\log(P/mmHg) = 6.9887 - 1677.43/(172.90 + t/^{\circ}C)$; temp range 131–302 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

5.73* (derived from compiled data, Zwolinski & Wilhoit 1971)

 $\log(P/mmHg) = 7.00756 - 1690.67/(107.20 + t/^{\circ}C)$; temp range 107.2–267.04 $^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971) $\log(P/mmHg) = [-0.2185 \times 12991.3/(T/K)] + 8.481732$; temp range 59.4–234 $^{\circ}C$ (Antoine eq., Weast 197–73)

4.55 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)

 $\log(P/mmHg) = 7.00925 - 1693.684/(t/^{\circ}C + 174.815)$; temp. range 139–236 $^{\circ}C$ (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1973) $\log(P/kPa) = 6.13542 - 1694.624/(t/^{\circ}C + 174.916)$; temp. range 139–236 $^{\circ}C$ (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984) $\log(P/mmHg) = 7.00756 - 1690.67/(174.22 + t/^{\circ}C)$; temp range 107–267 $^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log (P/\text{kPa}) = 6.13246 - 1690.67/(174.220 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P/\text{mmHg}) = 7.00756 - 1690.67/(t/^{\circ}\text{C} + 174.22)$; temp range 107–267°C, (Antoine eq., Dean 1985; 1992)
 $\log (P/\text{kPa}) = 6.13546 - 1690.67/(T/\text{K} - 98.93)$; temp range 417–511 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
 5.682* (recommended, Ruzicka & Majer 1994)
 $\ln [(P/\text{kPa})/(P_0/\text{kPa})] = [1 - (T_0/\text{K})/(T/\text{K})] \cdot \exp\{3.10403 - 2.071819 \times 10^{-3} \cdot (T/\text{K}) + 1.61160 \times 10^{-6} \cdot (T/\text{K})^2\}$; reference state at $P_0 = 101.325 \text{ kPa}$, $T_0 = 508.602 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log (P/\text{mmHg}) = 49.2391 - 4.9649 \times 10^3/(T/\text{K}) - 13.769 \cdot \log (T/\text{K}) - 2.1146 \times 10^{-9} \cdot (T/\text{K}) + 2.5902 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 268–676 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

233351 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

6.65 (HPLC- k' correlation, Coates et al. 1985)

6.50; 6.05 (calculated-fragment const.; calculated-molar volume, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 17.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)

$k_{\text{OH}} = 15.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K, $17.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 302 K (Atkinson 1989)

$k_{\text{OH}} = 16.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 2.1.1.1.29.1

Reported vapor pressures of *n*-tridecane at various temperatures and the coefficients for the vapor pressure equations

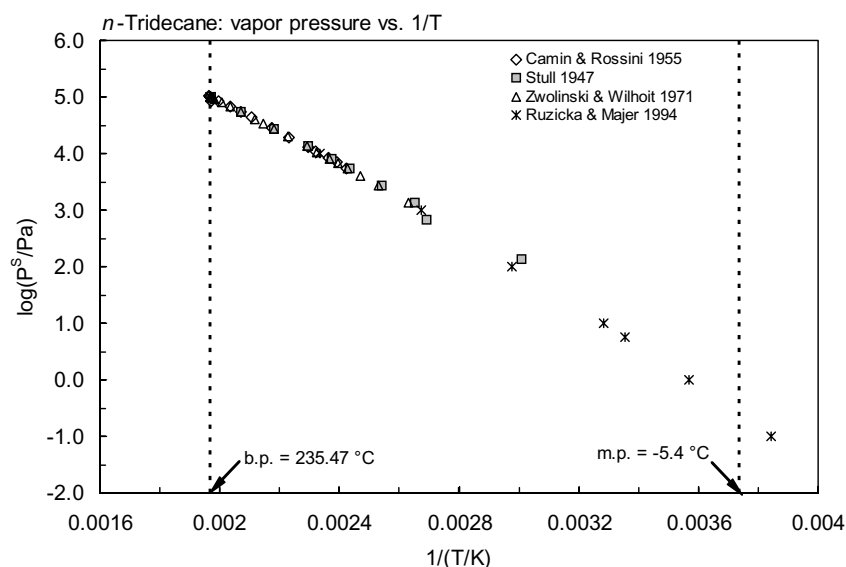
$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$		(5) - Cox eq.	

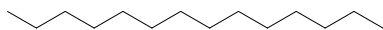
Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Ruzicka & Majer 1994	
summary of literature data		ebulliometry		selected values		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
59.4	133.3	139.3	5530	107.2	1333	260.30	0.1
98.3	666.6	145.16	6931	122.05	2666	280.31	1.0

(Continued)

TABLE 2.1.1.1.29.1 (Continued)

Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Ruzicka & Majer 1994	
summary of literature data		ebulliometry		selected values		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
104.0	1333	150.011	8326	131.48	4000	304.58	10
120.2	2666	157.603	10934	138.55	5333	335.89	100
137.7	5333	162.749	13079	144.258	6666	374.24	1000
148.2	7999	174.699	19416	149.08	7999	428.21	10000
162.5	13332	187.176	28544	156.993	10666	508.60	101325
185.0	26664	201.634	43155	163.404	13332	298.15	5.682
209.4	53329	209.788	53768	175.709	19998		
234.0	101325	218.367	67061	184.998	26664	Cox eq.	
		227.524	84040	192.55	33331	eq. 5	P/kPa
mp/°C	-6.2	234.052	85041	198.96	39997	P _{ref} /kPa	101.325
		235.316	101054	209.543	53329	T _{ref} /K	469.64
		236.065	102829	218.175	66661	a	3.10403
				225.521	79993	10 ³ b/K ⁻¹	-2.071819
				231.95	93326	10 ⁶ c/K ⁻²	1.712658
				233.148	95992		
				234.319	98659		
				235.466	101325		
				25.0	5.73		
				bp/°C	235.466		
				eq. 2	P/mmHg		
				A	7.00756		
				B	1690.67		
				C	174.220		
				ΔH _v /(kJ mol ⁻¹) =			
				at 25°C	66.23		
				at bp	45.65		

FIGURE 2.1.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-tridecane.

2.1.1.1.30 *n*-Tetradecane

Common Name: Tetradecane

Synonym:

Chemical Name: *n*-tetradecane

CAS Registry No: 629-59-4

Molecular Formula: $C_{14}H_{30}$; $CH_3(CH_2)_{12}CH_3$

Molecular Weight: 198.388

Melting Point ($^{\circ}C$):

5.82 (Lide 2003)

Boiling Point ($^{\circ}C$):

253.58 (Lide 2003)

Density (g/cm^3):0.76275, 0.75917 ($20^{\circ}C$, $25^{\circ}C$, Camin & Rossini 1955)0.7628, 0.7593 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)Molar Volume (cm^3/mol):260.1 ($20^{\circ}C$, Stephenson & Malanowski 1987)

318.2 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)

Enthalpy of Vaporization, ΔH_v (kJ/mol):71.13, 47.73 ($25^{\circ}C$, bp, Dreisbach 1961)

71.73 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

45.07 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

161.54, 147.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0069 (shake flask-GC, Frank 1966)

0.00655 (extrapolated, McAuliffe 1966)

0.0022; 0.0017 (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)

0.00033 (shake flask-GC, Coates et al. 1985)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($76.4^{\circ}C$, summary of literature data, temp range 76.4 – $252.5^{\circ}C$, Stull 1947)5532* ($154.860^{\circ}C$, ebulliometry, measured range 154.860 – $254.165^{\circ}C$, Camin & Rossini 1955)
 $\log(P/mmHg) = 7.01245 - 1739.623/(167.534 + t/^{\circ}C)$; temp range 165.9 – $254.2^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Camin & Rossini 1955)

1.56 (extrapolated-Antoine eq., Dreisbach 1959)

 $\log(P/mmHg) = 6.9957 - 1725.46/(165.75 + t/^{\circ}C)$; temp range 147 – $325^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)
1.27* (Antoine eq., temp range 121.80 – $286.0^{\circ}C$, Zwolinski & Wilhoit 1971)

1.867 (derived from compiled data, Zwolinski & Wilhoit 1971)

 $\log(P/mmHg) = 7.01300 - 1740.88/(167.720 + t/^{\circ}C)$; temp range 121.80 – $286.0^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

 $\log(P/mmHg) = [-0.2185 \times 13750.0/(T/K)] + 8.628699$; temp range 76.4 – $252.5^{\circ}C$ (Antoine eq., Weast 1972–73)

1.30 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)

 $\log(P/mmHg) = 7.02216 - 1747.452/(t/^{\circ}C + 168.437)$; temp range 155 – $254^{\circ}C$ (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1973)

 $\log(P/kPa) = 6.14914 - 1749.052/(t/^{\circ}C + 168.611)$; temp range 155 – $254^{\circ}C$ (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.01300 - 1740.88/(t/^\circ\text{C} + 167.72)$; temp. range 112–286°C (Antoine eq., Dean 1985; 1992)
 72.0* (70.01°C, gas saturation, measured temp range 343.16–394.73 K, Allemand et al. 1986)
 $\log (P_L/\text{kPa}) = 6.62828 - 2063.84/(T/\text{K} - 77.378)$; temp range 313–433 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.1379 - 1740.88/(T/\text{K} - 105.43)$; temp. range 432–529 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
 442.9* (99.926°C, static-differential pressure, measured range 99.926–314.982°C, Morgan & Kobayashi 1994)
 1.804* (recommended, Ruzicka & Majer 1994)
 $\ln [(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/K)/(T/K)] \cdot \exp\{3.13624 - 2.063853 \times 10^{-3} \cdot (T/K) + 1.541507 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_o = 101.325 \text{ kPa}$, $T_o = 526.691 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log (P/\text{mmHg}) = 106.1056 - 7.3461 \times 10^3/(T/\text{K}) - 31.5195 \cdot \log (T/\text{K}) + 1.2356 \times 10^{-2} \cdot (T/\text{K}) - 8.3955 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 279–692 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

347000 (calculated-P/C, Mackay & Shiu 1981)
 387000 (calculated-P/C, Eastcott et al. 1988)
 114497 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.20 (HPLC-k' correlation, Coates et al. 1985)
 7.88, 8.10 (RP-HPLC-MS correlation, Burkhard et al. 1985)
 7.00; 6.45 (calculated-fragment const.; calculated-molar volume, Wang et al. 1992)
 8.0 (recommended, Sangster 1989, 1993)
 6.49 (calculated-UNIFAC, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 19.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)

$k_{OH} = 19.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K (Atkinson 1989)

$k_{OH} = 19.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{OH} = 18.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation: microbial degradation $t_{1/2} < 15 \text{ d}$ by *Pseudomonas sp.* (Setti et al. 1993)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 2.1.1.1.30.1

Reported vapor pressures of *n*-tetradecane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

$$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2) \quad (5) - \text{Cox eq.}$$

1.

Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Allemand et al. 1986	
summary of literature data		ebulliometry		selected values		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
76.4	133.3	154.860	5532	121.8	1333	70.01	71.99
106.0	666.6	165.911	6325	137.06	2666	70.45	74.53
120.7	1333	173.737	10928	146.75	4000	80.0	136.8
135.6	2666	191.234	19417	154.01	5333	91.0	262.7
152.7	5333	204.019	28546	159.881	6666	106.78	634.6
164.0	7999	218.84	43156	164.836	7999	121.58	1324
178.5	13332	236.013	67061	172.967	10666		
201.8	26664	245.408	84041	179.553	13332		
226.8	53329	252.104	98106	192.196	19998		
252.5	101325	253.401	101061	201.739	26664		
		254.165	102850	209.497	33331		
mp/°C	5.5			216.082	39997		
		bp/°C	253.516	226.953	53329		
				235.819	66661		
				243.364	79993		
				249.967	93326		
				251.197	95992		
				252.4	98659		
				253.577	101325		

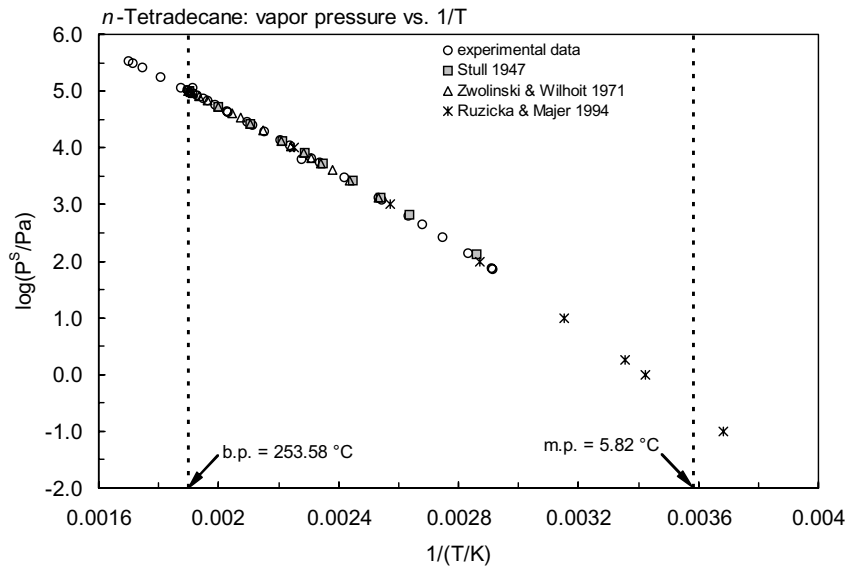
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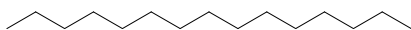
TABLE 2.1.1.1.30.1 (Continued)

2.

Morgan & Kobayashi 1994		Ruzicka & Majer 1994	
differential pressure gauge		recommended	
t/°C	P/Pa	T/K	P/Pa
99.926	442.9	271.60	0.1
119.936	1227	292.22	1.0
139.946	3026	317.21	10
159.956	6693	348.38	100
179.965	13526	388.82	1000
199.976	25267	444.22	10000
219.976	44274	526.69	101325
229.964	57442	298.15	1.804
239.977	73530		
249.979	93059	Cox eq.	
259.979	116500	eq. 5	P/kPa
249.979	116520	P _{ref} /kPa	101.325
279.980	177570	T _{ref} /K	526.691
299.980	261560	a	3.13624
309.982	314050	10 ³ b/K ⁻¹	-2.063853
314.982	343450	10 ⁶ c/K ⁻²	1.541507

data fitted to Wagner eq.

FIGURE 2.1.1.1.30.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-tetradecane.

2.1.1.1.31 *n*-Pentadecane

Common Name: Pentadecane

Synonym:

Chemical Name: *n*-pentadecane

CAS Registry No: 629-62-9

Molecular Formula: $C_{15}H_{32}$; $CH_3(CH_2)_{13}CH_3$

Molecular Weight: 212.415

Melting Point ($^{\circ}C$):

9.95 (Lide 2003)

Boiling Point ($^{\circ}C$):

270.6 (Camin & Rossini 1955; Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

0.76830, 0.76488 (20 $^{\circ}C$, 25 $^{\circ}C$, Camin & Rossini 1955)

0.7685, 0.7650 (20 $^{\circ}C$, 25 $^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

276.4 (20 $^{\circ}C$, calculated-density)

340.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

76.16, 49.41 (25 $^{\circ}C$, bp, Dreisbach 1961)

76.77 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.17, 34.6; 43.77 (–2.25, 9.95; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

156.02, 156.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25 $^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

7.6×10^{-5} (extrapolated from data of McAuliffe 1966, Coates et al. 1985)

0.0612; 0.0613 (measured; calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* (91.6 $^{\circ}C$, summary of literature data, temp range 91.6–270.5 $^{\circ}C$, Stull 1947)

5532* (169.686 $^{\circ}C$, ebulliometry, measured range 169.686–270.449 $^{\circ}C$, Camin & Rossini 1955)

$\log(P/mmHg) = 7.02445 - 1789.658/(161.291 + t/^{\circ}C)$; temp range 169.6–270.6 $^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Camin & Rossini 1955)

0.311 (extrapolated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 7.0017 - 1768.82/(158.60 + t/^{\circ}C)$; temp range 160–338 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

1333* (135.8 $^{\circ}C$, derived from compiled data, temp range 135.8–270.685 $^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.01359 - 1789.95/(161.380 + t/^{\circ}C)$; temp range 135.8–303.8 $^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 14635.9/(T/K)] + 8.822087$; temp range 91.6–270.5 $^{\circ}C$ (Antoine eq., Weast 1972–73)

0.356 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log P/mmHg = 7.03121 - 1797.239/(t/^{\circ}C + 164.128)$; temp range 170–270 $^{\circ}C$ (Antoine eq. from exptl. data of Camin & Rossini 1955, Boublik et al. 1973)

0.359 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.15888 - 1797.239/(t/^{\circ}C + 162.128)$; temp range 170–270.5 $^{\circ}C$ (Antoine eq. derived from exptl. data of Camin & Rossini 1955, Boublik et al. 1984)

$\log(P/mmHg) = 7.02359 - 1789.95/(161.38 + t/^{\circ}C)$; temp range 136–304 $^{\circ}C$ (Antoine eq., Dean 1985, 1992)

15.87* (60.0 $^{\circ}C$, gas saturation, measured temp range 60.0–136.0 $^{\circ}C$, Allemand et al. 1986)

$\log (P_L/kPa) = 6.38149 - 1945.469/(T/K - 97.875)$; temp range 366–409 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.14849 - 1789.95/(T/K - 111.77)$; temp range 447–546 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

0.576* (recommended, Ruzicka & Majer 1994)

$\ln [(P/kPa)/(P_o/kPa)] = [1 - (T_o/K)/(T/K)] \cdot \exp\{3.16144 - 2.062348 \times 10^{-3} \cdot (T/K) + 1.487263 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_o = 101.325$ kPa, $T_o = 543.797$ K (Cox equation, Ruzicka & Majer 1994)

$\log (P/mmHg) = 116.5157 - 8.041 \times 10^3/(T/K) - 38.799 \cdot \log (T/K) - 1.3398 \times 10^{-2} \cdot (T/K) - 4.4444 \times 10^{-6} \cdot (T/K)^2$; temp range 283–707 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

48535 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.72 (HPLC- k' correlation, Coates et al. 1985)

7.50; 6.78 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization: volatilization rate constant of $k = 0.69 \text{ d}^{-1}$ with a water column $t_{1/2} = 1.0 \text{ d}$ at 6–18°C, in spring; $k = 0.85 \text{ d}^{-1}$ with a water column $t_{1/2} = 0.8 \text{ d}$ at 20–22°C in summer; $k = 0.16 \text{ d}^{-1}$ with a water column $t_{1/2} = 4.3 \text{ d}$ at 3–7°C in winter for mesocosm experiment in coastal marine environment when volatilization dominates, volatilization $k = 0.343 \text{ d}^{-1}$ with a water column $t_{1/2} = 2.0 \text{ d}$ with HgCl_2 poisoned water tank and $k = 1.241 \text{ d}^{-1}$ with a water column $t_{1/2} = 0.56 \text{ d}$ for non-poisoned water tank in late summer (Wakeham et al. 1983).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 22.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)

$k_{OH} = 22.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K (Atkinson 1989)

$k_{OH} = 22.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{OH} = 22.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (experimental); $17.87 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atmospheric Oxidation Program); and $7.47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Fate of Atmospheric Pollutants) for gas-phase reaction with OH radicals (Meylan & Howard 1993)

$k_{OH} = 21.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation: microbial degradation $t_{1/2} < 15 \text{ d}$ by *Pseudomonas sp.* (Setti et al. 1993)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

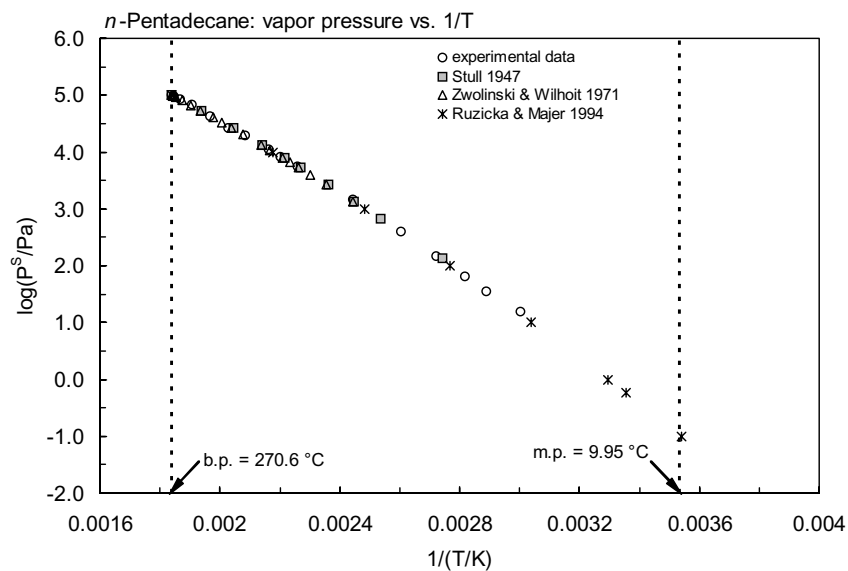
Half-Lives in the Environment:

Surface water: water column half-lives, $t_{1/2} = 1.0 \text{ d}$, 6–18°C, in spring; $t_{1/2} = 0.8 \text{ d}$, 20–22°C, in summer; $t_{1/2} = 4.3 \text{ d}$, 3–7°C, in winter for mesocosm experiment in coastal marine mesocosm; $t_{1/2} = 2.0 \text{ d}$ with HgCl_2 poisoned water tank and $t_{1/2} = 0.56 \text{ d}$ for non-poisoned water tank in late summer (Wakeham et al. 1983).

TABLE 2.1.1.1.31.1

Reported vapor pressures of *n*-pentadecane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)				
$\log P = A - B/(C + T/K)$		(3)							
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)							
$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$		(5) - Cox eq.							
Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Allemand et al. 1986			
summary of literature data		ebulliometry		selected values		gas saturation			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa		
91.6	133.3	169.686	5532	135.8	1333	60.0	15.87		
121.0	666.6	180.919	8325	151.41	2666	72.84	35.60		
135.4	1333	188.905	10927	161.45	4000	81.53	64.13		
150.2	2666	206.886	19417	168.78	5333	94.31	148.0		
167.7	5333	219.982	26546	174.785	6666	111.0	394.0		
178.4	7999	235.150	43159	179.859	7999	136.0	1465		
194.0	13332	151.703	67061	188.185	10666	Ruzicka & Majer 1994 recommended			
216.1	26664	262.310	84081	194.949	13332			T/K	P/Pa
242.8	53329	269.164	98106	207.872	19998				
270.5	101325	270.449	101069	217.641	26664				
mp/°C	10	bp/°C	270.613	225.582	33331				
				232.517	39997				
				243.446	53329	282.39	0.1		
				252.517	66661	303.58	1.0		
				260.237	79993	329.24	10		
				266.992	93326	361.22	100		
				268.25	95992	402.67	1000		
				269.48	98659	459.40	10000		
				270.685	101325	543.80	101325		
						298.15	0.576		
				bp/°C	270.685	Cox eq.			
				eq. 2	P/mmHg	eq. 5	P/kPa		
				A	7.02359	P _{ref} /kPa	101.325		
				B	1789.95	T _{ref} /K	543.64		
				C	161.380	a	3.16774		
						10 ³ b/K ⁻¹	-2.062348		
						10 ⁶ c/K ⁻²	1.487263		
		$\Delta H_v/(\text{kJ mol}^{-1}) =$							
		at 25°C							
		at bp							



2.1.1.1.32 *n*-Hexadecane

Common Name: Hexadecane

Synonym: cetane

Chemical Name: *n*-hexadecane

CAS Registry No: 544-76-3

Molecular Formula: $C_{16}H_{34}$; $CH_3(CH_2)_{14}CH_3$

Molecular Weight: 226.441

Melting Point ($^{\circ}C$):

18.12 (Lide 2003)

Boiling Point ($^{\circ}C$):

286.86 (Lide 2003)

Density (g/cm^3):

0.77344, 0.76996 ($20^{\circ}C$, $25^{\circ}C$, Camin et al. 1954; Dreisbach 1959)

0.7733 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

292.8 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

362.2 (calculated-Le Bas molar volume at normal boiling point, Eastcott et al. 1988)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

81.35 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

53.35, 51.46; 53.35 (18.15, $17.95^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

176.79, 165.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.28×10^{-3} (shake flask, Franks 1966)

2.1×10^{-5} (extrapolated data of McAuliffe 1966, Coates et al. 1985)

5.21×10^{-5} (extrapolated from data of McAuliffe 1996, Eastcott et al. 1988)

9.0×10^{-4} , 4.0×10^{-4} (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)

2.33×10^{-6} (calculated-TSA, Lande et al. 1985)

0.0272 (calculated-molar volume correlation, Wang et al. 1992)

4.95×10^{-5} (calculated-molar volume and mp., Ruelle Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($105.3^{\circ}C$, summary of literature data, temp range 105.3 – $287.5^{\circ}C$, Stull 1947)

6945* ($190.054^{\circ}C$, ebulliometry, measured range 190.054 – $286.704^{\circ}C$, Camin et al. 1954)

13.33* ($81.0^{\circ}C$, static method-Hg manometer, measured range 81.0 – $286.0^{\circ}C$, Myers & Fenske 1955)

$\log(P/mmHg) = 7.03044 - 1831.317/(154.528 + t/^{\circ}C)$; temp range 190.0 – $286.8^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Camin et al. 1954)

0.14 ($71.87^{\circ}C$, calculated-Antoine eq., Dreisbach 1959)

0.221* (derived from compiled data, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.02867 - 1830.51/(154.450 + t/^{\circ}C)$; temp range 149.18 – $320.7^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 15405.5/(T/K)] + 8.956267$; temp range 105.3 – $287.5^{\circ}C$ (Antoine eq., Weast 1972–73)

0.092 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)

$\log(P/mmHg) = 7.03519 - 1835.24/(t/^{\circ}C + 154.968)$; temp range 188 – $285^{\circ}C$ (Antoine eq. from exptl. data of Camin et al. 1945, Boublik et al. 1973)

$\log(P/kPa) = 6.16189 - 1836.287/(t/^{\circ}C + 155.125)$; temp range 190 – $287^{\circ}C$ (Antoine eq. from exptl. data of Camin et al. 1954, Boublik et al. 1984)

- $\log (P/\text{mmHg}) = 7.02867 - 1830.51/(154.45 + t/^{\circ}\text{C})$; temp range 149–321°C (Antoine eq., Dean 1985, 1992)
 $\log (P_L/\text{kPa}) = 6.77064 - 2273.168/(T/\text{K} - 80.252)$; temp range 323–425 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.15357 - 1830.57/(T/\text{K} - 118.7)$; temp range 467–563 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 7.02967 - 1830.51/(t/^{\circ}\text{C} + 154.45)$; temp range 149–321°C (Antoine eq., Dean 1992)
 $\log (P/\text{mmHg}) = 99.1091 - 7.5333 \times 10^3/(T/\text{K}) - 32.251 \cdot \log (T/\text{K}) + 1.0453 \times 10^{-2} \cdot (T/\text{K}) + 1.2328 \times 10^{-12} \cdot (T/\text{K})^2$; temp range 291–721 K (vapor pressure eq., Yaws 1994)
 317.6* (119.896°C, static-differential pressure, measured range 119.896–309.982°C, Morgan & Kobayashi 1994)
 0.191* (recommended, Ruzicka & Majer 1994)
 $\ln [(P/\text{kPa})/(P_o/\text{kPa})] = [1 - (T_o/\text{K})/(T/\text{K})] \cdot \exp\{3.18271 - 2.002545 \times 10^{-3} \cdot (T/\text{K}) + 1.384476 \times 10^{-6} \cdot (T/\text{K})^2\}$; reference state at $P_o = 101.325 \text{ kPa}$, $T_o = 559.978 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 0.190 (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 389000 (calculated-P/C, Eastcott et al. 1988)
 23072 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 8.25 (HPLC- k' correlation, Coates et al. 1985)
 8.00; 7.26 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$$k_{OH} = 25.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 312 \text{ K (Atkinson 1989)}$$

$$k_{OH} = 25.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1990)}$$

$$k_{OH} = 23.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)}$$

Hydrolysis:

Biodegradation: microbial degradation $t_{1/2} < 31 \text{ d}$ by *Pseudomonas* sp. (Setti et al. 1993)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Reported vapor pressures of *n*-hexadecane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll}
\log P = A - B/(T/K) & (1) \\
\log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\
\log P = A - B/(C + T/K) & (3) \\
\log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \\
\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2) & (5) - \text{Cox eq.}
\end{array}
\qquad
\begin{array}{ll}
\ln P = A - B/(T/K) & (1a) \\
\ln P = A - B/(C + t/^{\circ}\text{C}) & (2a)
\end{array}$$

1.

Stull 1947		Camin et al. 1954		Myers & Fenske 1955		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		static method-Hg manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
105.3	133.3	190.054	6945	81.0	13.33	149.18	1333
135.2	666.6	193.301	8330	94.2	66.66	165.14	2666
149.8	1333	199.273	9351	105.3	133.3	175.28	4000
164.7	2666	203.437	10951	117.2	266.6	182.87	5333
181.2	5333	208.962	13098	124.9	400.0	189.00	6666
193.2	7999	215.00	15824	130.7	533.3	194.184	7999
208.5	13332	221.78	19448	135.5	666.6	202.682	10666
231.7	26664	227.336	22886	138.2	799.9	209.565	13332
258.3	53329	235.145	28558	145.0	1067	222.774	19998
287.5	101325	242.432	34817	150.0	1333	232.743	26664
		250.605	43171	159.5	2000	240.846	33331
mp/°C	18.5	259.336	53777	166.0	2666	247.723	39997
		268.540	67076	176.0	4000	259.074	53329
		278.333	84.065	183.6	5333	268.33	66661
		285.337	98168	189.7	6666	276.205	79993
		286.704	101325	194.3	7999	283.097	93326
				202.6	10666	284.38	95992
		bp/°C	286.792	209.8	13332	285.635	98659
				222.3	19998	286.864	101325
		eq. 2	P/mmHg	232.2	26664	25.0	0.221
		A	7.03044	245.8	39997	bp/°C	286.854
		B	1831.317	258.0	53329		
		C	154.528	267.0	66661	eq. 2	P/mmHg
				274.5	79993	A	7.02867
				282.2	93326	B	1830.51
				286.0	101325	C	154.450
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	81.09
						at bp	51.21

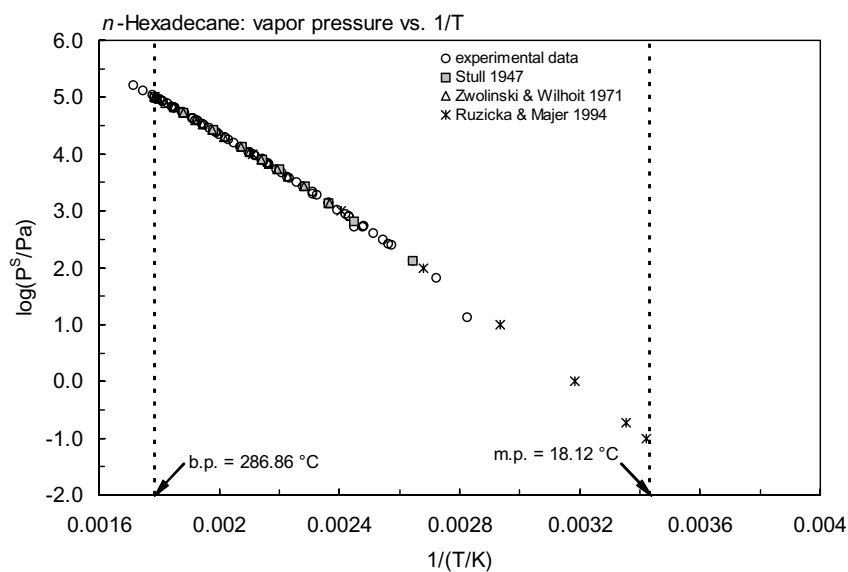
(Continued)

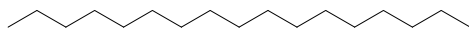
TABLE 2.1.1.1.32.1 (Continued)

2.

Morgan & Kobayashi 1994		Ruzicka & Majer 1994	
static method pressure gauge		recommended	
t/°C	P/Pa	T/K	P/Pa
119.896	317.6	292.41	0.1
129.903	541.2	314.20	1.0
139.909	886.1	340.55	10
149.916	1408	373.36	100
159.929	2172	415.82	1000
169.929	3273	473.84	10000
179.935	4810	559.98	101325
189.943	6912	298.15	0.191
199.976	9774		
209.956	13530	Cox eq.	
219.976	18418	eq. 5	P/kPa
229.969	24691	P _{ref} /kPa	101.325
239.977	32600	T _{ref} /K	469.64
249.979	42464	a	3.18271
259.979	54642	10 ³ b/K ⁻¹	-2.002545
269.979	69438	10 ⁶ c/K ⁻²	1.384476
279.980	87294		
289.980	108620		
299.980	133940		
309.982	163530		

data fitted to Wagner eq.

FIGURE 2.1.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-hexadecane.

2.1.1.1.33 *n*-Heptadecane

Common Name: Heptadecane

Synonym:

Chemical Name: *n*-heptadecane

CAS Registry No: 629-78-7

Molecular Formula: $C_{17}H_{36}$; $CH_3(CH_2)_{15}CH_3$

Molecular Weight: 240.468

Melting Point ($^{\circ}C$):

22 (Lide 2003)

Boiling Point ($^{\circ}C$):

302 (Lide 2003)

Density (g/cm^3):

0.7780, 0.7745 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

0.7780 (Weast 1982–83)

Molar Volume (cm^3/mol):

384.8 (calculated-Le Bas method at normal boiling point)

309.1 ($20^{\circ}C$, calculated-density)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

61.65, 53.12 ($25^{\circ}C$, bp, Dreisbach 1961)

86.47 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.96, 40.17; 51.13 (1.15, $21.95^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

174.61, 175.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.5×10^{-6} (extrapolated from data of McAuliffe 1966, Coates et al. 1985)

0.0014 (reported as $-\log S$ (mol/L) = 7.24, calculated-molar volume, Wang et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

1467* ($163.5^{\circ}C$, temp range 163.5 – $303.0^{\circ}C$, Krafft 1882; quoted, Boublik et al. 1984)

133.3* ($115.0^{\circ}C$, summary of literature data, temp range 115.0 – $303.0^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.0115 - 1847.82/(145.52 + t/^{\circ}C)$; temp range 188 – $374^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

0.0253* (derived from compiled data, temp range 160.9 – $337^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0143 - 1865.1/(149.20 + t/^{\circ}C)$; temp range 160.9 – $337^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 15608.5/(T/K)] + 8.847487$; temp range 115 – $303^{\circ}C$ (Antoine eq., Weast 1972–73)

0.030 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)

$\log(P/mmHg) = 6.97509 - 1851.699/(t/^{\circ}C + 149.263)$; temp range 164 – $303^{\circ}C$ (Antoine eq., Boublik et al. 1973)

$\log(P/kPa) = 6.09247 - 1845.726/(t/^{\circ}C + 148.633)$; temp range 164 – $303^{\circ}C$ (Antoine eq., Boublik et al. 1984)

$\log(P/mmHg) = 7.10143 - 1865.1/(t/^{\circ}C + 149.20)$; temp range 161 – $337^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.015 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 11.1197 - 4757.087/(T/K)$; temp range 289 – 320 K (Antoine eq.-I, liquid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.1392 - 1865.1/(T/K - 123.95)$; temp range 488 – 577 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

0.06148* (recommended, Ruzicka & Majer 1994)

$\ln[(P/kPa)/(P_o/kPa)] = [1 - (T_o/K)/(T/K)] \cdot \exp\{3.21826 - 2.036553 \times 10^{-3} \cdot (T/K) + 1.383899 \times 10^{-6} \cdot (T/K)^2\}$;
reference state at $P_o = 101.325$ kPa, $T_o = 575.375$ K (Cox equation, Ruzicka & Majer 1994)

$\log (P/\text{mmHg}) = 173.4039 - 1.0943 \times 10^4/(T/K) - 59.212 \cdot \log (T/K) + 2.0705 \times 10^{-2} \cdot (T/K) - 1.3433 \times 10^{-12} \cdot (T/K)^2$;
temp range 295–733 K (vapor pressure eq., Yaws 1994)
0.0627 (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

5415 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

8.92; 9.69 (estimated-RP-HPLC-MS; calculated-CLOGP, Burkhard et al. 1985)

8.79 (HPLC- k' correlation, Coates et al. 1985)

8.50; 7.68 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization: volatilization $k = 1.23 \text{ d}^{-1}$ with a water column $t_{1/2} = 0.6 \text{ d}$ at 6–18°C in spring; $k = 0.79 \text{ d}^{-1}$ with a water column $t_{1/2} = 0.9 \text{ d}$ at 20–22°C in summer; $k = 0.14 \text{ d}^{-1}$ with a water column $t_{1/2} = 5.0 \text{ d}$ at 3–7°C in winter for mesocosm experiments in coastal marine environment; volatilization $k = 0.359 \text{ d}^{-1}$ with a water column $t_{1/2} = 1.9 \text{ d}$ with HgCl poisoned water tank and $k = 1.362 \text{ d}^{-1}$ with a water column $t_{1/2} = 0.51 \text{ d}$ for non-poisoned water tank in late summer (Wakeham et al. 1983).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: microbial degradation $t_{1/2} < 31 \text{ d}$ by *Pseudomonas sp.* (Setti et al. 1993)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Surface water: water column $t_{1/2} = 0.6 \text{ d}$ at 6–18°C, in spring; $t_{1/2} = 0.9 \text{ d}$ at 20–22°C, in summer; $t_{1/2} = 5.0 \text{ d}$ at 3–7°C, in winter for mesocosm experiment in coastal marine environment; $t_{1/2} = 1.9 \text{ d}$ with HgCl poisoned water tank and $t_{1/2} = 0.51 \text{ d}$ for non-poisoned water tank in late summer (Wakeham et al. 1983).

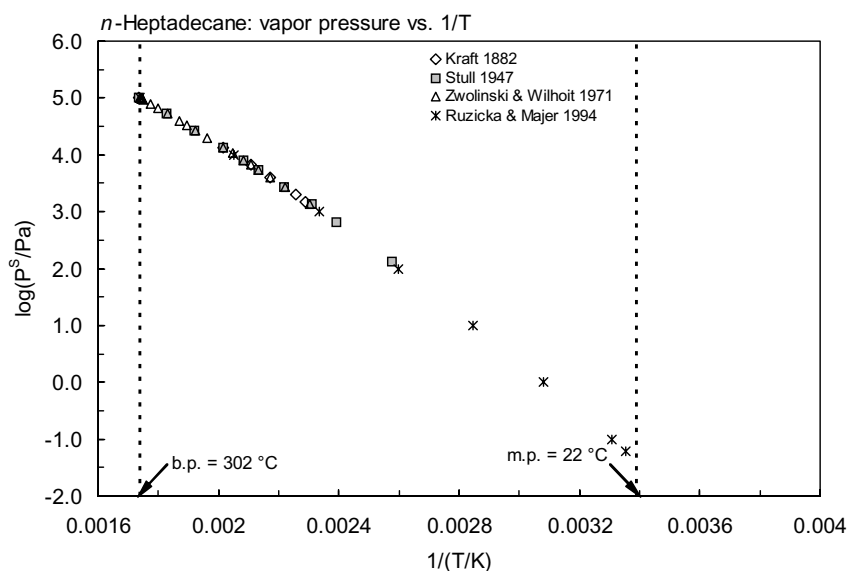
TABLE 2.1.1.1.33.1

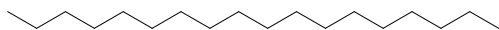
Reported vapor pressures of *n*-heptadecane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$	(5) - Cox eq.						
Stull 1947	Krafft 1882	Zwolinski & Wilhoit 1971	Ruzicka & Majer 1994				
summary of literature data	in Boublik et al. 1984	selected values	recommended				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
115.0	133.3	163.5	1467	160.9	1333	302.38	0.1
145.2	666.6	170.0	2000	177.3	2666	324.64	1.0
160.0	1333	187.5	4000	187.6	4000	351.56	10
177.7	2666	201.5	6666	195.4	5333	385.06	100
195.8	5333	223.0	13332	201.7	6666	428.4	1000

TABLE 2.1.1.1.33.1 (Continued)

Stull 1947		Krafft 1882		Zwolinski & Wilhoit 1971		Ruzicka & Majer 1994	
summary of literature data		in Boublik et al. 1984		selected values		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
207.3	7999	303.0	101325	207	7999	487.59	10000
223.0	13332			215.7	10666	575.38	101325
247.8	26664	bp/°C	303.003	222.76	13332	298.15	0.06148
274.5	53329			236.30	19998		
303.0	101325			246.50	26664	Cox eq.	
				254.82	33331	eq. 5	P/kPa
mp/°C	22.5			261.87	39997	P _{ref} /kPa	101.325
				273.51	53329	T _{ref} /K	469.64
				283.0	66661	a	3.21826
				291.08	79993	10 ³ b/K ⁻¹	-2.036553
				298.14	93326	10 ⁶ c/K ⁻²	1.383899
				299.47	95992		
				300.76	98659		
				302.02	101325		
				bp/°C	302.02		
				eq. 2	P/mmHg		
				A	7.0143		
				B	1865.10		
				C	149.20		
				$\Delta H_v/(\text{kJ mol}^{-1}) =$			
				at 25°C	86.20		
				at bp	52.89		

FIGURE 2.1.1.1.33.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-heptadecane.

2.1.1.1.34 *n*-Octadecane

Common Name: Octadecane

Synonym:

Chemical Name: *n*-octadecane

CAS Registry No: 543-45-3

Molecular Formula: $C_{18}H_{38}$; $CH_3(CH_2)_{16}CH_3$

Molecular Weight: 254.495

Melting Point ($^{\circ}C$):

28.2 (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

316.3 (Lide 2003)

Density (g/cm^3):

0.7819, 0.7785 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

0.7768 (Weast 1982–83)

Molar Volume (cm^3/mol):

325.5 ($20^{\circ}C$, calculated-density)

407.0 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)

Enthalpy of vaporization, ΔH_v (kJ/mol):

90.824, 54.84 ($25^{\circ}C$, bp, Dreisbach 1959)

91.6 ($25^{\circ}C$, Piacente et al. 1994)

91.44 (298.15K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

61.384 (Dreisbach 1959)

61.13 ($28^{\circ}C$, Piacente et al. 1994)

61.5 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

204.6, 184.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.930 (mp at $28.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

7.75×10^{-3} (Baker 1959)

2.1×10^{-3} ; 8.0×10^{-4} (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)

1.40×10^{-6} (extrapolated from data of McAuliffe 1966, Coates et al. 1988)

4.05×10^{-6} (extrapolated from data of McAuliffe 1966, Eastcott et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($119.6^{\circ}C$, summary of literature data, temp range 119.6 – $317.0^{\circ}C$, Stull 1947)

26.66* ($102.4^{\circ}C$, static method-Hg manometer, measured range 102.4 – $313^{\circ}C$, Myers & Fenske 1955)

$\log(P/mmHg) = 7.0156 - 1883.73/(139.46 + t/^{\circ}C)$; temp range 201 – $387^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

1333* ($172.3^{\circ}C$, derived from compiled data, temp range 172.3 – $316.3^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0022 - 1894.3/(143.3 + t/^{\circ}C)$; temp range 172.3 – $352^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 15447.0/(T/K)] + 8.619864$; temp range 119.6 – $317^{\circ}C$ (Antoine eq., Weast 1972–73)

0.013 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log(P/mmHg) = 7.14067 - 2012.745/(t/^{\circ}C + 155.492)$; temp range 174 – $317^{\circ}C$ (Antoine eq., Boublik et al. 1973)

0.0259 (liquid P_L , extrapolated-Antoine eq., Macknick & Prausnitz 1979)

0.220* ($45.0^{\circ}C$, gas saturation, measured range 45.0 – $88.10^{\circ}C$, Macknick & Prausnitz 1979)

$\ln(P_L/mmHg) = 25.548 - 10165/(T/K)$; temp range 45 – $88.1^{\circ}C$ (Antoine eq. on exptl. data, gas saturation, liquid state, Macknick & Prausnitz 1979)

0.0133 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.27065 - 2016.983/(t/^{\circ}\text{C} + 155.924)$; temp range 174–317°C (Antoine eq., Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 7.0022 - 1894.3/(143.30 + t/^{\circ}\text{C})$; temp range 172–352°C (Antoine eq., Dean 1985, 1992)
 1.15* (62.04°C, gas saturation, measured temp range 335.19–439.82 K, Allemand et al. 1986)
 0.0261 (extrapolated-Antoine eq.-I, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 10.18833 - 4404.095/(T/\text{K})$; temp range 310–361 K Antoine eq., liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.1392 - 1894.3/(T/\text{K} - 129.85)$; temp range 501–550 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 7.0022 - 1894.3/(t/^{\circ}\text{C} + 143.30)$; temp range 172–352°C (Antoine eq., Dean 1992)
 256.6* (139.919°C, static-differential pressure, measured range 139.919–314.982°C, Morgan & Kobayashi 1994)
 0.02007* (recommended, temp range 396–500 K, Ruzicka & Majer 1994)
 $\ln [(P/\text{kPa})/(P_0/\text{kPa})] = [1 - (T_0/K)/(T/K)] \cdot \exp\{3.24741 - 2.048039 \times 10^{-3} \cdot (T/K) + 1.362445 \times 10^{-6} \cdot (T/K)^2\}$;
 reference state at $P_0 = 101.325 \text{ kPa}$, $T_0 = 590.023 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)
 $\log (P/\text{mmHg}) = -15.0772 - 4.8702 \times 10^3/(T/K) + 14.501 \cdot \log (T/K) - 3.1625 \times 10^{-2} \cdot (T/K) + 1.3478 \times 10^{-5} \cdot (T/K)^2$;
 temp range 273–591 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated):

1013 (15°C, Wakeham et al. 1986)
 622200 (calculated-P/C, Eastcott et al. 1988)
 893 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

9.32 (HPLC- k' correlation, Coates et al. 1985)
 9.00; 8.13 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.90 (K_{OM} , Wakeham et al. 1986)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: volatilization rate constant $k_v = 0.03 \text{ d}^{-1}$, microcosm exptl. (Wakeham et al. 1986).

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: degradation rate constant of about 0.66 d^{-1} in a microcosm expt. (Wakeham et al. 1986); microbial degradation $t_{1/2} < 31 \text{ d}$ by *Pseudomonas sp.* (Setti et al. 1993).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Surface water: an estimated $t_{1/2} = 1.5 \text{ d}$ in Rhine River for a first order reduction process in river water (Zoeteman et al. 1980)

$t_{1/2} \sim 23 \text{ d}$ in a seawater microcosm experiment (Wakeham et al. 1986).

TABLE 2.1.1.1.34.1

Reported vapor pressures of *n*-octadecane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & \\ \ln(P/P_{\text{ref}}) &= [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2) & (5) - \text{Cox eq.} & \end{aligned}$$

1.

Stull 1947		Myers & Fenske 1955		Zwolinski & Wilhoit 1971		Macknick & Prausnitz 1979	
summary of literature data		ebulliometry		selected values		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
119.6	133.3	102.4	26.66	172.3	1333	45.0	0.220
152.1	666.6	115.9	66.66	189.0	2666	51.45	0.400
169.6	1333	127.0	133.3	199.6	4000	54.5	0.568
187.5	2666	139.6	266.6	207.5	5333	54.85	0.591
207.4	5333	147.0	400.0	213.9	6666	59.85	0.935
219.7	7999	153.3	533.3	219.3	7999	65.60	1.529
236.0	13332	157.7	666.6	228.2	10666	71.25	2.493
260.6	26664	161.8	799.9	234.39	13332	80.85	5.826
288.0	53329	167.7	1067	249.21	19998	84.10	7.148
317.0	101325	172.8	1333	259.64	26664	88.10	9.719
		182.8	2000	268.12	33331		
mp/°C	28	189.6	2666	275.32	39997	eq. 1a	P/mmHg
		199.9	4000	287.2	53329	A	25.548
		208.0	5333	296.9	66661	B	10165
		214.3	6666	305.2	79993		
		219.5	7999	312.4	93326		
		228.5	10666	313.7	95992		
		235.7	13332	315.0	98659		
		249.0	19998	316.3	101325		
		259.2	26664				
		273.8	39997	bp/°C	316.3		
		286.0	53329				
		294.7	66661	eq. 2	P/mmHg		
		302	79993	A	7.0022		
		308	93326	B	1894.3		
		313	101325	C	143.30		
				$\Delta H_v/(\text{kJ mol}^{-1}) =$			
				at 25°C	90.8		
				at bp	54.48		

TABLE 2.1.1.1.34.1 (Continued)

2.

Allemand et al. 1986		Morgan & Kobayashi 1994		Ruzicka & Majer 1994	
gas saturation		vapor-liquid equilibrium		recommended	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
62.04	1.1506	139.919	256.6	311.88	0.1
71.39	2.680	149.924	443.6	334.61	1.0
84.0	6.599	159.93	729.4	362.08	10
88.0	9.479	169.936	1148	396.24	100
97.0	18.40	179.974	1761	440.41	1000
100.4	22.00	189.948	2637	500.70	10000
110.0	43.86	199.976	3870	590.02	101325
124.21	106.1	209.976	5566	298.15	0.02007
130.0	152.0	219.976	7834		
140.0	264.0	229.977	10835	Cox eq.	
166.67	995.9	239.970	14744	eq. 5	P/kPa
		254.979	22736	P _{ref} /kPa	101.325
		254.979	27300	T _{ref} /K	469.64
		264.979	34026	a	3.24741
		284.980	49559	10 ³ b/K ⁻¹	-2.048039
		299.98	70490	10 ⁶ c/K ⁻²	1.362445
		314.982	98240		

data fitted to Wagner eq.

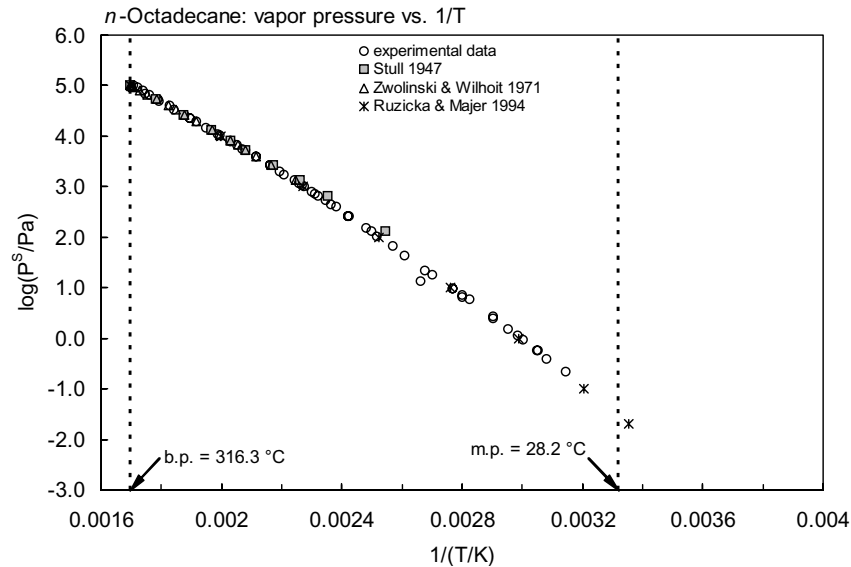


FIGURE 2.1.1.1.34.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-octadecane.

2.1.1.1.35 *n*-Eicosane

Common Name: Eicosane

Synonym: didecyl

Chemical Name: *n*-eicosane

CAS Registry No: 112-95-8

Molecular Formula: $C_{20}H_{42}$; $CH_3(CH_2)_{18}CH_3$

Molecular Weight: 282.547

Melting Point ($^{\circ}C$):

36.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

334.8 (Chirico et al. 1989)

Density (g/cm^3):0.7887, 0.7853 (20 $^{\circ}C$, 25 $^{\circ}C$, Dreisbach 1959)

0.7886 (Weast 1982–83)

Molar Volume (cm^3/mol):

451.4 (calculated-Le Bas molar volume at normal boiling point)

358.2 (20 $^{\circ}C$, calculated-density)

358 (Wang et al. 1992)

Enthalpy of vaporization, ΔH_v (kJ/mol):

63.93; 64.35 (exptl., calculated, Macknick & Prausnitz 1979b)

100.9; 110 (25, 94 $^{\circ}C$, Piacente et al. 1994)

101.81 (298.15 K, recommended, Ruzicka & Majer 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

69.875 (Dreisbach 1959)

69.5 (Piacente et al. 1994)

67.8 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

219.6, 203.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25 $^{\circ}C$ (assuming ΔS_{fus} = 56 J/mol K), F: 0.769 (mp at 36.6 $^{\circ}C$)Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$): 1.9×10^{-3} , 8.0×10^{-4} (shake flask-GC, distilled water; seawater, Sutton & Calder 1974) 1.10×10^{-7} (extrapolated from data of McAuliffe 1966, Coates et al. 1985) 3.11×10^{-7} (extrapolated from data of McAuliffe 1966, Eastcott et al. 1985)Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):13.33* (121.9 $^{\circ}C$, static method-Hg manometer, measured range 121.9–342.0 $^{\circ}C$, Myers & Fenske 1955) $\log(P/mmHg) = 7.0225 - 1948.7/(127.8 + t/^{\circ}C)$; temp range: 224–417 $^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1959)1333* (198.3 $^{\circ}C$, derived from compiled data, temp range 198.3–343.8 $^{\circ}C$, Zwolinski & Wilhoit 1971) $\log(P/mmHg) = 7.1522 - 2032.7/(132.1 + t/^{\circ}C)$; temp range: 198.3–379 $^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)0.41* (71.5 $^{\circ}C$, P_L , gas saturation-IR, Macknick & Prausnitz 1979) $\ln(P_L/mmHg) = 26.849 - 11230/(T/K)$; temp range: 71.15–107.3 $^{\circ}C$, (Antoine eq., gas saturation, liquid state, Macknick & Prausnitz 1979) $\log(P_L/kPa) = 10.77373 - 4872.63/(T/K)$; temp range: 344–380 K (Antoine eq., liquid, Stephenson & Malanowski 1987) $\log(P_L/kPa) = 6.2771 - 2032.7/(T/K - 141.05)$; temp range 528–620 K (Antoine eq., liquid, Stephenson & Malanowski 1987)0.201* (79.97 $^{\circ}C$, pressure gauge, measured range 90.07–194.21 $^{\circ}C$, Sasse et al. 1988)

$\log (P/\text{mmHg}) = 7.95834 - 2665.762/(t/^{\circ}\text{C} + 167.047)$; (Antoine eq. derived from exptl. data, liquid phase, pressure gauge measurement, Sasse et al. 1988)

15.6* (115°C, inclined piston measurement, temp range 115–215°C, Chirico et al. 1989)

$\ln (P/\text{kPa}) = 19.36 - 9083/(T/\text{K})$; temp range 406–472 K (transpiration method, Piacente et al. 1991)

$\ln (P/\text{kPa}) = 22.53 - 10649/(T/\text{K})$; temp range 345–393 K (torsion method, Piacente et al. 1991)

$\ln (P/\text{kPa}) = 18.10 - 7889/[(T/\text{K}) + 32]$; temp range 315–472 K (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)

$\log (P/\text{mmHg}) = 7.1522 - 2032.1/(t/^{\circ}\text{C} + 132.10)$; temp range 198–379°C (Antoine eq., Dean 1992)

0.32*, 0.641 (74, 78°C, torsion-effusion method, measured range 74–115°C, Piacente et al. 1994)

$\log (P/\text{kPa}) = 13.37 - 5785/(T/\text{K})$; temp range 351–384 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

$\log (P/\text{kPa}) = 12.96 - 5709/(T/\text{K})$; temp range 347–389 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

$\log (P/\text{kPa}) = 13.16 - 5747/(T/\text{K})$; temp range ~ 347–388 K, $\Delta H_v = 110 \text{ kJ mol}^{-1}$ (selected Antoine eq. based on exptl. data, torsion-effusion method, Piacente et al. 1994)

0.002091* (recommended, Ruzicka & Majer 1994)

$\ln [(P/\text{kPa})/(P_0/\text{kPa})] = [1 - (T_0/K)/(T/K)] \cdot \exp\{3.31181 - 2.102218 \times 10^{-3} \cdot (T/K) + 1.348780 \times 10^{-6} \cdot (T/K)^2\}$; reference state at $P_0 = 101.325 \text{ kPa}$, $T_0 = 617.415 \text{ K}$ (Cox equation, Ruzicka & Majer 1994)

$\log (P/\text{mmHg}) = 19.4193 - 5.8699 \times 10^3/(T/\text{K}) - 44.282 \cdot \log (T/\text{K}) - 1.2606 \times 10^{-2} \cdot (T/\text{K}) + 5.2241 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 310–767 K (vapor pressure eq., Yaws 1994)

0.00209* (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

198300 (calculated-P/C, Eastcott et al. 1988)

32.73 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

10.39 (HPLC- k' correlation, Coates et al. 1985)

10.0; 8.92 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Biodegradation: microbial degradation $t_{1/2} < 31 \text{ d}$ by *Pseudomonas* sp. (Setti et al. 1993)

Half-Lives in the Environment:

TABLE 2.1.1.1.35.1

Reported vapor pressures of eicosane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C/T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log(T/K)$	(4)		
$\ln(P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2)$	(5)		

1.

Myers & Fenske 1955		Zwolinski & Wilhoit 1971		Macknick & Prausnitz 1979		Sasse et al. 1988	
Hg manometer		selected values		gas saturation		electronic manometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
121.9	13.33	198.3	1333	71.15	0.4106	90.07	2.333
136.5	66.6	215.3	2666	79.90	0.973	90.12	2.360
148.6	133.3	326.1	4000	86.70	1.693	100.17	5.526
162.0	266.6	234.1	5333	90.35	2.333	100.17	5.266
170.0	400.0	240.7	6666	94.50	3.266	110.16	11.49
176.7	533.3	246.1	7999	102.95	6.719	110.16	11.43
182.0	666.6	255.15	10666	107.30	9.133	120.06	22.53
185.7	799.9	262.41	13332			120.10	22.80
192.6	1067	276.39	19998			130.11	43.20
198.0	1333	286.91	26664	eq. 1a	P/mmHg	130.13	43.73
208.8	2000	295.45	33331	A	26.849	139.99	80.66
215.7	2666	302.70	39997	B	11230	140.03	79.86
226.4	4000	314.60	53329			149.88	141.61
234.7	5333	324.4	66661			149.97	144.9
241.3	6666	332.6	79993			159.73	243.7
246.5	7999	339.8	93326			159.83	245.7
255.7	10666	341.2	95992			169.61	404.2
262.5	13332	342.5	98659			169.68	410.6
276.1	19998	343.8	101325			179.49	657.3
286.4	26664					189.25	1025
300.2	39997	bp/ $^{\circ}\text{C}$	343.8			194.21	1266
312.0	53329						
320.0	66661	eq. 2	P/mmHg			eq. 2	P/mmHg
327.0	79993	A	7.1522			A	7.99897
333.0	93326	B	2032.7			B	2067.622
342.0	101325	C	132.1			C	177.32
$\Delta H_v/(\text{kJ mol}^{-1}) =$							
at 25 $^{\circ}\text{C}$							
at bp							

TABLE 2.1.1.1.35.1 (Continued)

2.

Chirico et al. 1989				Piacente et al. 1991			
ebulliometry		inclined piston gauge		transpiration method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				1 st set		2 nd set data	
250.795	9596	115.0	15.6	150.85	114.8	124.85	23.99
254.896	10897	120.001	21.9	155.85	138.0	129.85	43.65
259.013	12348	125.001	30.7	160.35	182.0	134.35	37.15
263.144	13961	130.0	42.3	163.85	218.8	149.35	97.72
267.291	15752	135.0	58.3	166.85	275.4	152.85	123.0
271.454	17737	140.0	78.7	169.85	309.0	154.35	134.9
275.628	19933	150.0	139.9	171.85	371.5	156.35	147.9
284.032	25023	170.0	397.9	175.85	416.9	159.35	177.8
292.481	31177	180.0	641.9	177.85	537.0	165.85	218.8
300.985	38565	190.0	1007.7	180.35	537.0	169.85	281.8
309.540	46375	200.0	1539.6	182.85	537.0	172.35	275.4
318.146	57817	210.0	2300.3	185.85	645.7	174.35	354.8
326.761	70120	215.0	2789.0	188.35	831.8	176.35	426.6
335.416	84533			190.35	812.8	179.85	489.8
344.053	101325	Cox vapor pressure eq.		192.35	871.0	184.85	537.0
352.842	120790	eq. 5	P/kPa	193.85	912.0	188.85	645.7
		P _{ref} /kPa	101.325	196.85	1096.5	191.85	741.3
		T _{ref} /K	617.456	198.85	1175	194.35	851.1
		a	3.31018			196.35	831.8
enthalpy of vaporization:							
ΔH _v /(kJ mol ⁻¹) =							
380 K	89.07	10 ³ b/K ⁻¹	-2.09538				
400 K	86.133	10 ⁶ c/K ⁻²	1.34198				
420 K	83.448	temp range: 388–626 K					
440 K	80.78						
460 K	78.20						
480 K	75.68						
500 K	73.21						
520 K	70.75						
540 K	68.27						
560 K	65.74						
580 K	63.12						
600 K	60.37						
620 K	57.44						

(Continued)

TABLE 2.1.1.1.35.1 (Continued)

3.

Piacente et al. 1991 (cont'd)

transpiration (cont'd)		torsion method				Knudsen method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
3 rd set data		cell B, #1		cell B, #3		cell AK	
131.35	64.57	71.85	0.575	66.35	0.3802	42	0.0288
135.35	67.61	77.85	1.148	73.85	0.7586	51	0.10
141.35	107.15	81.85	1.514	78.85	1.148	60	0.269
145.85	114.82	84.35	1.905	82.85	1.698	70	0.5888
150.35	158.49	87.85	2.455	84.85	2.089	cell AK	
157.35	194.98	90.85	3.020	87.85	2.630	70	0.741
159.85	229.09	96.85	4.169	89.85	3.388	77	1.318
162.35	257.04	97.85	5.888	91.85	3.981	83	1.738
163.85	295.12	101.85	6.761	95.85	4.786	93	4.467
166.35	281.84	104.35	8.710	97.85	6.026		
179.35	338.84	105.35	9.333	101.85	7.943		
174.35	436.52	108.35	11.48	110.35	15.14	Eq. for transpiration, torsion and Knudsen effusion	
177.85	524.81	112.35	16.22	117.35	25.12		
183.35	707.95	112.85	17.38	117.85	25.70	eq. 3a	P/kPa
185.35	691.83	114.85	19.20	118.85	26.92	A	18.10 ± 0.23
187.85	812.83	cell B #2		cell B, #4		B	7889 ± 230
191.85	977.24	88.85	2.8184	71.35	0.5754	C	-32 ± 10
192.85	1023.3	89.85	3.388	78.35	1.148		
		90.85	3.388	82.85	1.698		
		91.85	3.802	86.85	2.291	bp /°C	343.65
Antoine eq. for transpiration		95.85	4.571	89.85	3.388	mp/°C	36.65
eq. 1a	P/kPa	96.85	4.898	104.85	10.0		
A	19.36 ± 0.46	97.35	5.129	107.85	11.48	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 69.882$ at 298.15 K	
B	9083 ± 207	1-2.35	7.943	109.35	13.18		
		104.35	8.710	110.85	15.49	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 152.3$ at 298.15 K	
		106.83	9.550	112.85	18.62		
		107.85	10.72	115.85	22.91		
		108.85	12.02	117.85	28.18		
		109.85	13.18	119.85	32.36		
		110.85	14.79				
		111.85	16.98	Antoine eq. for torsion			
		112.85	19.50	eq. 1a	P/kPa		
				A	22.53 ± 0.30		
				B	10649 ± 230		

TABLE 2.1.1.1.35.1 (Continued)

4.

Piacente et al. 1994				Morgan & Kobayashi 1994		Ruzicka & Majer 1994	
torsion-effusion				static pressure gauge		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
run a		run b		top-cut			
77.85	0.641	73.85	0.32	159.903	244	330.01	0.1
79.85	0.961	77.85	0.481	169.91	401.8	353.55	1.0
81.85	1.28	80.85	0.641	179.918	641.1	381.97	10
83.85	1.52	82.85	0.801	189.926	1006	417.30	100
85.85	1.84	85.85	1.28	199.934	1537	462.95	1000
88.85	2.40	88.85	1.60	199.976	1538	525.23	10000
91.85	3.36	91.85	2.40	209.976	2301	617.41	101325
93.85	4.17	94.85	3.04	219.947	3358	298.15	0.002091
94.85	4.97	97.85	4.17	229.954	4812		
98.85	6.57	100.85	4.65	239.961	6771	Cox eq.	
101.85	8.33	103.85	6.89	249.969	9359	eq. 5	P/kPa
103.85	10.40	106.85	8.65	259.979	12738	P _{ref} /kPa	101.325
107.85	15.1	112.85	14.3	269.979	17040	T _{ref} /K	617.415
110.85	19.4	114.85	17.1	284.980	25728	a	3.31181
				299.980	37745	10 ³ b/K ⁻¹	-2.102218
				314.982	54210	10 ⁶ c/K ⁻²	1.248780
eq. for run a		eq. for run b		mid-cut			
eq. 1	P/kPa	eq. 1	P/kPa				
A	13.37	A	12.96	159.847	244.9		
B	5785	B	5709	169.853	401		
temp range: 351–384 K		temp range: 347–388 K		179.860	639		
				189.875	999.1		
ΔH _v /(kJ mol ⁻¹) =		By weighing the slopes and		199.874	1541		
at 298.15 K	100.9	intercepts of above 2 eq.,		209.884	2302		
at 367 K	110 ± 2	selected vapor pressure eq.		219.894	3349		
		eq. 1	P/kPa	229.911	4813		
mp/°C	28	A	13.16	239.915	6773		
ΔH _{fus} /(kJ mol ⁻¹) = 61.10		B	5747	249.931	9349		
				259.938	12736		
ΔH _{subl} /(kJ mol ⁻¹) = 152.7		ΔH _v /(kJ mol ⁻¹) = 110 ± 2		269.949	17029		
		at 367 K		279.957	22549		
				289.970	29252		
				299.970	37754		
				309.982	48080		
				data fitted to Wagner eq.			

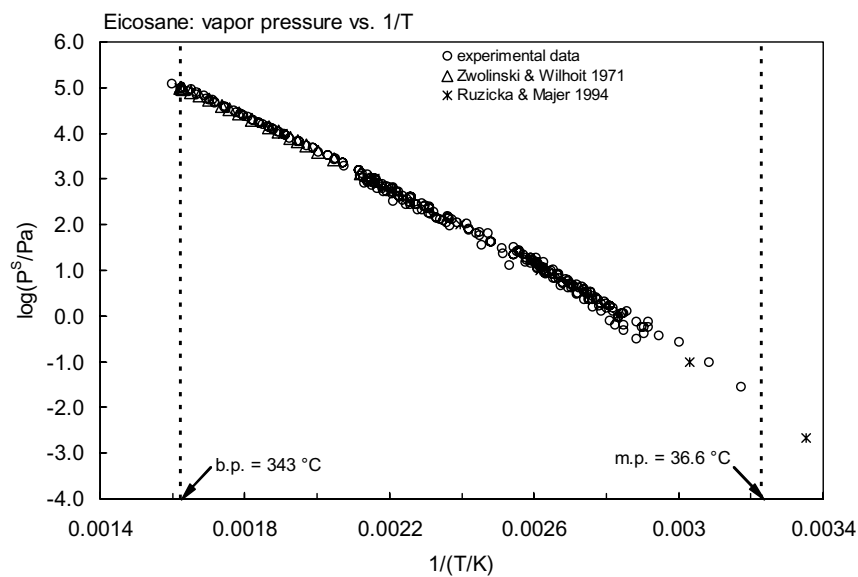
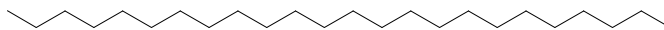


FIGURE 2.1.1.1.35.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-eicosane.

2.1.1.1.36 *n*-Tetracosane

Common Name: Tetracosane

Synonym:

Chemical Name: *n*-tetracosane

CAS Registry No: 646-31-1

Molecular Formula: $C_{24}H_{50}$; $CH_3(CH_2)_{22}CH_3$

Molecular Weight: 338.654

Melting Point ($^{\circ}C$):

50.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

391.3 (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

0.7991, 0.7958 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

540.2 (calculated-Le Bas method at normal boiling point)

423.8 ($20^{\circ}C$, calculated-density)

Enthalpy of vaporization, ΔH_v (kJ/mol):

126 ($132^{\circ}C$, Piacente et al. 1994)

121.9 (calculated, Chickos & Hanshaw 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

54.9 (Dreisbach 1959; Piacente et al. 1994)

31.3, 54.89; 86.19 (48.15 , $50.95^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

266.79, 240.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.563 (mp at $50.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.8×10^{-10} (extrapolated from data of McAuliffe 1966, Coates et al. 1985)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($183.8^{\circ}C$, summary of literature data, temp range 183.8 – $386.4^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.53923 - 2591.9/(165.1 + t/^{\circ}C)$; temp range 260 – $500^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

$\log(P/mmHg) = 7.0976 - 2112.0/(109.6 + t/^{\circ}C)$ (Antoine eq., Kudchadker & Zwolinski 1966)

66.66* ($175.9^{\circ}C$, derived from compiled data, temp range 175.9 – $391.3^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0976 - 2112.0/(109.6 + t/^{\circ}C)$; temp range 175.9 – $391.3^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 19642.5/(T/K)] + 9.408166$; temp range 183.8 – $386.4^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P_L/kPa) = 6.44051 - 2289.02/(T/K - 147.92)$; temp range 498 – $573\ K$ (liquid, Antoine eq., Stephenson & Malanowski 1987)

0.253* ($100.26^{\circ}C$, pressure gauge, Sasse et al. 1988)

$\log(P/mmHg) = 7.17666 - 2243.665/(t/^{\circ}C + 126.236)$; temp range 100.26 – $149.23^{\circ}C$ (Antoine eq. derived from exptl. data, liquid phase, Sasse et al. 1988)

$\log(P/kPa) = (8.76 \pm 0.50) - (4501 \pm 250)/(T/K)$; temp range 451 – $497\ K$ (Antoine eq. from exptl. data, transpiration method, Piacente & Scardala 1990; quoted, Pompili & Piacente 1990)

$\ln(P/kPa) = 21.25 - 10946/(T/K)$; temp range 501 – $523\ K$ (transpiration method, Piacente et al. 1991)

$\ln(P/kPa) = 25.35 - 12399/(T/K)$; temp range 376 – $438\ K$ (torsion method, Piacente et al. 1991)

$\ln(P/kPa) = 18.38 - 8349/[(T/K) + 58]$; temp range 343 – $523\ K$ (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)

90.1* (179.916°C, static-differential pressure, measured range 179.916–314.820°C, Morgan & Kobayashi 1994)
 0.721*, 0.801 (114, 115°C, torsion-effusion, measured range 386–425 K, Piacente et al. 1994)
 $\log(P/\text{kPa}) = 13.57 - 6459/(T/\text{K})$; temp range 388–413 K (torsion-effusion, Antoine eq., Piacente et al. 1994)
 $\log(P/\text{kPa}) = 14.25 - 6726/(T/\text{K})$; temp range 387–423 K (torsion-effusion, Antoine eq., Piacente et al. 1994)
 $\log(P/\text{kPa}) = 13.92 - 6591/(T/\text{K})$; temp range 386–425 K (torsion-effusion, Antoine eq., Piacente et al. 1994)
 $\log(P/\text{kPa}) = 13.96 - 6608/(T/\text{K})$; temp range ~ 386–425 K, $\Delta H_v = 126 \text{ kJ mol}^{-1}$ (selected Antoine eq. based on exptl. data, torsion-effusion method, Piacente et al. 1994)
 3.30×10^{-5} (quoted from Daubert & Danner 1997, Goss & Schwarzenbach 1999)
 2.37×10^{-5} (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

12.53 (HPLC- k' correlation, Coates et al. 1985)
 12.0; 10.5 (calculated-fragment const; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Biodegradation: microbial degradation $t_{1/2} < 31 \text{ d}$ by *Pseudomonas* sp. (Setti et al. 1993)

Half-Lives in the Environment:

TABLE 2.1.1.1.36.1

Reported vapor pressures of tetracosane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/\text{K})$	(1)	$\ln P = A - B/(T/\text{K})$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/\text{K})$	(3)	$\ln P = A - B/(C + t/\text{K})$	(3a)
$\log P = A - B/(T/\text{K}) - C \cdot \log(T/\text{K})$	(4)		

1.

Stull 1947		Zwolinski & Wilhoit 1971		Sasse et al. 1988		Piacente et al. 1990	
summary of literature data		selected values		electronic manometry		transpiration	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
183.8	133.3	175.9	66.66	100.26	0.255	run A	
219.6	666.6	188.0	133.3	110.25	0.613	183.85	85.11
237.6	1333	201.1	266.6	120.21	1.560	185.85	100.0
255.3	2666	220.5	666.6	130.15	3.506	187.85	97.72
276.3	5333	236.8	1333	139.93	7.386	189.85	107.2
288.4	7999	391.3	101325	140.09	7.506	193.85	134.9
305.2	13332			149.92	14.80	195.85	151.4
330.3	66661	bp/°C	391.3	149.97	14.80	For run A:-	
358.0	53329			159.77	28.53	eq. 1	P/kPa
386.4	101325	eq. 2	P/mmHg	159.62	52.13	A	8.17
		A	7.0976	179.45	91.06	B	4221
mp/°C	51.1	B	2112.0	189.23	148.9	For temp range: 457–469 K	
						Run B	

TABLE 2.1.1.1.36.1 (Continued)

Stull 1947		Zwolinski & Wilhoit 1971		Sasse et al. 1988		Piacente et al. 1990	
summary of literature data		selected values		electronic manometry		transpiration	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		C	109.6			187.85	104.7
				eq. 2	P/mmHg	192.85	138.0
				A	7.16777	197.85	182.0
				B	2243.665	206.85	288.4
				C	126.336	209.85	295.1
						212.35	316.2
						215.85	426.6
						216.85	436.5
						217.35	446.7
						217.88	457.1
						222.35	588.8
						223.35	616.6
						for run B:-	
						eq. 1	P/kPa
						A	9.53
						B	4843
						for temp range: 461–496 K	

2.

Piacente et al. 1990 (cont'd)

Piacente et al. 1991

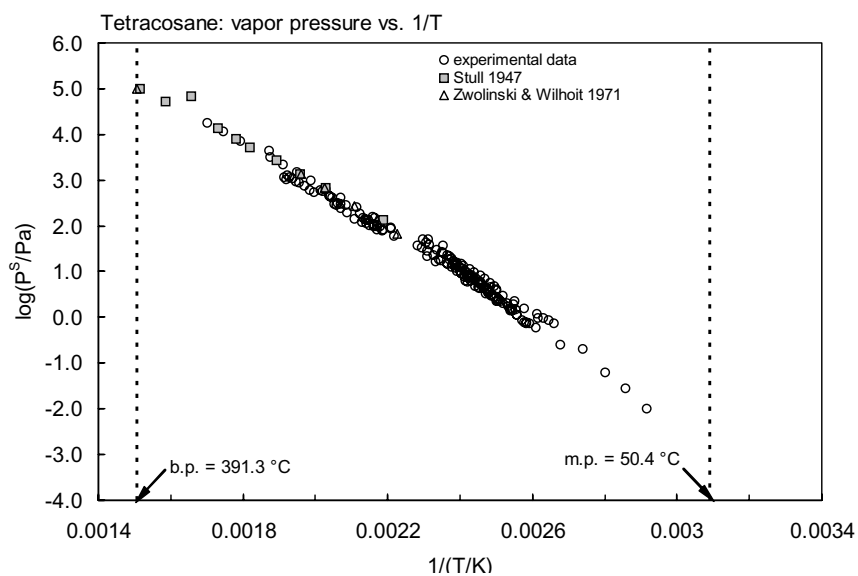
transpiration method		transpiration method		torsion method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
run C				cell B		cont'd	
177.85	61.66	227.85	537.0	109.05	0.955	136.85	9.772
184.85	79.43	230.85	602.6	118.35	1.514	138.85	11.22
187.85	85.11	234.85	741.3	122.35	2.089	141.85	13.49
189.85	97.72	238.85	871.0	126.35	2.291	142.85	14.79
192.35	102.3	240.85	933.3	129.35	3.020	144.85	15.85
193.85	117.5	242.85	1096	131.35	3.388	147.85	19.05
194.85	141.25	245.85	1175	134.35	4.365	148.85	21.38
196.85	123.0	246.85	1259	136.35	4.898	149.85	23.44
201.35	141.25	247.85	1047	138.35	6.457	152.35	26.30
205.85	199.5	249.85	1148	141.35	7.943	154.85	29.51
209.85	245.5			143.35	10.23	158.85	39.81
212.85	288.4	For transpiration data:		145.35	11.75	160.35	44.67
213.85	302.0	eq. 1a	P/kPa	147.35	13.80	162.35	51.29
		A	21.25 ± 1.08	cell D		cell D	
		B	10946 ± 554	123.85	2.951	126.85	2.344
for transpiration data:				126.85	3.981	130.85	3.548
eq. 1	P/kPa			129.85	4.677	134.85	4.577
A	8.31 ± 1.08			133.85	5.888	139.85	5.888
B	4314 ± 211			135.85	7.079	140.85	6.457
for temp range: 451–487 K				137.85	8.128	142.85	9.333
				139.85	8.128	144.85	10.47
overall vapor pressure eq. by				142.85	9.333	147.85	12.88

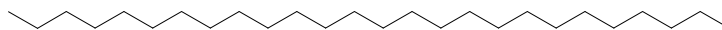
(Continued)

TABLE 2.1.1.1.36.1 (Continued)

Piacente et al. 1991 (cont'd)		Piacente et al. 1994			
Knudsen effusion		torsion-effusion			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
209.939	415.6				
219.946	652.9			mp/K	322
229.950	1001			$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 54.9$	
239.960	1506			$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 180.9 \pm 2$	
249.971	2209			at 298.15 K	
259.979	3176				
260.979	4489				
284.980	7303				
299.980	11470				
314.820	17460				

data fitted to Wagner eq.

FIGURE 2.1.1.1.36.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-tetracosane.

2.1.1.1.37 *n*-Hexacosane

Common Name: Hexacosane

Synonym: cerane

Chemical Name: *n*-hexacosane

CAS Registry No: 631-01-3

Molecular Formula: $C_{26}H_{54}$; $CH_3(CH_2)_{24}CH_3$

Molecular Weight: 366.707

Melting Point ($^{\circ}C$):

56.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

412.2 (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):0.8032, 0.7998 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)0.8032 ($20^{\circ}C$, Weast 1982–83)Molar Volume (cm^3/mol):

584.6 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)

456.6 ($20^{\circ}C$, calculated-density)

457 (Wang et al. 1992)

Enthalpy of vaporization, ΔH_v (kJ/mol):

64.806 (bp, Dreisbach 1959)

131.2 (calculated, Chickos & Hanshaw 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):32.3, 59.5; 95.3 (53.35, $56.35^{\circ}C$, total phase change enthalpy, Chickos et al. 1999)Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

289.03, 259.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$): F: 0.495 (mp at $56.1^{\circ}C$)Water Solubility (g/m^3 or mg/L at $25^{\circ}C$): 1.7×10^{-3} ; 1.0×10^{-4} (shake flask-GC, distilled water; seawater, Sutton & Calder 1974) 1.33×10^{-10} (extrapolated from data of McAuliffe 1966, Eastcott et al. 1988)Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):133.3* ($204.0^{\circ}C$, summary of literature data, temp range 204.0 – $399.8^{\circ}C$, Stull 1947) $\log(P/mmHg) = 7.57689 - 2692.73/(161.2 + t/^{\circ}C)$; temp range 278 – $500^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959) $\log(P/mmHg) = 7.1096 - 2164.3/(99.6 + t/^{\circ}C)$ (Antoine eq., Kudchadker & Zwolinski 1966)66.66* ($192.5^{\circ}C$, derived from compiled data, temp range 192.5 – $412.2^{\circ}C$, Zwolinski & Wilhoit 1971) $\log(P/mmHg) = 7.1096 - 2164.3/(99.6 + t/^{\circ}C)$; temp range 192.6 – $412.2^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971) $\log(P/mmHg) = [-0.2185 \times 21605.7/(T/K)] + 9.899820$; temp range 204 – $399.8^{\circ}C$ (Antoine eq., Weast 1972–73) $\log(P_L/kPa) = 6.2345 - 2164.3/(T/K - 173.55)$; temp range 466 – $685\ K$ (Antoine eq., liquid, Stephenson & Malanowski 1987) $\log(P_L/kPa) = 9.44384 - 4935.969/(T/K)$; temp range 478 – $530\ K$ (Antoine eq., liquid, Stephenson & Malanowski 1987) $\log(P/kPa) = (9.93 \pm 0.50) - (5168 \pm 200)/(T/K)$; temp range 455 – $519\ K$, (Antoine eq. from exptl. data, transpiration, Piacente & Scardala 1990; Pompili & Piacente 1990) $\ln(P/kPa) = 18.63 - 9892/(T/K)$; temp range 506 – $546\ K$ (transpiration method, Piacente et al. 1991) $\ln(P/kPa) = 28.91 - 14285/(T/K)$; temp range 391 – $442\ K$ (torsion method, Piacente et al. 1991) $\ln(P/kPa) = 17.76 - 8050/[(T/K) + 72]$; temp range 356 – $546\ K$ (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991) $\log(P/kPa) = 14.50 - 7084/(T/K)$; temp range 420 – $437\ K$ (torsion-effusion, Antoine eq., Piacente et al. 1994)

$\log (P/\text{kPa}) = 13.75 - 6765/(T/\text{K})$; temp range 391–433 K (torsion-effusion, Antoine eq., Piacente et al. 1994)
 $\log (P/\text{kPa}) = 13.65 - 6748/(T/\text{K})$; temp range 392–431 K (torsion-effusion, Antoine eq., Piacente et al. 1994)
 $\log (P/\text{kPa}) = 14.01 - 6682/(T/\text{K})$; temp range ~ 392–437 K, $\Delta H_v = 132 \text{ kJ mol}^{-1}$ (selected Antoine eq. based on exptl. data, torsion-effusion method, Piacente et al. 1994)

5.03×10^{-6} (quoted from Daubert & Danner 1997, Goss & Schwarzenbach 1999)

2.82×10^{-6} (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$):

21200 (calculated-P/C, Eastcott et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

13.0, 11.4 (calculated-fragment const., calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Biodegradation: microbial degradation $t_{1/2} < 31 \text{ d}$ by *Pseudomonas* sp. (Setti et al. 1993)

Half-Lives in the Environment:

TABLE 2.1.1.1.37.1

Reported vapor pressures of hexacosane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/\text{K})$	(1)	$\ln P = A - B/(T/\text{K})$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/\text{K})$	(3)	$\ln P = A - B/(C + T/\text{K})$	(3a)
$\log P = A - B/(T/\text{K}) - C \cdot \log (T/\text{K})$	(4)		

1.

Stull 1947		Zwolinski & Wilhoit 1971		Piacente et al. 1990			
summary of literature data		selected values		transpiration		transpiration (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
204.0	133.3	192.5	66.66	run A		run C	
240.0	666.6	204.8	133.3	187.85	64.57	182.35	37.15
257.4	1333	218.3	266.6	194.35	74.13	188.85	54.95
275.8	2666	138.0	666.6	197.35	91.20	193.35	70.79
295.2	5333	254.6	527.75	197.85	100.0	196.85	89.13
307.8	7999	412.2	101325	198.35	97.72	199.85	104.7
323.2	13332			199.85	109.65	202.35	123.0
348.4	66661			202.85	129.8	203.85	131.8
374.5	53329	bp/°C	412.2	205.85	131.8	204.85	112.2
399.8	101325			208.85	162.2	206.85	134.9
				211.85	251.2	210.85	229.1
		eq. 2	P/mmHg	214.85	263.0	215.35	288.4
mp/°C	56.6	A	7.1096	eq. for run A:-		218.85	263.0
		B	2164.3	eq. 1	P/kPa	221.85	309.0
		C	99.6	A	10.40 ± 0.42	223.35	346.7

(Continued)

TABLE 2.1.1.1.37.1 (Continued)

Stull 1947		Zwolinski & Wilhoit 1971		Piacente et al. 1990			
summary of literature data		selected values		transpiration		transpiration (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				B	5355 ± 198	243.35	691.8
				for temp range: 461–488 K		245.85	812.8
				run B		eq. for run C:-	
				202.35	100	eq. 1	P/kPa
				209.35	128.8	A	9.53 ± 0.21
				215.85	166.0	B	4979 ± 103
				220.85	269.2	temp range: 455.5–519 K	
				224.85	295.1		
				227.35	331.1	overall vapor pressure eq. by	
				229.35	407.4	weighted slopes and intercepts	
				234.85	457.1	eq. 1	P/kPa
						A	9.93 ± 0.50
				eq. 1	P/kPa	B	5168 ± 200
				A	10.09 ± 0.64		
				B	5289 ± 315	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				for temp range: 475.5–508 K		at 488 K	99 ± 4

2.

Piacente et al. 1991

transpiration method		torsion method		torsion (continued)		torsion (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		cell E		cell A		cell B	
232.85	354.8	131.35	1.202	141.35	1.479	138.85	3.020
238.35	616.6	132.35	1.380	143.35	1.950	142.85	4.571
242.85	616.6	134.35	1.585	145.35	2.692	144.85	4.169
242.85	616.6	136.35	1.778	146.35	3.162	144.85	4.898
246.35	575.4	137.35	1.995	146.85	3.715	147.35	6.166
247.85	660.7	139.35	2.570	147.35	4.169	150.35	6.457
249.35	758.6	140.85	3.020	147.85	4.898	153.85	9.550
251.35	871.0	142.35	3.388	148.35	5.623	154.35	9.120
252.35	933.3	146.35	5.129	148.85	6.310	154.35	9.550
254.35	933.3	148.35	6.166	149.35	7.586	154.85	9.550
255.85	1023	150.35	6.918	150.35	9.120	155.85	10.72
256.35	871.0	153.35	7.762	152.35	10.47	155.85	10.96
258.85	1047	155.35	9.120	154.35	11.22	158.85	13.80
259.35	1148	158.35	12.30	165.35	12.88	cell A	
261.85	1288	160.35	14.13	158.35	15.49	132.85	2.455
262.85	1288	163.35	17.38	160.35	18.62	135.35	2.951
266.35	1230	165.35	20.42	cell A		138.85	3.890
266.35	1259	167.35	23.99	117.85	0.490	142.35	5.129
268.35	1445	169.35	28.18	123.85	0.741	143.85	5.623
269.35	1413			126.85	0.977	145.35	6.310
271.85	1380			128.35	0.977	146.85	7.586
272.85	1585			129.35	1.230	147.35	7.413
272.85	1514			131.35	1.479	147.85	8.511
				133.35	1.698	148.85	9.550
eq. 1a	P/kPa			134.35	1.950	150.35	9.120

TABLE 2.1.1.1.37.1 (Continued)

Piacente et al. 1991							
transpiration method		torsion method		torsion (continued)		torsion (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
A	18.63 ± 1.03			135.35	2.188	150.85	10.00
B	9892 ± 552			136.35	2.455	151.85	10.47
				137.35	2.951	152.35	12.88
				138.35	3.467	152.85	13.18
				139.35	3.890	153.85	14.13
				141.35	4.677	155.85	15.85
				143.35	5.379		
						eq. 1a	P/kPa
						A	28.91 ± 0.40
						B	14285 ± 345

3.

Piacente et al. 1991 (cont'd)				Piacente et al. 1994			
Knudsen effusion		torsion-effusion		torsion-effusion (continued)		torsion-effusion (continued)	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		run a		run b		run c	
83	0.01995	146.85	4.01	117.85	0.320	118.85	0.320
92	0.04677	147.85	4.49	120.85	0.401	124.85	0.481
102	0.1514	148.85	5.13	124.85	0.481	127.85	0.641
111	0.2818	149.85	5.77	128.85	0.801	130.85	0.801
119	0.5623	150.85	6.42	131.85	1.120	133.85	1.12
		151.85	7.05	134.85	1.52	136.85	1.60
bp/K	658.2	152.85	7.69	137.85	2.08	139.85	2.08
mp/K	329.4	153.85	8.33	141.85	2.88	142.85	2.72
		154.85	9.13	145.85	4.17	146.85	3.85
eq. for transpiration, torsion		155.85	9.61	149.85	5.77	151.85	6.09
and Knudsen effusion		156.85	10.9	156.85	10.7	154.85	7.85
eq. 3a	P/kPa	157.85	11.7	159.85	13.5	157.85	10.4
A	17.76 ± 0.46	159.85	13.3				
B	8050 ± 460	161.85	15.5				
C	72 ± 10	163.85	18.9				
				eq. 1	P/kPa	eq. 1	P/kPa
		eq. 1	P/kPa	A	13.75 ± 0.29	A	13.65 ± 0.29
		A	14.50 ± 0.36	B	6765 ± 119	B	6748 ± 120
		B	7084 ± 153	temp range: 391–433 K		temp range: 392–431 K	
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 60.70$		temp range: 420–437 K					
$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 177.2$		overall vapor pressure eq.					
at 298.15 K				eq. 1	P/kPa		
				A	14.01 ± 0.30		
				B	6882 ± 50		
				$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) =$			
				at 414 K	132 ± 1		
				mp/K	329		
				$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 59.9$			
				$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 191.5 \pm 1$			
				at 298.15 K			

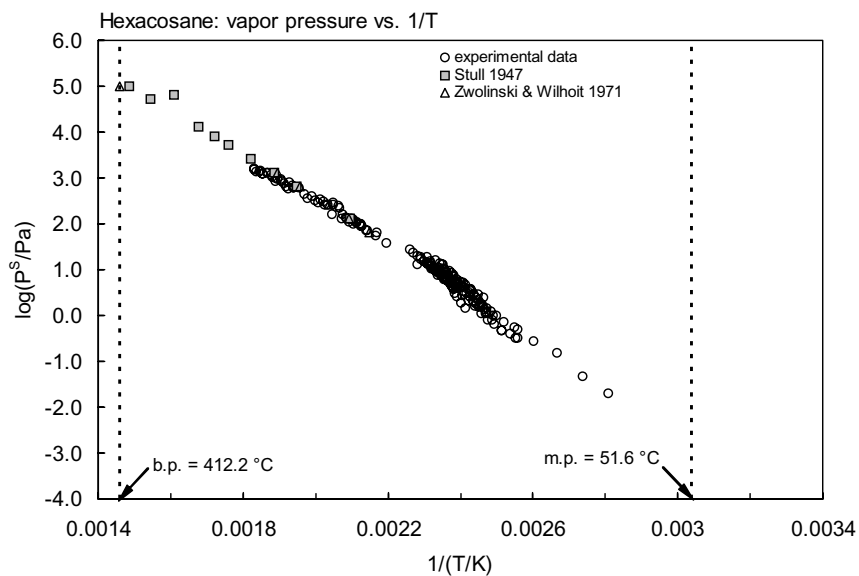


FIGURE 2.1.1.1.37.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-hexacosane.

2.1.1.2 Cycloalkanes

2.1.1.2.1 Cyclopentane



Common Name: Cyclopentane

Synonym: pentamethylene

Chemical Name: cyclopentane

CAS Registry No: 287-92-37

Molecular Formula: C_5H_{10}

Molecular Weight: 70.133

Melting Point ($^{\circ}C$):

−93.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

49.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7457 (Weast 1984)

0.7454, 0.7440 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

94.10 ($20^{\circ}C$, calculated-density; McAuliffe 1966)

99.5 (calculated-Le Bas method at normal boiling point, Abernethy et al. 1988; Mackay & Shiu 1990)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

28.527, 27.296 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

0.609 (Riddick et al. 1986)

4.9, 0.34, 0.60; 5.84 (-151.15 , -135.15 , $-93.45^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

45.96, 40.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$. Additional data at other temperatures designated * are compiled at the end of this section.):

156 (shake flask-GC, McAuliffe 1963, 1966)

342* (shake flask-GC, measured range 5.11 – $45.21^{\circ}C$, Pierotti & Liabastre 1972)

160* (shake flask-GC, measured range 25 – $153.1^{\circ}C$, Price 1976)

160 (shake flask-GC, Krzyzanowska & Szeliga 1978)

164 (shake flask-GC, Groves 1988)

156* (IUPAC “tentative” best, IUPAC Solubility Data Series, Shaw 1989)

166* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2 – $426.3 K$, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

27250* ($14.25^{\circ}C$, static method-manometry, measured range -47.24 to $14.25^{\circ}C$, Ashton et al. 1943)

34890* ($20.2^{\circ}C$, ebulliometry-manometer, measured range 15.7 – $50^{\circ}C$, Willingham et al. 1945)

$\log(P/mmHg) = 6.87798 - 1119.208/(230.738 + t/^{\circ}C)$; temp range 15.7 – $50.0^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

43150* (Antoine eq. regression, temp range -68 to $49.4^{\circ}C$, Stull 1947)

42330 (calculated from exptl. determined data, Dreisbach 1955; quoted, Hine & Mookerjee 1975)

$\log(P/mmHg) = 6.88676 - 1124.162/(231.361 + t/^{\circ}C)$; temp range -25 to $110^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

29036* (selected exptl. data, temp range -39 to $230^{\circ}C$, Pasek & Thodos 1962)

- 42400 (interpolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981)
- 42330* (derived from compiled data, temp range -40.4 to 71.6°C , Zwolinski & Wilhoit 1971)
- $\log(P/\text{mmHg}) = 6.88676 - 1124.162/(231.361 + t/^{\circ}\text{C})$; temp range -40.4 to 71.6°C (Antoine eq., Zwolinski & Wilhoit 1971)
- $\log(P/\text{mmHg}) = [-0.2185 \times 7411.1/(T/\text{K})] + 7.940722$; temp range -68 to 49.3°C (Antoine eq., Weast 1972–73)
- $\log(P/\text{atm}) = [1 - 322.386/(T/\text{K})] \times 10^{\{0.818603 - 7.52365 \times 10^{-4} \cdot (T/\text{K}) + 8.27395 \times 10^{-7} \cdot (T/\text{K})^2\}}$; temp range: 190.20 – 503.20 K (Cox eq., Chao et al. 1983)
- 42570, 42320 (calculated-Antoine equations, Boublik et al. 1984)
- $\log(P/\text{kPa}) = 6.25832 - 1240.438/(242.957 + t/^{\circ}\text{C})$; temp range -47.25 to 14°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log(P/\text{kPa}) = 6.82877 - 1133.199/(232.415 + t/^{\circ}\text{C})$, temp range 15.7 – 50.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
- 42320 (interpolated-Antoine eq., Dean 1985, 1992)
- $\log(P/\text{mmHg}) = 6.88676 - 1124.162/(231.36 + t/^{\circ}\text{C})$; temp range -40 to 72°C (Antoine eq., Dean 1985, 1992)
- 42400 (selected lit., Riddick et al. 1986)
- $\log(P/\text{kPa}) = 6.04584 - 1142.30/(233.463 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
- 42340 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.0080 - 1122.21/(-42.011 + T/\text{K})$; temp range 280 – 311 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.08918 - 1174.132/(-34.864 + T/\text{K})$; temp range 322 – 384 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.41769 - 1415.096/(-0.66 + T/\text{K})$ temp range 381 – 455 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.77782 - 1749.65/(48.533 + T/\text{K})$; temp range 452 – 511 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log(P/\text{mmHg}) = 29.1547 - 2.3512 \times 10^3/(T/\text{K}) - 7.6965 \cdot \log(T/\text{K}) - 1.6212 \times 10^{-10} \cdot (T/\text{K}) + 3.125 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 179 – 512 K (vapor pressure eq., Yaws 1994)
- 35000* (20.14°C , differential pressure gauge, measured range -68.59 to 70.06°C , Mokbel et al. 1995)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 18800 (calculated as $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
- 13310; 18380 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
- 18500; 19100, 18600 (recommended; calculated-P/C, Mackay & Shiu 1981)
- 17550 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 19030 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 16617* (27.9°C , EPICS-GC, measured range 27.9 – 45°C , Hansen et al. 1993)
- $\ln[H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -3351/(T/\text{K}) + 14.0$; temp range 27.9 – 45°C (EPICS-GC, Hansen et al. 1993)
- 12796 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
- $\log K_{\text{AW}} = 5.162 - 1302/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.05 (calculated- π substituent constant, Hansch et al. 1968)
- 3.00 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979)
- 3.00 (recommended, Sangster 1989, 1993)
- 3.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{O(3P)}} = 1.30 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O(}^3\text{P)}$ (Herron & Huie 1973)

$k_{\text{OH}} = (4.72 \pm 0.28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} (\text{calc}) = 5.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)

$k_{\text{OH}} = 5.40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1979)

$k_{\text{OH}} = 5.40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{O(3P)}} = 1.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O(}^3\text{P)}$ atoms at room temp. (Gaffney & Levine 1979)

$k_{\text{OH}} = 6.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and $5.18 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and $5.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K and $4.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson 1985)

$k_{\text{OH}} = (3.12 \pm 0.23) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (flash photolysis-resonance absorption technique, Jolly et al. 1985)

$k_{\text{OH}} = 5.02 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–491 K (Droege & Tully 1987)

$k_{\text{OH}}^* = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}} = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K with an estimated lifetime of 27 h in summer daylight (Altshuller 1991)

$k_{\text{OH}}^* = 5.02 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

$k_{\text{OH}}^* = 4.83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction rate constant $k = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radical in air at 298 K (Atkinson 1990; Altshuller 1991) with an estimated lifetime of 27 h, based on reaction rate with OH radical in summer daylight (Altshuller 1991).

TABLE 2.1.1.2.1.1

Reported aqueous solubilities of cyclopentane at various temperatures

Pierotti & Liabastre 1972		Price 1976		Shaw 1989a		Mączyński et al. 2004	
shake flask-GC/FID		shake flask-GC/FID		IUPAC "tentative" values		calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
5.11	338.6	25.0	160	5	339	25	168
15.21	341.7	40.1	163	15	342	40.1	175
25.11	341.9	55.7	180	25	156	55.7	195
35.21	368.5	99.1	296	30	160	99.1	343
45.21	341.5	118.0	372	40	350	118	468
		137.3	611	60	500	137.3	701
		153.1	792	80	750	153.1	974
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = -2.50$ 25°C				100	1100		
				120	1600		
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = -2.80$ 25°C		140	2600		
				160	3850		
				180	6700		
				200	14000		

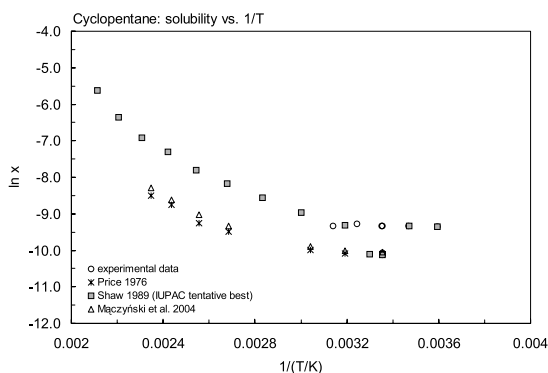


FIGURE 2.1.1.2.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for cyclopentane.

TABLE 2.1.1.2.1.2

Reported vapor pressures of cyclopentane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A + B/(T/K) + C \cdot \log (T/K) + D[P/(T/K)^2]$			(5)
$\log P = A - B/T(T/K) - C \cdot \log (T/K) + D \times 10^{-3}(T/K) - E \times 10^{-8}(T/K)^2$			(6)

1.

Ashton et al. 1943		Willingham et al. 1945		Stull 1947		Pasek & Thodos 1962	
static method-manometry		ebulliometry		summary of literature data		selected experimental data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−47.24	830.6	15.707	28956	−68.0	133.3	−39.064	1571
−38.35	1570	20.196	34892	−49.6	666.6	9.335	21949
−31.63	2446	25.598	43322	−40.4	1333	15.722	29036
−24.7	3753	31.172	53656	−30.1	2666	48.146	97608
−18.6	5360	37.119	66760	−18.6	5333	57.885	133322
−12.91	7350	43.574	83722	−11.3	7999	71.612	1999836
−7.29	9875	48.131	97608	−1.30	13332	100.005	4197790
−1.93	12931	48.621	99205	13.8	26664	230.065	4023402
4.47	17569	49.073	100698	31.0	53329		
9.33	21949	49.587	102401	49.3	101325	bp/°C	49.307
14.25	27250	50.031	103921				
				mp/°C	−93.7	Frost-Kalkwarf equation: derived from exptl. data eq 5 P/mmHg A 21.62180 B −2131.85 C −4.83947 D 1.41701	
bp/°C	49.20						
mp/°C	−93.62	bp/°C	49.262				
eq. 6	P/mmHg	eq. 2	P/mmHg				
A	30.957385	A	6.87798				
B	2298.386	B	1119.208			Frost-Kalkwarf equation: calculated from molecular structures, normal bp and	
C	8.91170	C	230.738				
D	4.385677						
E	1.054940						

TABLE 2.1.1.2.1.2 (Continued)

Ashton et al. 1943		Willingham et al. 1945		Stull 1947		Pasek & Thodos 1962	
static method-manometry		ebulliometry		summary of literature data		selected experimental data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
ΔH_v /(kJ mol ⁻¹) = 29.21 at 25°C						deviations of resulting v.p.: eq 5 P/mmHg	
						A	21.63300
						B	-2132.5
						C	-4.84313
						D	1.41701

2.

Zwolinski & Wilhoit 1971		Mokbel et al. 1995	
selected values		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa
−40.4	1333	−68.59	138
−30.1	2666	−59.24	313
−23.6	4000	−49.42	692
−18.6	5333	−39.51	1446
−14.7	6666	−39.42	1456
−11.3	7999	−29.66	2775
−5.80	10666	−29.53	2781
−1.30	13332	−19.77	5034
7.28	19998	−19.64	5057
13.78	26664	−9.86	8679
19.08	33331	−9.73	8718
23.57	39997	0.15	14340
31.01	53329	0.22	14430
37.08	66661	10.11	22750
42.35	79993	10.17	22840
46.78	93326	20.08	34860
47.627	95992	20.14	35000
48.453	98659	30.27	51930
49.262	101325	40.23	74670
		50.14	104580
		60.12	143100
eq. 2	P/mmHg	65.10	166090
A	6.88676	70.06	191640
B	1124.162		
C	231.361	Wagner eq. given in ref.	
bp/°C	49.262		
$\Delta H_v/(\text{kJ mol}^{-1}) =$			
at 25°C	28.53		
at bp	27.30		

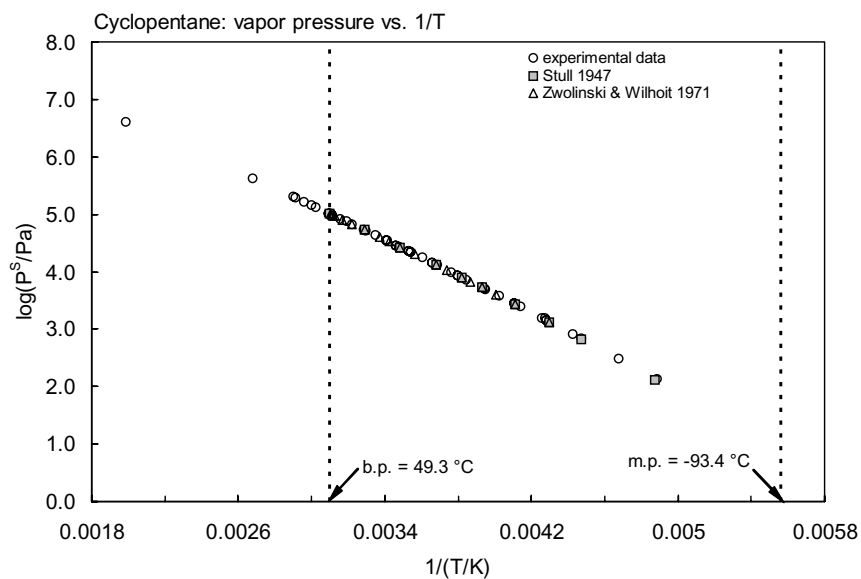


FIGURE 2.1.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for cyclopentane.

TABLE 2.1.1.2.1.3

Reported Henry's law constants of cyclopentane at various temperatures

Hansen et al. 1993

EPICS-GC

t/°C	H/(kPa m ³ /mol)
27.9	16.617
35.8	24.318
45.0	30.398
ln [H/(Pa m ³ /mol)] = A – B/(T/K)	
H/(kPa m ³ /mol)	
A	14 ± 2.03
B	3351 ± 633

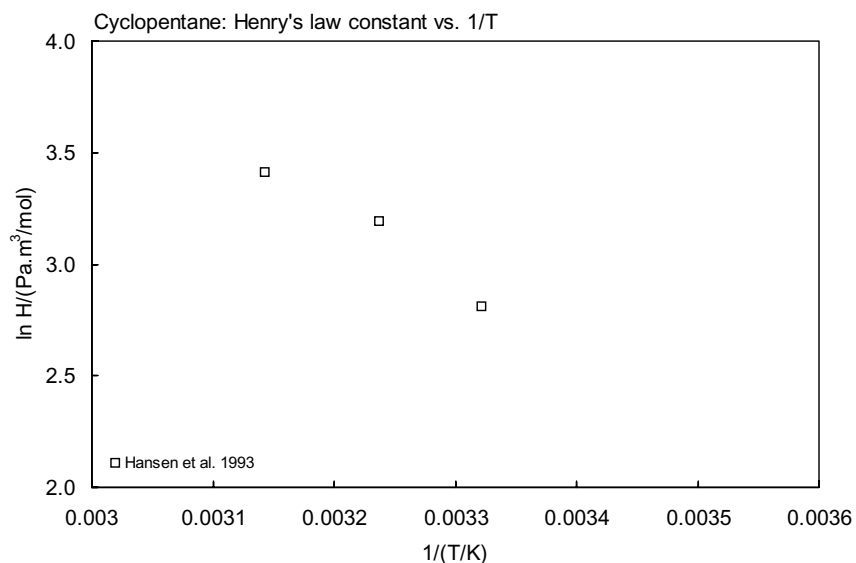


FIGURE 2.1.1.2.1.3 Logarithm of Henry's law constant versus reciprocal temperature for cyclopentane.

2.1.1.2.2 *Methylcyclopentane*

Common Name: Methylcyclopentane

Synonym:

Chemical Name: methylcyclopentane

CAS Registry No: 96-37-3

Molecular Formula: C_6H_{12}

Molecular Weight: 84.159

Melting Point ($^{\circ}C$):

-142.42 (Lide 2003)

Boiling Point ($^{\circ}C$):

71.8 (Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):0.7487, 0.7439 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955; Riddick et al. 1986)Molar Volume (cm^3/mol):112.4, 113.1 ($20^{\circ}C$, $25^{\circ}C$, calculated from density)

121.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):41.59, 29.08 ($25^{\circ}C$, bp, Riddick et al. 1986)Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.929 (Riddick et al. 1986)

6.93 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

53.01, 43.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

42.6 (shake flask-GC, McAuliffe 1963)

42.0 (shake flask-GC, McAuliffe 1966)

41.8 (shake flask-GC, Price 1976)

45.0 (partition coefficient-GC, Rudakov & Lutsyk 1979)

43.0 (recommended, IUPAC Solubility Data Series, Shaw 1989)

74.8 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):16680 ($22.75^{\circ}C$, ebulliometry-manometer, measured range 15.0 – $22.6^{\circ}C$, Willingham et al. 1945) $\log(P/mmHg) = 6.86283 - 1186.059/(229.042 + t/^{\circ}C)$; temp range 15.0 – $22.6^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)17870 (Antoine eq. regression, temp range -53.7 to $71.8^{\circ}C$, Stull 1947)

18330 (calculated from exptl. determined data, Dreisbach 1955)

 $\log(P/mmHg) = 6.86283 - 1186.059/(226.042 + t/^{\circ}C)$; temp range -5 to $125^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)18302 (interpolated-Antoine eq., temp range -23.7 to $95.7^{\circ}C$, Zwolinski & Wilhoit 1971) $\log(P/mmHg) = 6.86283 - 1186.059/(226.042 + t/^{\circ}C)$; temp range -23.7 to $95.7^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)17850 (interpolated-Antoine eq., temp range -53.7 to $71.8^{\circ}C$, Weast 1972–73) $\log(P/mmHg) = [-0.2185 \times 7490.0/(T/K)] + 7.945471$; temp range -53.7 to $71.8^{\circ}C$ (Antoine eq., Weast 1972–73) $\log(P/atm) = [1 - 344.830/(T/K)] \times 10^{0.872156 - 9.88091 \times 10^{-4} \cdot (T/K) + 10.8367 \times 10^{-7} \cdot (T/K)^2}$; temp range: 183.15 – $513.15\ K$ (Cox eq., Chao et al. 1983)

18330 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 5.99178 - 1188.32/(226.307 + t/^{\circ}\text{C})$; temp range 15.035–72.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

18330 (interpolated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 6.86283 - 1186.059/(226.04 + t/^{\circ}\text{C})$; temp range –24 to 96°C (Antoine eq., Dean 1985, 1992)

18400 (lit. average, Riddick et al. 1986)

$\log(P/\text{kPa}) = 5.98773 - 1186.059/(226.042 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

18340 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.98551 - 1184.874/(-47.232 + T/\text{K})$; temp range 288–346 K (Antoine eq., Stephenson & Malanowski 1987)

18400, 17066 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 32.4766 - 2.6434 \times 10^3/(T/\text{K}) - 8.733 \cdot \log(T/\text{K}) + 2.0749 \times 10^{-11} \cdot (T/\text{K}) + 3.2158 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 131–533 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

36664 (calculated as $1/K_{\text{AW}}$, C_W/C_A reported as exptl., Hine & Mookerjee 1975)

22090, 27810 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

36700; 36700, 36800 (recommended, calculated-P/C, Mackay & Shiu 1981)

25370 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

36934 (calculated-P/C, Eastcott et al. 1988)

36180 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.35 (calculated- π substituent constant, Hansch et al. 1968)

3.37 (shake flask, Log P Database, Hansch & Leo 1987)

3.37 (recommended, Sangster 1989)

3.37 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 7.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1990, 1991)

$k_{\text{OH}} = 7.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a estimated lifetime $\tau = 20 \text{ h}$ in summer daylight (Altshuller 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

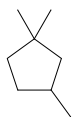
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

rate constant $k = 7.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in air (Atkinson 1990, 1991, Altshuller 1991); and an estimated reaction lifetime $\tau = 20 \text{ h}$ in summer daylight (Altshuller 1991).

2.1.1.2.3 1,1,3-Trimethylcyclopentane



Common Name: 1,1,3-Trimethylcyclopentane

Synonym:

Chemical Name: 1,1,3-trimethylcyclopentane

CAS Registry No: 4516-69-2

Molecular Formula: C_8H_{16}

Molecular Weight: 112.213

Melting Point ($^{\circ}C$):

-142.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

104.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7483, 0.7430 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

Molar Volume (cm^3/mol):

146.0 ($20^{\circ}C$, calculated-density, Wang et al. 1992)

166.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

36.23, 32.35 ($25^{\circ}C$, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.73 (shake flask-GC, Price 1976)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/mmHg) = 6.80948 - 1275.998/(219.899 + t/^{\circ}C)$; temp range 28.9 – $105.8^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

5300 (calculated from determined data, Dreisbach 1955)

$\log (P/mmHg) = 6.80947 - 1275.988/(219.899 + t/^{\circ}C)$; temp range 20 – $140^{\circ}C$ (interpolated-Antoine eq. for liquid state, Dreisbach 1955)

5300 (interpolated-Antoine eq., temp range -0.30 to $131.3^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.80947 - 1275.998/(219.899 + t/^{\circ}C)$; temp range -0.30 to $131.3^{\circ}C$ (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/atm) = [1 - 378.056/(T/K)] \times 10^{0.848231 - 8.28174 \times 10^{-4} \cdot (T/K) + 8.81168 \times 10^{-7} \cdot (T/K)^2}$; temp range: 272.85 – $404.45\ K$ (interpolated-Cox eq., Chao et al. 1983)

5300 (interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.93423 - 1275.928/(219.893 + t/^{\circ}C)$; temp range 28.944 – $105.8^{\circ}C$ (extrapolated-Antoine eq. from reported exptl. data, Boublik et al. 1984)

5070 (extrapolated-Antoine eq., temp range 29 – $106^{\circ}C$, Dean 1985, 1992)

$\log (P/mmHg) = 6.80931 - 1275.92/(219.89 + t/^{\circ}C)$; temp range 29 – $106^{\circ}C$ (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P_L/kPa) = 5.93036 - 1273.902/(-53.454 + T/K)$; temp range 301 – $379\ K$ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

159000 (calculated-P/C, Mackay & Shiu 1981)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.28 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
- 3.34 (calculated-molar volume V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

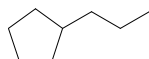
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

- Air: atmospheric $t_{1/2} \sim 2.4\text{--}24$ h for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976).

2.1.1.2.4 *n*-Propylcyclopentane

Common Name: *n*-Propylcyclopentane

Synonym:

Chemical Name: *n*-propylcyclopentane

CAS Registry No: 2040-96-2

Molecular Formula: C₈H₁₆

Molecular Weight: 112.213

Melting Point (°C):

−117.3 (Dreisbach 1955; Lide 2003)

Boiling Point (°C):

130.937 (Willingham et al. 1945)

131 (Lide 2003)

Density (g/cm³ at 20°C):

0.7763, 0.7723(20°C, 25°C, Dreisbach 1955)

Molar Volume (cm³/mol):

144.6 (20°C, calculated-density)

166.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.197, 34.746(25°C, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.04 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

64.45, 57.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

2.04 (shake flask-GC, Price 1976)

1.77 (shake flask-GC, Krzyzanowska & Szeliga 1978)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

log (P/mmHg) = 6.89887 − 1380.391/(212.610 + t/°C); temp range 51.7–131.9°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

log (P/mmHg) = 6.30392 − 1384.386/(213.159 + t/°C); temp range 51.9–131.9°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

1650 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.90392 − 1384.386/(213.159 + t/°C); temp range 40–170°C (extrapolated-Antoine eq. for liquid state, Dreisbach 1955)

1640 (interpolated-Antoine eq., temp range −21.3 to 158.2°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.30392 − 1384.386/(213.159 + t/°C); temp range −21.3 to 158.2°C (Antoine eq., Zwolinski & Wilhoit 1971)

1646 (extrapolated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 6.91061 − 1388.511/(213.615 + t/°C); temp range 51.88–131.97°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1973)

1640, 5320 (quoted, calculated-bp, Mackay et al. 1982)

log (P/atm) = [1 − 427.713/(T/K)] × 10⁴{0.865420 − 7.04026 × 10^{−4}·(T/K) + 5.98562 × 10^{−7}·(T/K)²}; temp range: 313.35–458.95 K (Cox eq., Chao et al. 1983)

1644 (extrapolated-Antoine eq., temp range 40–186°C, Dean 1985, 1992)

log (P/mmHg) = 6.88646 − 1460.80/(207.94 + t/°C); temp range 40–186°C (Antoine eq., Dean 1985, 1992)

log (P_L/kPa) = 6.04236 − 1393.284/(−58.949 + T/K); temp range 323–406 K (Antoine eq., Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 33.922 - 3.2097 \times 10^3/(T/K) - 8.9914 \cdot \log (T/K) - 3.2992 \times 10^{-11} \cdot (T/K) + 2.0684 \times 10^{-6} \cdot (T/K)^2; \text{ temp range } 156\text{--}603 \text{ K (vapor pressure eq., Yaws 1994)}$$

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

90200 (calculated-P/C, Mackay & Shiu 1981)

90430 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.95 (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)

2.65 (calculated-molar volume V_M , Wang et al. 1992)

4.37 (calculated-fragment const., Müller & Klein 1992)

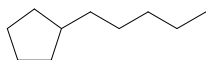
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

2.1.1.2.5 *Pentylcyclopentane*

Common Name: Pentylcyclopentane

Synonym: 1-cyclopentylpentane

Chemical Name: pentylcyclopentane

CAS Registry No: 3741-00-2

Molecular Formula: $C_{10}H_{20}$

Molecular Weight: 140.266

Melting Point ($^{\circ}C$):

-83 (Dreisbach 1955; Lide 2003)

Boiling Point ($^{\circ}C$):

180 (Dreisbach 1955; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7912, 0.7874 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

177.3, 178.1 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

210.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

51.12, 39.94 (25° , bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.115 (shake flask-GC, Price 1976)

0.13 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

159 (calculated by formula, Dreisbach 1959)

$\log(P/mmHg) = 6.929 - 1526.0/(197.0 + t/^{\circ}C)$; temp range $85-220^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

152 (extrapolated-Antoine eq., temp range $60-210^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.9414 - 1540.6/(198.8 + t/^{\circ}C)$; temp range $60-210^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

18500 (calculated-P/C, Mackay & Shiu 1981)

18600 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

2.1.1.2.6 Cyclohexane



Common Name: Cyclohexane

Synonym: hexahydrobenzene, hexamethylene

Chemical Name: cyclohexane

CAS Registry No: 110-82-7

Molecular Formula: C_6H_{12}

Molecular Weight: 84.159

Melting Point ($^{\circ}C$):

6.59 (Lide 2003)

Boiling Point ($^{\circ}C$):

80.73 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7786, 0.7739 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm^3/mol):

108.1 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Lande & Banerjee 1981)

118.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.89, 30.05 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

2.677 (Riddick et al. 1986)

5.84, 2.68; 9.41 (-87.05 , $6.65^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

45.77, 44.55 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$, additional data at other temperatures designated * are compiled at the end of this section.):

80.0 (shake flask-gravitational method, McBain & Lissant 1951)

55.0 (shake flask-GC, McAuliffe 1963, 1966)

88.84* (shake flask-GC/FID, measured range 5.11 – $45.21^{\circ}C$, Pierotti & Liabastre 1972)

56.7 (shake flask-GC/FID, Leinonen & Mackay 1973)

57.5 (shake flask-vapor extraction-GC/FID, Mackay & Shiu 1975)

55.8, 50.2, 61.7 (shake flask-GC, Mackay et al. 1975)

66.5 (shake flask-GC/FID, Price 1976)

66.5 (shake flask-GC, Krzyzanowski & Szeliga 1978)

52.0 ($23.5^{\circ}C$, elution chromatography, Schwarz 1980)

72.4 (calculated-HPLC- k' correlation, converted from reported γ_w , Hafkenscheid & Tomlinson 1983)

72.8* ($40^{\circ}C$, shake flask-GC, measured range 40 – $209.06^{\circ}C$, Tsonopoulos & Wilson 1983)

58.4 (shake flask-GC, Groves 1988)

58.0* (IUPAC recommended best value, Shaw 1989a)

$\ln x = -301.366 + 12924.45/(T/K) + 43.2980 \cdot \ln (T/K)$; temp range 290 – 400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 2001)

$\ln x = -219.863 + 6693.78/(T/K) + 31.3744 \cdot \ln (T/K)$; temp range 290 – 400 K (eq. derived from direct fit of solubility data, Tsonopoulos 2001)

60.78 (calculated-liquid-liquid equilibrium LLE data, temp range 278.2 – 482.2 K, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

12972 (gas saturation/air-bubbling method, Washburn & Handorf 1935)

16212* ($30^{\circ}C$, vapor-liquid equilibrium VLE data, measured range 30 – $80^{\circ}C$, Scatchard et al. 1939)

- log (P/mmHg) = $6.65859 - 1040.641/(T/K) - 104.865/(T/K)^2$; temp range 30–60°C (VLE data, Scatchard et al. 1939)
- 10910* (20.97°C, manometry, measured range 6.33–20.97 °C, Aston et al. 1943b)
- 11700* (20.96°C, ebulliometry-manometer, measured range 19.9–81.6°C, Willingham et al. 1945)
- log (P/mmHg) = $6.84498 - 1203.526/(222.863 + t/°C)$; temp range 19.9–81.6°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
- 12280* (calculated-Antoine eq. regression, temp range –45.3 to 80.7°C, Stull 1947)
- 10253*; 10375 (20.015°C, selected exptl., calculated-Frost-Kalkwarf vapor pressure eq., temp range 293.185–551.225 K, Pasek & Thodos 1962)
- log (P/mmHg) = $23.14002 - 2411.8/(T/K) - 5.17900 \cdot \log (T/K) + 1.84394 \cdot [(P/\text{mmHg})/(T/K)^2]$; temp range 293.185–551.225 K (Frost-Kalkwarf eq., Pasek & Thodos 1962)
- 13040* (static method, measured range 25–75°C, Cruickshank & Cutler 1967)
- log (P/mmHg) = $6.85875 - 1212.014/(233.956 + t/°C)$; temp range 25–75°C (static method, Cruickshank & Cutler 1967)
- 13010 (calculated from determined data, Dreisbach 1955)
- log (P/mmHg) = $6.84498 - 1203.526/(222.863 + t/°C)$; temp range –20 to 142°C (Antoine eq. for liquid state, Dreisbach 1955)
- 13159* (25.26°C, temp range 17.55–80.22°C, Boublik 1960; quoted, Boublik et al. 1984)
- 13014* (interpolated-Antoine eq., temp range 6.59–105.2°C, Zwolinski & Wilhoit 1971)
- log (P/mmHg) = $6.84130 - 1201.531/(222.647 + t/°C)$; temp range 6.59–105.2°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 11170 (interpolated-Antoine eq., temp range –45.3 to 257.5°C, Weast 1972–73)
- log (P/mmHg) = $[-0.2185 \times 7830.9/(T/K)] + 7.662126$; temp range –45.3 to 257.5°C (Antoine eq., Weast 1972–73)
- log (P/atm) = $[1 - 353.663/(T/K)] \times 10^{[0.881199 - 9.58655 \times 10^{-4} \cdot (T/K) + 9.72305 \times 10^{-7} \cdot (T/K)^2]}$; temp range 227.85–553.64 K (Cox eq., Chao et al. 1983)
- 13010, 13040 (interpolated-Antoine equations, Boublik et al. 1984)
- log (P/kPa) = $5.97561 - 1206.731/(223.223 + t/°C)$, temp range 19.9–81.6°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
- log (P/kPa) = $6.98226 - 1211.248/(223.869 + t/°C)$; temp range 25–75°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- log (P/kPa) = $6.00569 - 1223.273/(225.089 + t/°C)$; temp range 17.55–80.22°C (Antoine eq. from reported exptl. data of Cruickshank & Cutler 1967, Boublik et al. 1984)
- 13020 (interpolated-Antoine eq., temp range 20–81°C, Dean 1985, 1992)
- log (P/mmHg) = $6.84130 - 1201.53/(222.65 + t/°C)$; temp range 20–81°C (Antoine eq., Dean 1985, 1992)
- 13040 (lit. average, Riddick et al. 1986)
- log (P/kPa) = $5.96407 - 1200.31/(222.504 + t/°C)$; temp range not specified (Antoine eq., Riddick et al. 1986)
- 13070 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P_S/kPa) = $7.2778 - 1747.2/(26.84 + T/K)$; temp range 223–280 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $5.9682 - 1201.531/(-50.503 + T/K)$; temp range 293–335 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.03245 - 1244.124/(-44.911 + T/K)$; temp range 353–414 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.36849 - 1519.732/(-4.032 + T/K)$; temp range 412–491 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $7.37347 - 2683.075/(159.31 + T/K)$; temp range 489–533 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- 12920, 1730 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)
- log (P/mmHg) = $48.5529 - 3.0874 \times 10^3/(T/K) - 15.521 \cdot \log (T/K) + 7.383 \times 10^{-3} \cdot (T/K) + 6.3563 \times 10^{-12} \cdot (T/K)^2$; temp range 280–554 K (vapor pressure eq., Yaws 1994)
- 12068* (23.363°C, comparative ebulliometry, measured range 281–552 K, data fitted to Wagner eq., Ewing & Ochoa 2000)
- 16230, 36180 (30, 50°C, VLE equilibrium data, Carmona et al. 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 19860 (calculated-P/C, Mackay & Shiu 1975)
- 19690 (calculated as $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
- 18380, 27810 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 18000 (recommended; Mackay & Shiu 1981)
- 22092 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 5532, 17935, 19353, 1450 (bubble column non-equilibrium measurement, EPICS-GC, direct concentration. ratio, calculated-UNIFAC activity coeff., Ashworth et al. 1988)
- 17935* (EPICS-GC/FID, measured range $10\text{--}30^\circ\text{C}$, Ashworth et al. 1988)
- $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 9.141 - 3238/(T/K)$; temp range: $10\text{--}30^\circ\text{C}$ (EPICS measurements, Ashworth et al. 1988)
- 19980 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 37190* (40°C , equilibrium headspace-GC, measured range $40\text{--}80^\circ\text{C}$, Kolb et al. 1992)
- $\ln (1/K_{\text{AW}}) = -12.90 + 3228/(T/K)$; temp range: $40\text{--}80^\circ\text{C}$ (equilibrium headspace-GC measurements, Kolb et al. 1992)
- 15062 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
- $\log K_{\text{AW}} = 5.154 - 1279/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.46 (calculated- π substituent constant, Hansch et al. 1968)
- 3.44 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979)
- 3.40 (Cramer 1977)
- 3.18, 3.48, 3.48 (calculated-fragment const., Rekker 1977)
- 3.69 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
- 3.70 (from activity coefficient measurement, Berti et al. 1986)
- 3.44 (recommended, Sangster 1989, 1993)
- 3.73 (from activity coefficient measurement, Tse & Sandler 1994)
- 3.44 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated. Additional data at other temperatures designated* are compiled at the end of this section:

- 2.83* (20.29°C , from GC-determined γ^∞ in octanol, measured range $20.29\text{--}50.28^\circ\text{C}$, Gruber et al. 1997)
- 2.71 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 2.38 (estimated, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.68 (estimated-S, Howard 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 2.8$ h from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982, quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}^*(\text{exptl}) = 5.38 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 4.79 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–497 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

$k_{\text{OH}}(\text{exptl}) = 6.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K; $k_{\text{OH}}(\text{calc}) = 6.7 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 300 K (Darnall et al. 1978)

$k_{\text{O}(3\text{P})} = 1.40 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atoms at room temp. (Herron & Huie 1973)

$k_{\text{OH}} = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979)

$k_{\text{OH}} = (7.57 \pm 0.05) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{\text{OH}} = (6.20 \pm 0.44) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(24.4 \pm 0.4)^\circ\text{C}$ with an atmospheric lifetime of 1.9 d for an average OH radical concentration of $1.0 \times 10^6 \text{ molecules/cm}^3$ (Edney et al. 1986)

$k_{\text{OH}} = 7.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (Atkinson 1986; quoted, Edney et al. 1986)

$k_{\text{OH}} = 7.14 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K, measured range 292–491 K (Droege & Tully 1987)

$k_{\text{OH}} = 7.38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Dilling et al. 1988)

$k_{\text{OH}}^* = 7.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}^* = 7.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 13.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{\text{NO}_3} = 1.35 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1991)

$k_{\text{NO}_3}(\text{exptl}) = 1.35 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}(\text{calc}) = 2.04 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Aschmann & Atkinson 1995)

$k_{\text{OH}}^* = 7.21 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

$k_{\text{OH}}^* = 6.69 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation: highly resistant to biodegradation (Howard 1990);

$t_{1/2}(\text{aq. aerobic}) = 672 \text{ to } 4032 \text{ h}$, based on unacclimated grab sample of aerobic soil and aerobic aqueous screening test data (Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 2688 \text{ to } 16280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

atmospheric lifetime $\tau = 1.9 \text{ d}$ for an average OH radical concentration of $1.0 \times 10^6 \text{ molecules/cm}^3$ (Edney et al. 1986);

$t_{1/2} = 52 \text{ h}$, based on photooxidation rate constant (Howard 1990);

an atmospheric lifetime $\tau \sim 19 \text{ h}$ in summer daylight, based on the photooxidation reaction rate constant of $7.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in air during summer daylight (Altshuller 1991);

will degrade photochemically by hydroxyl radicals with $t_{1/2} = 52 \text{ h}$ and much faster under photochemical smog conditions with $t_{1/2} = 6 \text{ h}$ (Howard 1990);

$t_{1/2} = 8.7\text{--}87 \text{ h}$, based on reaction with OH radical half-life in air (Howard et al. 1991).

Surface water: volatilization $t_{1/2} = 2 \text{ h}$ in a model river (Howard 1990);

$t_{1/2} = 672\text{--}4320 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

photooxidation $t_{1/2} = 1.4 \times 10^9 \text{ to } 6.9 \times 10^{10} \text{ h}$ (16000 to 780000 yr), based on measured rate data for alkylperoxyl radicals in aqueous solution (Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated grab sample of aerobic soil and aerobic aqueous screening test data (Howard et al. 1991).

Biota:

TABLE 2.1.1.2.6.2

Reported vapor pressures of cyclohexane at various temperatures and the coefficients for the vapor pressure equations:

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) + D[P/(T/K)^2] & (5) \\ \log P = A - B/T(T/K) - C/(T/K)^2 & (6) \end{array}$$

$$\begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

1.

Ashton et al. 1943b		Willingham et al. 1945		Stull 1947		Pasek & Thodos 1962	
manometry		ebulliometry		summary of literature data		selected exptl. data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
6.33	5388	19.915	10303	-45.3	133.3	20.015	10253
9.89	6421	22.657	11695	-25.4	666.6	52.693	39997
13.63	7697	26.347	13821	-15.9	1333	82.469	106658
17.65	9327	30.556	16610	-5.0	2666	105.215	199984
20.97	10910	34.821	19917	6.7	5333	160.015	670345
		38.789	23453	14.7	7999	219.905	1813184
mp/°C	6.69	44.108	28960	25.5	13332	240.395	3420467
bp/°C	80.8	48.991	43324	42.0	26664	278.075	3959408
		54.884	53659	60.8	53329		
$\Delta H_v/(\text{kJ mol}^{-1}) = 33.33$		60.969	66762	80.7	101325	bp/°C	80.75
at 25°C		67.467	83723				
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 2.627$		74.520	97609	mp/°C	6.60	Frost-Kalkwarf equation derived from exptl. data eq. 5 P/mmHg A 23.14002 B -2411.8 C -5.27900 D 1.84394	
		79.052	99209				
		80.037	100701				
		80.534	102403				
		81.093	103923				
Scatchard et al. 1939		81.582	103923			Frost-Kalkwarf equation calculated from molecular structures, normal bp and deviations of resulting v.p. eq. 5 P/mmHg A 23.09550 B -2411.82 C -5.26151 D 1.84394	
vapor-liquid equilibrium							
t/°C	P/Pa						
30	16212	bp/°C	80.738				
40	24613	eq. 2	P/mmHg				
50	36237	A	6.84498				
60	51901	B	1203.526				
70	72521	C	222.863				
80	88995						
eq. 6	P/mmHg						
A	6.65859						
B	1040.641						
C	116.197						

(Continued)

2.

Boublik 1960		Cruickshank & Cutler 1966		Zwolinski & Wilhoit 1971		Ewing & Ochoa 2000	
in Boublik et al. 1984		static method-manometry		selected values		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
17.55	9210	25	13040	6.69	5333	8.188	5777
20.16	10426	35	20104	11.01	6666	9.698	6243
22.98	11876	45	30008	14.66	7999	11.356	6791
25.26	13159	55	43538	20.666	10666	15.215	8225
28.77	15372	65	61551	25.536	13332	17.163	9039
32.77	18252	75	85012	34.904	19998	19.868	10284
37.10	21891			41.991	26664	22.608	11675
40.66	25264	mp/°C	6.55	47.763	33331	23.263	12086
45.77	30864	bp/°C	80.728	52.669	39997	28.346	15109
50.96	37543	density, d ²⁵	0.77386	60.784	53329	44.379	29290
56.18	45356			67.415	66661	49.393	35456
62.46	56448	$\Delta H_v/(kJ\ mol^{-1}) =$		73.067	79993	55.302	44015
68.71	69467	at 20°C	33.23	78.021	93326	60.881	53541
75.42	86053	25°C	32.97	78.944	95992	66.269	64227
80.22	99818	54.1°C	31.45	79.848	98659	71.034	75023
		73.3°C	30.44	80.292	99992	75.094	86306
bp/°C	80.731	80.7°C	30.03	80.732	101325	78.498	94753
						80.80	101589
		eq. 2	P/mmHg	eq. 2	P/mmHg	83.489	110504
		A	6.85875	A	6.84130	87.149	122451
		B	1212.014	B	1201.531		
		C	233.956	C	222.647		
				bp/°C	80.732	temp range 281–552 K data fitted to Wagner eq.	
				$\Delta H_v/(kJ\ mol^{-1}) =$			
				at 25°C	33.04		
				at bp	29.96		

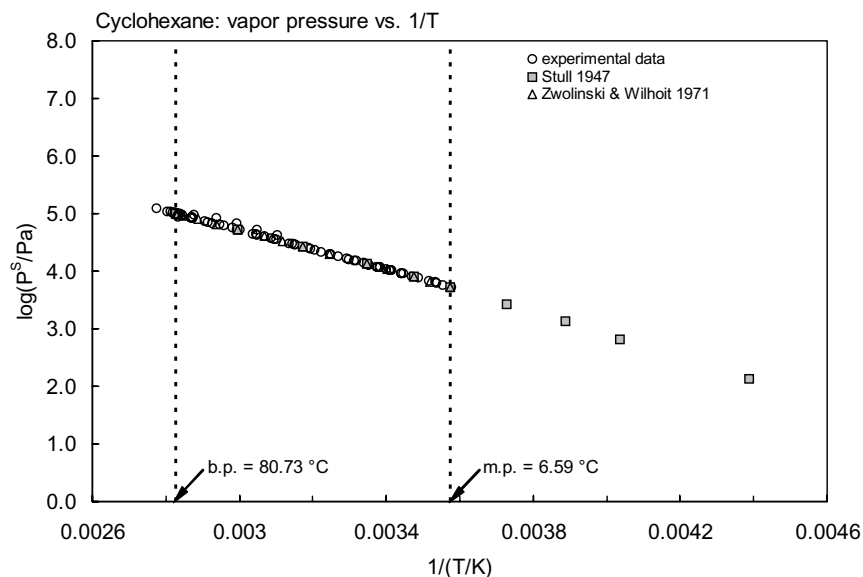


FIGURE 2.1.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexane.

TABLE 2.1.1.2.6.3

Reported Henry's law constants and octanol-air partition coefficients of cyclohexane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Henry's law constant				log K_{OA}	
Ashworth et al. 1988		Kolb et al. 1992		Gruber et al. 1997	
EPICS-GC		equilibrium headspace-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OA}
10	10436	40	37190	20.29	2.835
15	12767	60	55400	30.3	2.652
20	14189	70	95100	40.4	2.511
25	17935	80	146800	50.28	2.365
30	22595				
		eq. 2	1/ K_{AW}		
		A	-12.90		
eq. 4a	H/(atm m ³ /mol)	B	-3228		
A	9.141				
B	3238				

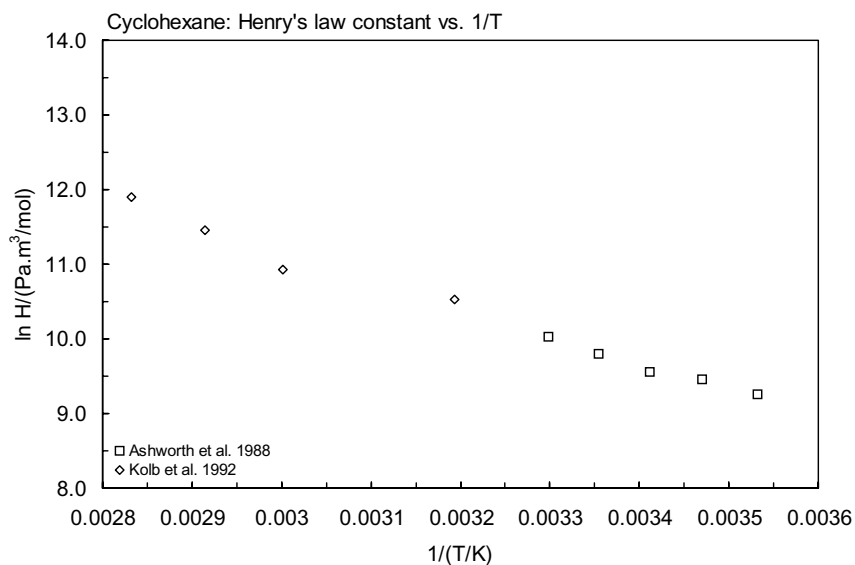


FIGURE 2.1.1.2.6.3 Logarithm of Henry's law constant versus reciprocal temperature for cyclohexane.

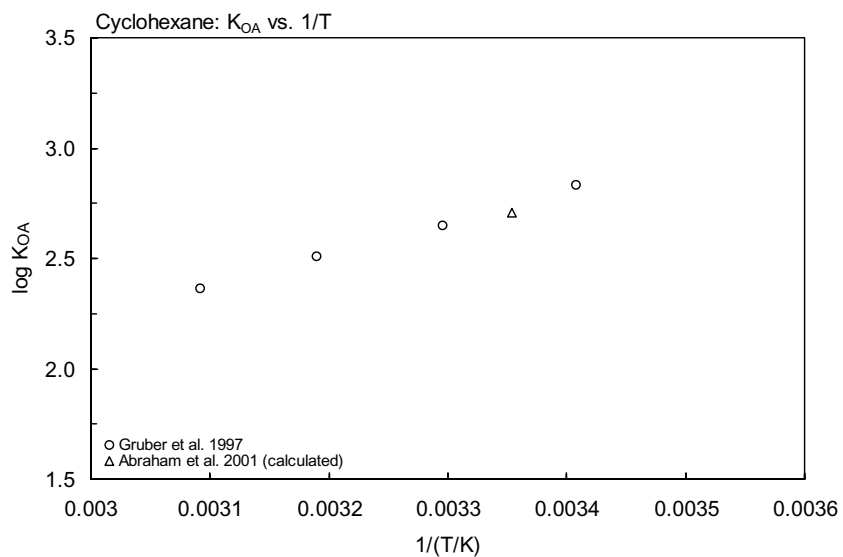
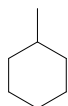


FIGURE 2.1.1.2.6.4 Logarithm of K_{OA} versus reciprocal temperature for cyclohexane.

2.1.1.2.7 Methylcyclohexane



Common Name: Methylcyclohexane

Synonym: hexahydrotoluene, cyclohexylmethane

Chemical Name: methylcyclohexane

CAS Registry No: 108-87-2

Molecular Formula: C_7H_{14}

Molecular Weight: 98.186

Melting Point ($^{\circ}C$):

-126.6 (Dreisbach 1959; Weast 1984; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

100.93 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7694, 0.7651 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm^3/mol):

127.6 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.359, 31.13 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.757 (Riddick et al. 1986)

6.75 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

46.1, 47.3 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

14.0 (shake flask-GC, McAuliffe 1963, 1966)

16.0* (shake flask-GC, measured range 25 – $149.5^{\circ}C$, Price 1976; quoted, Eastcott et al. 1988)

15.3 (partition coefficient-GC, Rudakov & Lutsyk 1979)

15.2 ($20^{\circ}C$, shake flask-GC, Burris & MacIntyre 1986)

16.7 (shake flask-GC, Groves 1988)

15.1* (IUPAC recommended, temp range 25 – $150^{\circ}C$, Shaw 1989)

15.82* (calculated-liquid-liquid equilibrium LLE data, temp range 298.2 – $410.5 K$, Mączyński et al. 2004)

16.15* ($26.1^{\circ}C$, shake flask-GC, measured range 26.1 – $170.8^{\circ}C$, Marche et al. 2004)

$\ln(S/ppm) = 13.091 - 7085.522/(T/K) + 1055594/(T/K)^2$ (Marche et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6128 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log(P/mmHg) = 6.95423 - 1336.93/(T/K - 45.52)$; temp range 4 – $75^{\circ}C$ (Antoine eq. based on exptl. data, Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)

6354* ($25.59^{\circ}C$, ebulliometry-manometer, Willingham et al. 1945)

$\log(P/mmHg) = 6.82689 - 1272.864/(221.630 + t/^{\circ}C)$; temp range 25.6 – $101.8^{\circ}C$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

5887* (calculated-Antoine eq. regression, temp range -35.9 to $100.0^{\circ}C$, Stull 1947)

6180 (calculated from determined data, Dreisbach 1955)

$\log(P/mmHg) = 6.82689 - 1272.864/(221.630 + t/^{\circ}C)$; temp range 10 – $155^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

10207* ($35.901^{\circ}C$, temp range 35.901 – $95.946^{\circ}C$, Varushchenko et al. 1970)

- 6180* (interpolated-Antoine eq., temp range -3.20 to 127.0°C , Zwolinski & Wilhoit 1971)
 $\log(P/\text{mmHg}) = 6.82300 - 1272.763/(221.416 + t/^{\circ}\text{C})$; temp range -3.20 to 127.0°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 5880 (interpolated-Antoine eq., temp range -35.9 to 100°C , Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 8549.2/(T/\text{K})] + 7.909762$; temp range -35.9 to 100°C (Antoine eq., Weast 1972–73)
- 5806 (calculated-bp, Mackay et al. 1982)
 $\log(P/\text{atm}) = [1 - 373.957/(T/\text{K})] \times 10^{\{0.862568 - 8.71426 \times 10^{-4} \cdot (T/\text{K}) + 8.69685 \times 10^{-7} \cdot (T/\text{K})^2\}}$; temp range 203.20 – 563.20 K (Cox eq., Chao et al. 1983)
- 5364, 6111, 6177 (Antoine equations, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.95366 - 1273.962/(221.755 + t/^{\circ}\text{C})$; temp range 25.6 – 101.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.95497 - 1275.047/(221.678 + t/^{\circ}\text{C})$; temp range 35.9 – 95.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.92856 - 1253.199/(216.058 + t/^{\circ}\text{C})$; temp range 58.645 – 113.6°C (Antoine eq. from reported exptl. data of Meyer et al. 1976, Boublik et al. 1984)
- 6180 (interpolated-Antoine eq., temp range -3 to 127°C , Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.82300 - 1270.763/(221.42 + t/^{\circ}\text{C})$; temp range -3 to 127°C (Antoine eq., Dean 1985, 1992)
- 6100 (quoted lit., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.94790 - 1270.763/(221.416 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
- 6160 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.9428 - 1266.954/(-52.282 + T/\text{K})$; temp range 308 – 368 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.14677 - 1413.495/(-32.726 + T/\text{K})$; temp range 373 – 511 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.29186 - 2700.205/(147.549 + T/\text{K})$; temp range 501 – 573 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 38.0955 - 3.0738 \times 10^3/(T/\text{K}) - 10.684 \cdot \log(T/\text{K}) - 5.1766 \times 10^{-11} \cdot (T/\text{K}) + 3.5282 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 147 – 572 K (vapor pressure eq., Yaws 1994)
- 5205* (21.46°C , static method-manometry, measured range -76.96 to 41.44°C , Mokbel et al. 1995)
 $\ln x = -328.666 + 14073.29/(T/\text{K}) + 47.1467 \cdot \ln(T/\text{K})$; temp range 290 – 400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 2001)
 $\ln x = -491.070 + 22132.10/(T/\text{K}) + 70.9150 \cdot \ln(T/\text{K})$; temp range 290 – 400 K (eq. derived from direct fit of solubility data, Tsionopoulos 2001)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 44080 (calculated as $1/K_{\text{AW}}, C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
- 31030, 41340 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 40000 (recommended; Mackay & Shiu 1981)
- 31934 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 37930 (calculated-P/C, Eastcott et al. 1988)
- 43300 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 12666* (27.3°C , EPICS-GC, measured range 27.3 – 45°C , Hansen et al. 1993)
 $\ln[H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -9406/(T/\text{K}) + 34.0$; temp range 27.3 – 45°C (EPICS-GC, Hansen et al. 1993)
- 6410 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 13.507 - 3836/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.76 (calculated- π substituent constant, Hansch et al. 1968)
- 2.96 (calculated- MCI π , Murray et al. 1975)
- 2.82 (Hansch & Leo 1979)
- 3.88 (recommended, Sangster 1989, 1993)
- 4.10 (calculated-fragment const. per Lyman 1982, Thoms & Lion 1992)
- 2.89 (calculated-molar volume V_{M} , Wang et al. 1992)

- 3.87 (calculated-fragment const., Müller & Klein 1992)
 3.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.14* (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.29–50.28°C Gruber et al. 1997)
 3.05 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (10.6 \pm 0.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 1.04 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = 1.04 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K with an estimated half-life of 13 h (Altshuller 1991)

$k_{OH} = 1.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biotransformation:

Biodegradation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: an atmospheric lifetime was estimated to be 13 h in summer daylight, based on the photooxidation rate constant of $1.04 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radicals in air (Altshuller 1991).

TABLE 2.1.1.2.7.1

Reported aqueous solubilities of methylcyclohexane at various temperatures

Price 1976		Shaw 1989a		Marche et al. 2004		Mączyński et al. 2004	
Shake flask-GC		IUPAC recommended		Shake flask-GC		Calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
		25	15.1	26.1	16.15	25	15.82
25.0	16.0	30	17.0	70.5	27.49	40.1	16.91
40.1	18.0	40	18.0	100.5	54.88	55.7	19.64
55.7	18.9	50	19.0	131.0	133.1	99.1	44.18
99.1	33.8	70	22.0	151.4	230.7	120	76.37
120.0	79.5	90	29.0	170.8	386.2	137.3	125.5
137.3	139	110	52.0	$S = A - B/(T/K) + C/(T/K)^2$ S g/m ³ A 13.091 B 7085.522 C 1055594			
149.5	244	130	110				
		150	250				

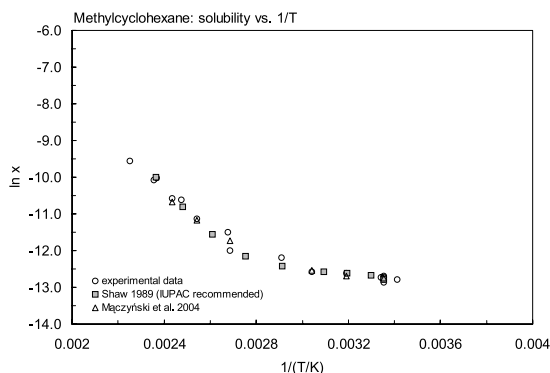


FIGURE 2.1.1.2.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for methylcyclohexane.

TABLE 2.1.1.2.7.2

Reported vapor pressures of methylcyclohexane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot \log (T/K) + D[P/(T/K)^2]$	(5)		

1.

Willingham et al. 1945		Stull 1947		Varushchenko et al. 1970		Zwolinski & Wilhoit 1971	
ebulliometry		summary of literature data				selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
25.585	6354	−35.9	133.3	35.901	10207	−3.20	1333
29.533	7655	−14.0	666.6	45.809	15552	8.70	2666
32.976	8962	−3.2	1333	50.799	19018	16.3	4000
36.089	10303	8.7	2666	55.419	22754	21.98	5333
38.998	11696	22.0	5333	61.644	28719	26.585	6666
42.929	13820	35.0	7999	67.476	35390	30.477	7999
47.407	16919	42.1	13332	74.177	44530	36.874	10666
51.964	19918	59.6	26664	81.020	55721	42.063	13332
56.194	23453	79.6	53329	88.101	69542	52.048	19998
61.857	28958	100.0	101325	93.567	81944	59.604	26664
67.067	34896			94.159	93376	65.758	33331
73.349	43323	mp/°C	−126.4	94.766	84890	70.990	39997
79.842	53657			95.307	86243	79.646	53329
86.771	66760			95.946	87847	86.720	66661
94.299	83721					92.752	79993
99.614	97628					98.039	93326
100.185	99205					99.025	95992
100.715	100697					99.989	98659
101.312	102398					100.464	99992
101.832	103919					100.934	101325

TABLE 2.1.1.2.7.2 (Continued)

Willingham et al. 1945		Stull 1947		Varushchenko et al. 1970		Zwolinski & Wilhoit 1971	
ebulliometry		summary of literature data				selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
100.715	100697					99.989	98659
101.312	102398					100.464	99992
101.832	103919					100.934	101325
bp/°C	100.934					eq. 2	P/mmHg
						A	6.82300
eq. 2	P/mmHg					B	1270.763
A	6.82689					C	221.416
B	1272.864					bp/°C	100.934
C	221.630					$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	35.36
						at bp	31.13

2.

Mokbel et al. 1995

static method-manometry					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-76.96	1.68	-28.28	240	21.46	5205
-67.0	5.87	-18.38	497	31.45	8368
-58.55	15.8	-8.44	970	41.44	12950
-48.64	42.4	1.50	1785		
-38.15	108	11.47	3128	data fitted to Wagner eq.	

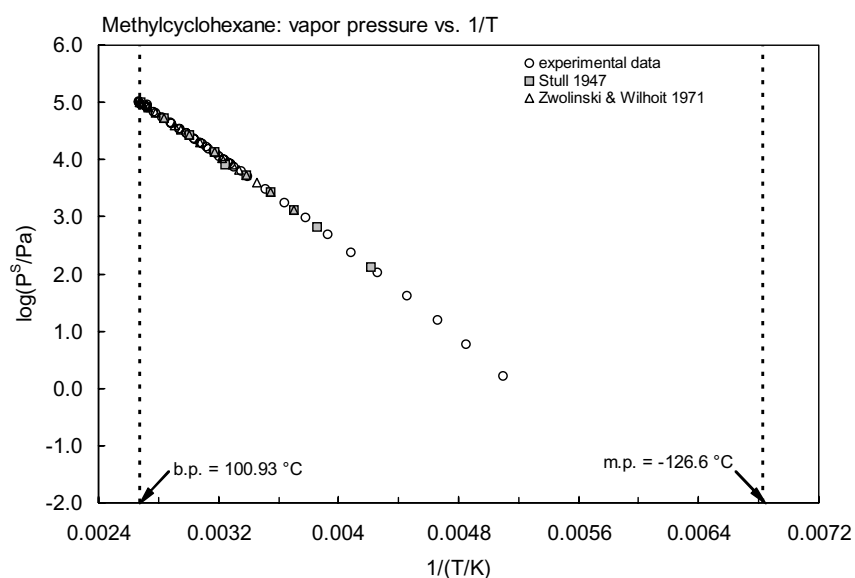


FIGURE 2.1.1.2.7.2 Logarithm of vapor pressure versus reciprocal temperature for methylcyclohexane.

TABLE 2.1.1.2.7.3

Reported Henry's law constants and octanol-air partition coefficients of methylcyclohexane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)		
Henry's law constant		$\log K_{OA}$		
Hansen et al. 1993		Gruber et al. 1997		
EPICS-GC		GC det'd activity coefficient		
t/°C	H/(kPa m ³ /mol)	t/°C	.log K _{OA}	
27.3	12.666	20.29	3.142	
35.8	34.653	30.3	2.943	
45.0	72.447	40.4	2.784	
		50.28	2.632	
eq. 4	H/(kPa m ³ /mol)			
A	34 ± 3.39			
B	9406 ± 1046			

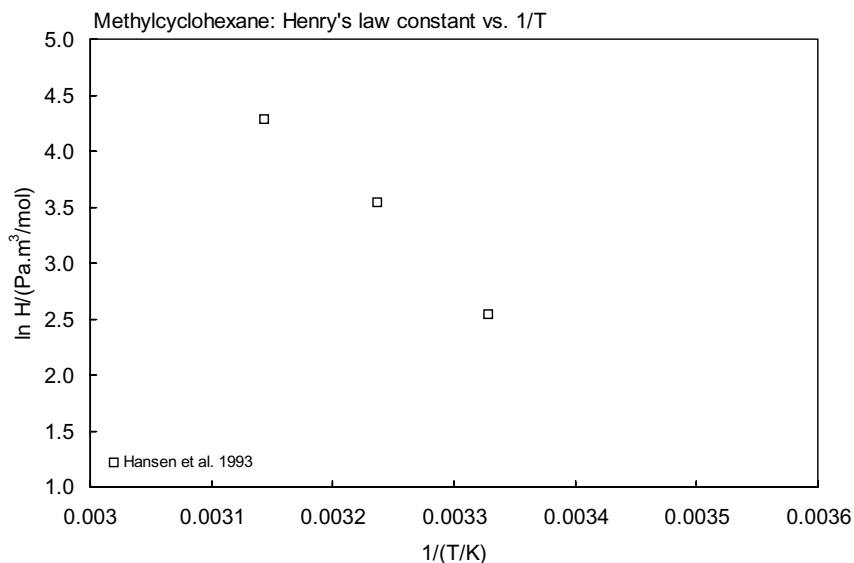


FIGURE 2.1.1.2.7.3 Logarithm of Henry's law constant versus reciprocal temperature for methylcyclohexane.

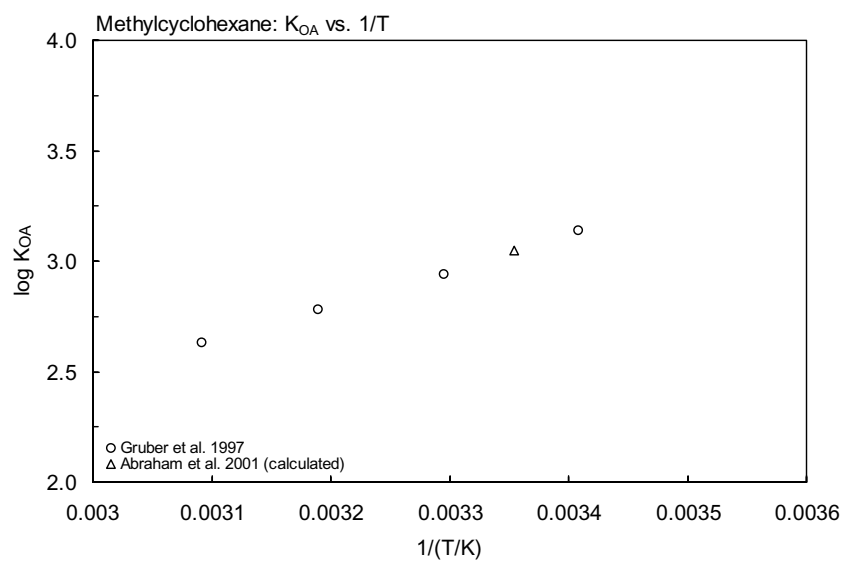
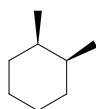


FIGURE 2.1.1.2.7.4 Logarithm of K_{OA} versus reciprocal temperature for methylcyclohexane.

2.1.1.2.8 1,2-*cis*-Dimethylcyclohexane

Common Name: 1,2-*cis*-Dimethylcyclohexane

Synonym: *cis*-1,2-dimethylcyclohexane

Chemical Name: 1,2-*cis*-dimethylcyclohexane

CAS Registry No: 2207-01-4

Molecular Formula: C₈H₁₆

Molecular Weight: 112.213

Melting Point (°C):

−49.8 (Lide 2003)

Boiling Point (°C):

129.8 (Lide 2003)

Density (g/cm³ at 20°C):

0.7963, 0.7922 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm³/mol):

140.9 (20°C, calculated-density, McAuliffe 1966)

141.6 (25°C, calculated-density; Ruelle & Kesselring 1997)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.715, 34.196 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

1.644 (Dreisbach 1955; Riddick et al. 1986)

8.26, 1.64 (−100.65, −39.05°C, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

55.22, 50.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6.0 (shake flask-GC, McAuliffe 1966)

5.01 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

5.94* (generator column-GC, measured range 273.15–313.15 K, Dohányosová et al. 2004)

$\ln x = -59.7348 + 45.8700/\tau + 46.6282 \cdot \ln \tau$; $\tau = T/298.15$ K (empirical eq., generator column-GC, Dohányosová et al. 2004)

$\ln (S/\text{ppm}) = 11.610 - 8455.943/(T/K) + 961943.2/(T/K)^2$, temp range 30.3–170°C (Marche et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6352* (49.185°C, ebulliometry, measured range 49.185–130.684°C, Willingham et al. 1945)

1333* (18.4°C, summary of literature data, temp range −15.9 to 129.7°C, Stull 1947)

$\log (P/\text{mmHg}) = 6.84164 - 1369.525/(216.040 + t/^\circ\text{C})$; temp range 49.2–130.7°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

1929 (calculated by formula, Dreisbach 1955)

$\log (P/\text{mmHg}) = 6.84164 - 1369.525/(216.040 + t/^\circ\text{C})$; temp range 40–170°C (Antoine eq. for liquid state, Dreisbach 1955)

1933* (interpolated-Antoine eq., temp range 18.4–157.6°C, Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 6.83746 - 1367.311/(215.835 + t/^\circ\text{C})$; temp range 18.4–157.6°C (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 9364.9/(T/K)] + 8.001159$; temp range −15.9 to 129.7°C (Antoine eq., Weast 1972–73)

$\log (P/\text{atm}) = [1 - 402.894/(T/K)] \times 10^{\{0.841813 - 8.56119 \times 10^{-4} \cdot (T/K) + 5.01855 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 257.25–430.75 K (Cox eq., Chao et al. 1983)

1927 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.96885 - 1370.962/(216.202 + t/^{\circ}\text{C})$; temp range 49.2–130.68°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

1928 (interpolated-Antoine eq., temp range 18–158°C, Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.83746 - 1367.311/(215.84 + t/^{\circ}\text{C})$; temp range 18–158°C (Antoine eq., Dean 1985, 1992)

$\log (P/\text{kPa}) = 5.96654 - 1369.525/(216.040 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 5.96232 - 1367.306/(-57.314 + T/K)$; temp range 322–405 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 32.1535 - 3.0728 \times 10^3/(T/K) - 8.4344 \cdot \log (T/K) + 6.8943 \times 10^{-10} \cdot (T/K) + 1.9558 \times 10^{-6} \cdot (T/K)^2$; temp range 223–606 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

36000 (calculated-P/C, Mackay & Shiu 1981)

35830 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

53000, 62270 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

44080 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

36045 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

36180* (derived from solute fugacity and mole fraction solubility, temp range 273.15–313.15 K, Dohányosová et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.06 (calculated- π substituent constant, Hansch et al. 1968)

3.33 (calculated-MCI χ , Murray et al. 1975)

3.21 (calculated-molar volume V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24$ h for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.8.1

Reported aqueous solubilities and Henry's law constants of 1,2-*cis*-dimethylcyclohexane at various temperatures

Aqueous solubility				Henry's law constant	
Dohányosová et al. 2004				Dohányosová et al. 2004	
generator column-GC/FID		smoothed raw exptl data		from solute fugacity f and x	
T/K	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	H/(Pa m ³ /mol)
raw data					
274.15	6.608	273.15	6.59	273.15	7218
274.15	6.670	278.15	6.27	278.15	10566
274.15	6.421	283.15	6.05	283.15	14994
278.15	6.184	288.15	5.93	288.15	20700
278.15	6.234	293.15	5.90	293.15	27720
278.15	6.078	298.15	5.94	298.15	36180
283.75	6.159	303.15	6.06	303.15	46260
283.75	6.041	308.15	6.25	308.15	57780
288.15	5.767	313.15	6.51	313.15	70740
288.15	6.234				
288.15	6.147	$\ln x = A + B/\tau + C \ln \tau$			
293.15	5.960	$\tau = T/298.15$			
293.15	5.679	A	-59.7348		
293.15	5.980	B	45.8700		
298.15	5.979	C	46.6282		
298.15	5.866				
298.15	6.003	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$			
303.15	6.190	25°C			
308.15	6.483				
308.15	6.016				
313.15	6.546				
313.15	6.483				
313.15	6.795				

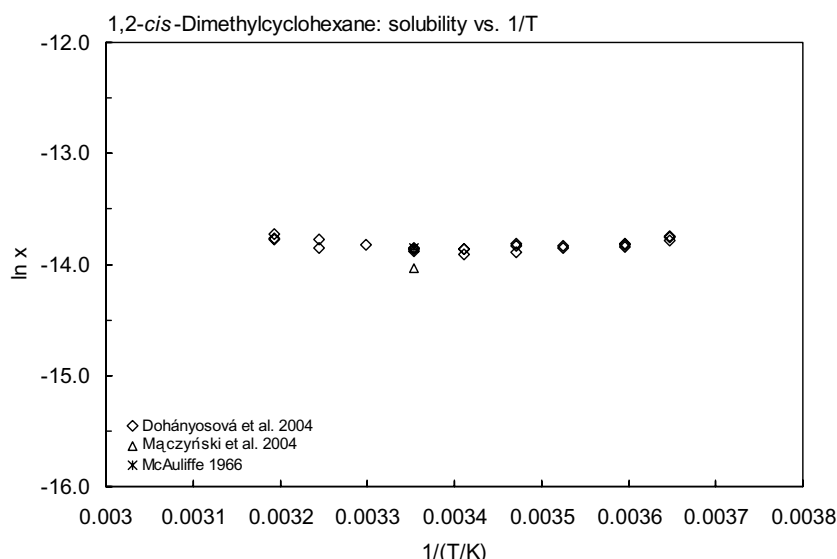


FIGURE 2.1.1.2.8.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,2-*cis*-dimethylcyclohexane.

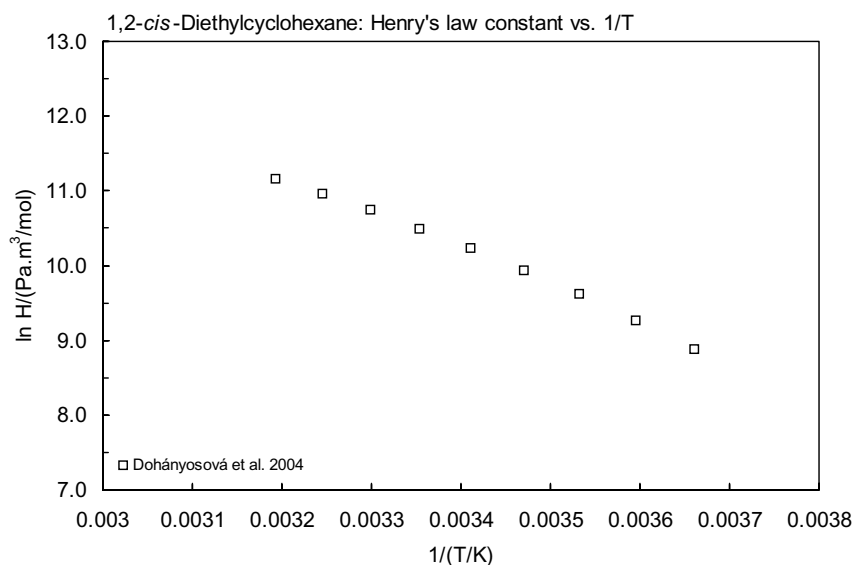


FIGURE 2.1.1.2.8.2 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-*cis*-dimethylcyclohexane.

TABLE 2.1.1.2.8.2

Reported vapor pressures of 1,2-*cis*-dimethylcyclohexane at various temperatures and the coefficients for the vapor pressure equations

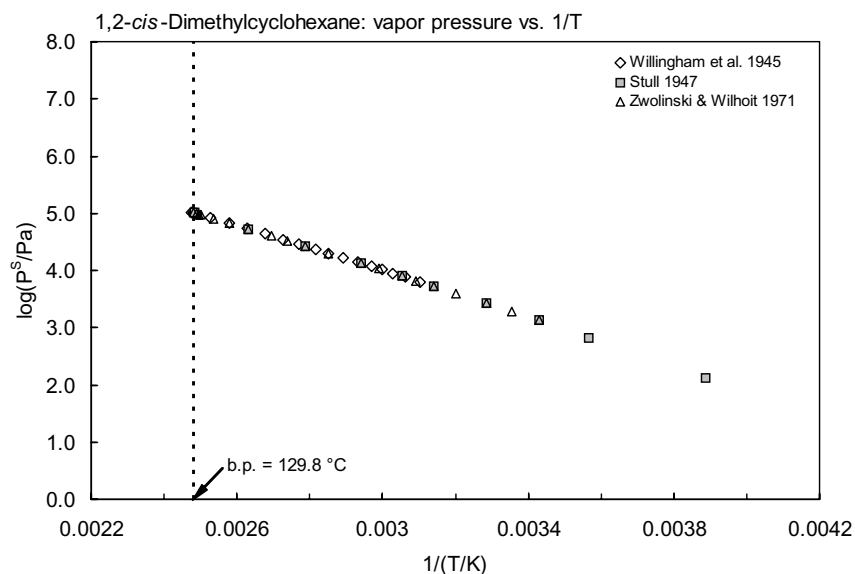
$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & \ln P = A - B/(C + T/K) & (3a) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \\ \ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)] \cdot \exp(a + bT + cT^2) & (5) & & \end{array}$$

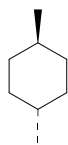
Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
49.185	6352	-15.9	133.3	18.4	1333
53.413	7655	7.30	666.6	31.1	2666
57.094	8966	18.4	1333	39.24	4000
60.429	10304	31.1	2666	45.33	5333
63.543	11696	45.3	5333	50.257	6666
67.742	13820	54.4	7999	54.421	7999
72.553	16608	66.8	13332	61.264	10666
77.402	19924	85.6	26664	66.815	13332
81.921	23451	107.0	53329	77.493	19998
87.974	28955	129.7	101325	85.572	26664
93.548	34897			92.151	33331
100.258	43324	mp/°C	-50	97.744	39997
107.192	53656			106.944	53329
114.600	66759			114.554	66661
122.639	83718			120.998	79993
128.315	97607			126.647	93326
128.926	99203			127.699	95992
129.491	100694			128.729	98659
130.125	102389			129.738	101325

(Continued)

TABLE 2.1.1.2.8.2 (Continued)

Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971	
ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
130.684	103909			25.0	1933
bp/°C	124.450			eq. 2	P/mmHg
				A	6.83746
eq. 2	P/mmHg			B	1367.311
A	6.83866			C	215.835
B	1345.859			bp/°C	129.738
C	215.598			$\Delta H_v/(kJ\ mol^{-1}) =$	
temp range 45.2–125.4°C				a 25°C	39.71
pressure range 48–780 mmHg				a bp	33.64

FIGURE 2.1.1.2.8.3 Logarithm of vapor pressure versus reciprocal temperature for 1,2-*cis*-dimethylcyclohexane.

2.1.1.2.9 1,4-*trans*-Dimethylcyclohexane

Common Name: 1,4-*trans*-Dimethylcyclohexane

Synonym: *trans*-1,4-dimethylcyclohexane

Chemical Name: 1,4-*trans*-dimethylcyclohexane

CAS Registry No: 2207-04-7

Molecular Formula: C₈H₁₆

Molecular Weight: 112.213

Melting Point (°C):

−36.93 (Lide 2003)

Boiling Point (°C):

119.4 (Lide 2003)

Density (g/cm³ at 20°C):

0.7626, 0.7584 (20°C, 25°C, Dreisbach 1955)

Molar Volume (cm³/mol):

147.2, 148 (20°C, 25°C, calculated-density)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

38.14, 33.05 (25°, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.422 (Dreisbach 1955)

12.34 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

52.26, 50.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

3.84 (shake flask-GC, Price 1976; quoted, Shaw 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

log (P/mmHg) = 6.82180 − 1332.613/(218.791 + t/°C); temp range 40.3–120.3°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

3025 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.82180 − 1332.613/(218.791 + t/°C); temp range 30–155°C (Antoine eq. for liquid state, Dreisbach 1955)

3026 (interpolated-Antoine eq., temp range 10.1–146.8°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.81773 − 1330.437/(218.581 + t/°C); temp range 10.1–146.8°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [−0.2185 × 8951.2/(T/K)] + 7.898079; temp range −24.3 to 119.5°C (Antoine eq., Weast 1972–73)

log (P/atm) = [1 − 396.346/(T/K)] × 10⁴{0.827486 − 6.12608 × 10^{−4}·(T/K) + 4.53086 × 10^{−7}·(T/K)²}; temp range: 252.05–424.25 K (Cox eq., Chao et al. 1983)

3024 (interpolated-Antoine eq., temp range 10–147°C, Dean 1985, 1992)

log (P/mmHg) = 6.81773 − 1330.437/(218.58 + t/°C); temp range 10–147°C (Antoine eq., Dean 1985, 1992)

log (P_L/kPa) = 5.94449 − 1331.612/(−54.43 + T/K); temp range 313–395 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 32.5731 − 2.9872 × 10³/(T/K) − 8.6494·log (T/K) − 2.1355 × 10^{−9}·(T/K) + 2.2946 × 10^{−6}·(T/K)²; temp range 236–590 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

88200 (calculated-P/C, Mackay & Shiu 1981)

88360 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

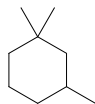
Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24$ h for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

2.1.1.2.10 1,1,3-Trimethylcyclohexane



Common Name: 1,1,3-Trimethylcyclohexane

Synonym:

Chemical Name: 1,1,3-trimethylcyclohexane

CAS Registry No: 3073-66-3

Molecular Formula: C_9H_{18}

Molecular Weight: 126.239

Melting Point ($^{\circ}C$):

-65.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

136.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$): 0.7664

Molar Volume (cm^3/mol):

164.7 ($20^{\circ}C$, calculated-density, Ruelle & Kesselring 1997)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.77 (shake flask-GC, Price 1976)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/mmHg) = 6.83705 - 1393.299/(215.551 + t/^{\circ}C)$; temp range 54.7 – $137.6^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

$\log (P/atm) = [1 - 409.802/(T/K)] \times 10^{0.838270 - 6.63916 \times 10^{-4} \cdot (T/K) + 5.61172 \times 10^{-7} \cdot (T/K)^2}$; temp range: 327.82 – $410.80\ K$ (Cox eq., Chao et al. 1983)

1480 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.96492 - 1395.206/(215.77 + t/^{\circ}C)$; temp range 54.67 – $137.6^{\circ}C$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

$\log (P/kPa) = 5.96816 - 1397.161/(215.961 + t/^{\circ}C)$; temp range 54.69 – $137.65^{\circ}C$ (Antoine eq. from reported exptl. data of Pasek & Thodos 1962, Boublik et al. 1984)

1480 (interpolated-Antoine eq., temp range 55 – $137^{\circ}C$, Dean 1985, 1992)

$\log (P/mmHg) = 6.83951 - 1394.88/(215.73 + t/^{\circ}C)$; temp range 55 – $137^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log (P_L/kPa) = 5.96449 - 1395.396/(-57.308 + T/K)$; temp range 348 – $411\ K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

105600 (calculated-P/C from selected data)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 8.73 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson 1989)

$k_{OH} = 8.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

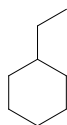
Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.1.2.11 Ethylcyclohexane



Common Name: Ethylcyclohexane

Synonym:

Chemical Name: ethylcyclohexane

CAS Registry No: 1678-91-7

Molecular Formula: C_8H_{16} , $C_2H_5C_6H_{11}$

Molecular Weight: 112.213

Melting Point ($^{\circ}C$):

-111.3 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

131.9 (Lide 2003)

Density (g/cm^3):

0.7880 ($20^{\circ}C$, Weast 1982–82)

Molar Volume (cm^3/mol):

142.4 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

7.0* ($40^{\circ}C$, shake flask-solid phase extraction-GC, measured range 38.35 – $280^{\circ}C$, Heidman et al. 1985)

$\ln x = -334.2468 + 14105.21/(T/K) + 47.93102 \cdot \ln (T/K)$; measured range 40 – $280^{\circ}C$ (shake flask-solid phased extraction-GC, Heidman et al. 1985)

7.0* ($40^{\circ}C$, IUPAC tentative value, temp range 40 – $280^{\circ}C$, Shaw 1989a)

3.89* (generator column-GC/FID, measured range 273.15 – 313.15 K, Dohányosová et al. 2004)

$\ln x = -53.6687 + 39.4055/\tau + 41.1210 \cdot \ln \tau$, $\tau = [(T/K)/298.15]$, temp range 273.15 – 313.15 K (generator column-GC/FID, Dohányosová et al. 2004)

4.36* ($30.3^{\circ}C$, shake flask-GC, measured range 30.3 – $170.8^{\circ}C$, Marche et al. 2004)

$\ln x = -344.02468 + 14105.21/(T/K) + 47.93102 \cdot \ln (T/K)$; temp range 30.3 – $170.8^{\circ}C$ (Marche et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6351* ($51.412^{\circ}C$, ebulliometry, measured range 51.4 – $132.7^{\circ}C$, Willingham et al. 1945)

1612 (extrapolated-Antoine eq., Willingham et al. 1945)

$\log (P/mmHg) = 6.87041 - 1384.036/(214.128 + t/^{\circ}C)$; temp range 51.4 – $132.7^{\circ}C$ (Antoine eq., ebulliometry, Willingham et al. 1945)

1333* ($20.6^{\circ}C$, summary of literature data, temp range -14.5 to $131.9^{\circ}C$, Stull 1947)

1705* (extrapolated-Antoine eq., temp range 20.6 – $159.5^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.86728 - 1382.466/(214.995 + t/^{\circ}C)$; temp range 20.6 – $159.5^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P_L/kPa) = 5.99043 - 1381.396/(-58.271 + T/K)$; temp range 323 – 407 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C Additional data at other temperatures designated * are compiled at the end of this section.):

$$\ln(k_H/\text{MPa}) = 325.570 - 18496.5/(T/K) - 10.9666 \cdot (T/K)^2 - 44.7690 \cdot \ln(T/K); \text{ maximum } k_H = 1.186 \times 10^4 \text{ MPa at } 385.2 \text{ K (Heidman et al. 1985)}$$

48960* (derived from solute fugacity and mole fraction solubility, temp range 273.15–323.15 K, Dohányosová et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

TABLE 2.1.1.2.11.1

Reported aqueous solubilities of ethylcyclohexane at various temperatures

$$\ln x = A + B/(T/K) + C \ln(T/K) \quad (1)$$

Heidman et al. 1985		Shaw 1989a		Dohányosová et al. 2004		Marche et al. 2004	
shake flask-GC		IUPAC "tentative" best		generator column-GC		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	t/°C	S/g·m ⁻³
38.35	6.8	40	7.0	274.15	3.803	30.3	4.358
94.45	15.0	50	7.0	274.15	4.108	70.4	8.790
150.25	120	60	7.0	278.15	3.996	100.5	28.18
206.35	750	70	10	278.15	3.678	131.0	67.95
263.15	7300	80	13	283.15	3.734	151.2	110.8
279.65	14600	90	16	288.15	3.759	170.8	183.3
		100	21	288.15	3.666		
eq. 1	x	120	55	293.15	3.766		
A	-334.2468	140	95	293.15	3.797		
B	14105.21	160	160	298.15	3.965		
C	47.93102	180	280	303.15	3.971		
		200	550	303.15	4.034		
		220	1600	313.15	4.358		
		240	3400	313.15	4.520		
		260	6500	313.15	4.364		
		280	15000				
empirical eq.							
$\ln x = A + B/\tau + C \ln \tau$							
$\tau = (T/K)/298.15$							
				A	-53.6887		
				B	39.4055		
				C	41.1210		

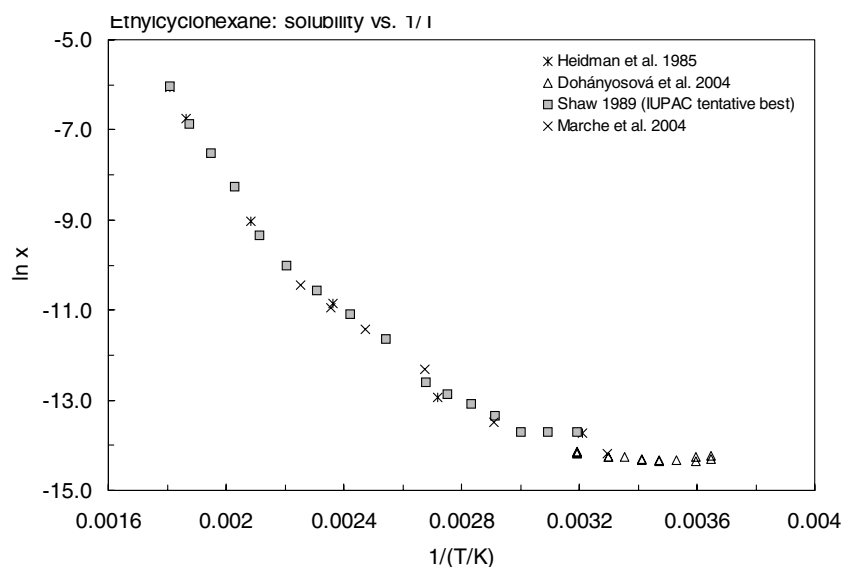


FIGURE 2.1.1.2.11.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for ethylcyclohexane.

TABLE 2.1.1.2.11.2

Reported vapor pressures and Henry's law constants of ethylcyclohexane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Vapor pressure						Henry's law constant	
Willingham et al. 1945		Stull 1947		Zwolinski & Wilhoit 1971		Dohányosová et al. 2004	
Ebulliometry		Summary of literature data		Selected values		From solute fugacity f and x	
$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	$H/(Pa \text{ m}^3 \text{ mol}^{-1})$
51.412	6351	-14.5	133.3	20.6	1333	0	10422
55.636	7653	9.2	666.6	33.4	2666	5	14994
59.315	8959	20.6	1333	41.48	4000	10	20880
62.655	10299	33.4	2666	47.57	5333	15	28440
65.755	11691	47.6	5333	51.494	6666	20	37800
69.948	13818	56.7	7999	56.656	7999	25	48960
74.738	16615	69.0	13332	63.493	10666	30	62100
79.587	19916	87.8	26664	69.093	13332	35	77040
84.115	23451	109.1	53329	79.699	19998	40	93780
90.158	28956	131.8	101325	87.762	26664		
95.716	34893			94.327	33331		
102.412	43320	mp/ $^{\circ}C$	-111.3	99.906	39997		
109.327	53657			109.13	53329		
116.709	66760			116.666	66661		
124.723	83722			123.088	79993		
130.379	97609			128.715	93326		

(Continued)

TABLE 2.1.1.2.11.2 (Continued)

Willingham et al. 1945		Vapor pressure		Zwolinski & Wilhoit 1971		Henry's law constant	
		Stull 1947				Dohányosová et al. 2004	
Ebulliometry		Summary of literature data		Selected values		From solute fugacity f and x	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3 \text{ mol}^{-1})$
130.988	99208			129.764	95992		
131.551	100700			130.79	98659		
132.181	102404			131.795	101325		
132.742	103922			25.0	1707		
bp/ $^{\circ}\text{C}$	131.783			eq. 2	P/mmHg		
Antoine eq.				A	6.86728		
eq. 2	P/mmHg			B	1382.466		
A	6.87041			C	214.995		
B	1384.036			bp/ $^{\circ}\text{C}$	131.795		
C	214.128			$\Delta H_v/(\text{kJ mol}^{-1}) =$			
temp range 51.4–132.7 $^{\circ}\text{C}$				at 25 $^{\circ}\text{C}$	40.48		
pressure range 48–780 mmHg				at bp	34.31		

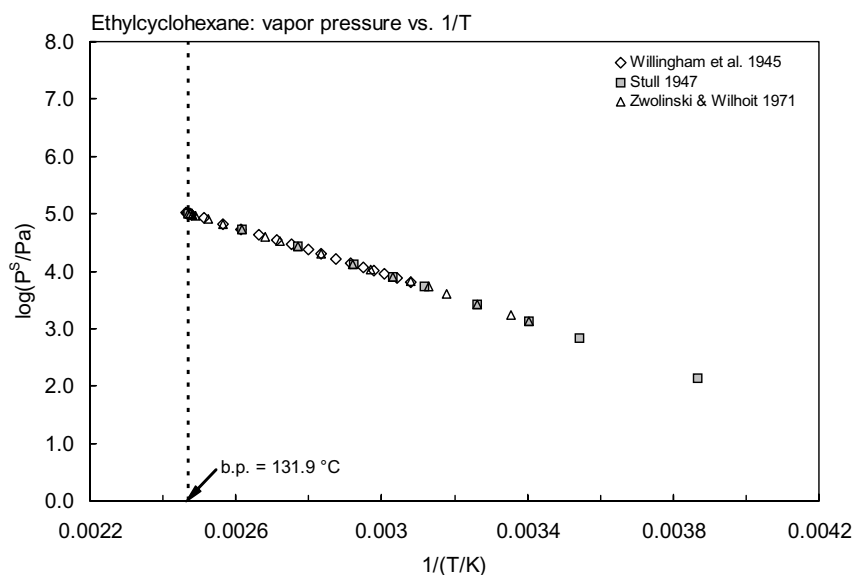


FIGURE 2.1.1.2.11.2 Logarithm of vapor pressure versus reciprocal temperature for ethylcyclohexane.

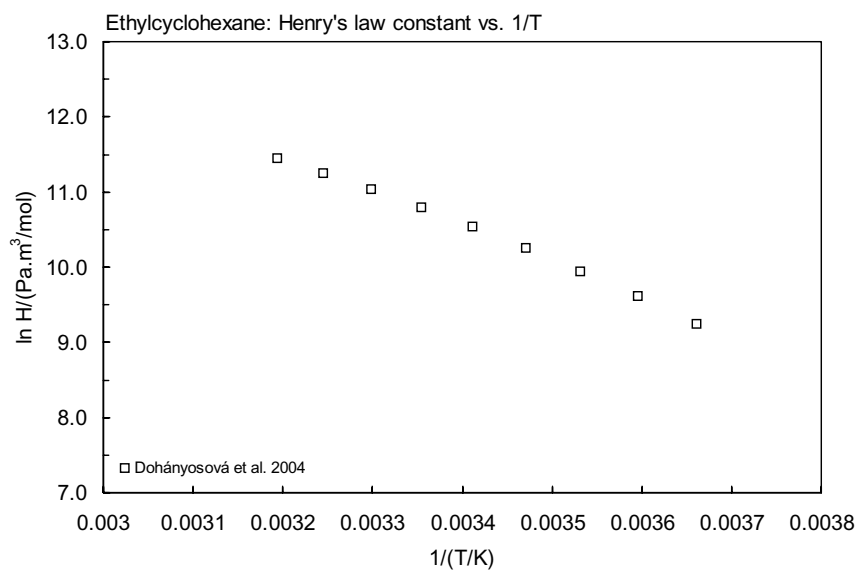


FIGURE 2.1.1.2.11.3 Logarithm of Henry's law constant versus reciprocal temperature for ethylcyclohexane.

2.1.1.2.12 Cycloheptane



Common Name: Cycloheptane

Synonym: suberane

Chemical Name: cycloheptane

CAS Registry No: 291-64-5

Molecular Formula: C_7H_{14}

Molecular Weight: 98.186

Melting Point ($^{\circ}C$): -12

-8.46 (Lide 2003)

Boiling Point ($^{\circ}C$): 118.5

118.4 (Lide 2003)

Density (g/cm^3):

0.8098 ($20^{\circ}C$, Weast 1984)

0.80656 (measured, Anand et al. 1975)

Molar Volume (cm^3/mol):

121.3 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

136.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.98, 0.29, 0.45, 1.88 (-138.35 , -74.95 , -60.75 , $-8.05^{\circ}C$, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

47.6, 48.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

30.0 (shake flask-GC, McAuliffe 1966)

27.1 ($30^{\circ}C$, shake flask-GC, Groves 1988)

23.5, 23.5 (25 , $30^{\circ}C$, calculated-liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

19920* ($68.2^{\circ}C$, ebulliometry, measured range 68.2 – $159^{\circ}C$, Finke et al. 1956)

$\log(P/mmHg) = 6.85271 - 1330.742/(t/^{\circ}C + 216.246)$; temp range 68.2 – $159^{\circ}C$ (Antoine eq., ebulliometry, Finke et al. 1956)

2924* (static method-quartz spiral gauge, measured range 283.048 – $323.551 K$, Anand et al. 1975)

$\log(P/kPa) = 6.19317 - 1450.17/(T/K - 44.91)$; temp range 283.048 – $323.551 K$ (static method, vapor-liquid equilibria study, Anand et al. 1975)

16312* ($63.03^{\circ}C$, comparative ebulliometry, measured range 60 – $121.7^{\circ}C$, Meyer & Hotz 1976)

$\log(P/mmHg) = 5.85683 - 1333.780/(t/^{\circ}C + 216.6438)$; temp range 60 – $121.7^{\circ}C$ (Antoine eq., comparative ebulliometry, Meyer & Hotz 1976)

$\log(P/atm) = [1 - 391.896/(T/K)] \times 10^4 \{0.885524 - 8.19621 \times 10^{-4} \cdot (T/K) + 7.88065 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 284.35 – $432.17 K$ (Cox eq., Chao et al. 1983)

2895, 2898 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.97858 - 1331.383/(214.325 + t/^{\circ}C)$; temp range 60.2 – $159^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 5.98198 - 1333.899/(216.657 + t/^{\circ}C)$; temp range 63.03 – $121.68^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

2895 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.85395 - 1331.57/(216.35 + t/^{\circ}C)$; temp range: 68 – $159^{\circ}C$ (Antoine eq., Dean 1985, 1992)

2930 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.98143 - 1333.833/(-56.458 + T/\text{K})$; temp range 341–433 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.12682 - 1417.738/(-47.665 + T/\text{K})$; temp range 282–333 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.97596 - 1329.98/(-56.968 + T/\text{K})$; temp range 333–398 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.05325 - 2475.271/(108.392 + T/\text{K})$; temp range 476–604 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 54.0858 - 3.6109 \times 10^3/(T/\text{K}) - 17.331 \cdot \log (T/\text{K}) + 7.5292 \times 10^{-3} \cdot (T/\text{K}) + 1.7553 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 265–604 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

9977 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.87 (calculated- π substituent constant, Hansch et al. 1968)

3.06 (calculated-MCI χ , Murray et al. 1975)

3.76 (calculated-fragment const., Yalkowsky & Morozowich 1980)

2.72 (calculated-molar volume V_M , Wang et al. 1992)

3.91 (calculated-fragment const., Müller & Klein 1992)

3.1648 (calculated-UNIFAC group contribution, Chen et al. 1993)

4.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 13.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985)

$k_{OH} = (7.88 \pm 1.38) \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance absorption, Jolly et al. 1985)

$k_{OH} = (11.8 - 13.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298–300 K (review, Atkinson 1989)

$k_{OH} = 1.25 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1990)

$k_{OH} = 13.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.12.1

Reported vapor pressures of cycloheptane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

$$\log P = A'[1 - (T_B/K)/(T/K)] \quad (5) \text{ where } A' = a + bT + cT^2$$

Finke et al. 1956		Anand et al. 1975		Meyer & Hotz 1976	
ebulliometric method		static-quartz spiral gauge		comparative ebulliometry	
t/ $^{\circ}\text{C}$	P/Pa	T/K	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
68.204	19920	283.043	1272	63.03	16312
74.338	25007	288.237	1711	68.929	20748
80.529	31160	292.906	2218	77.747	28258
86.771	38547	298.150	2924	85.702	37172
93.068	47359	301.924	3550	96.324	52481
99.416	57803	309.193	5080	106.462	71394
105.820	70109	312.723	6006	117.547	97871
112.281	84525	317.813	7573	121.681	109500
118.793	101325	323.551	9741		
125.364	120798			bp/ $^{\circ}\text{C}$	118.813
131.985	143268	Antoine eq.			
138.665	169052	eq. 3	P/kPa	Antoine eq.	
145.387	198530	A	6.19317	eq. 2	P/cmHg
152.178	232087	B	1450.17	A	5.85683
159.022	270110	C	-44.91	B	1333.780
				C	216.6438
bp/ $^{\circ}\text{C}$	118.79			temp range:	63–122 $^{\circ}\text{C}$
$\Delta H_v =$	38.53 kJ/mol				
	at 25 $^{\circ}\text{C}$				
Antoine eq.				Cox equation:	
eq. 2	P/mmHg			eq 5	P/atm
A	6.85271			a	0.878453
B	1330.742			$-b \times 10^3$	0.916539
C	216.246			$c \times 10^6$	0.965009
Cox eq.					
eq. 5	P/atm				
T_B	391.953				
a	0.839608				
$-b \times 10^4$	6.9133				
$c \times 10^7$	6.4035				

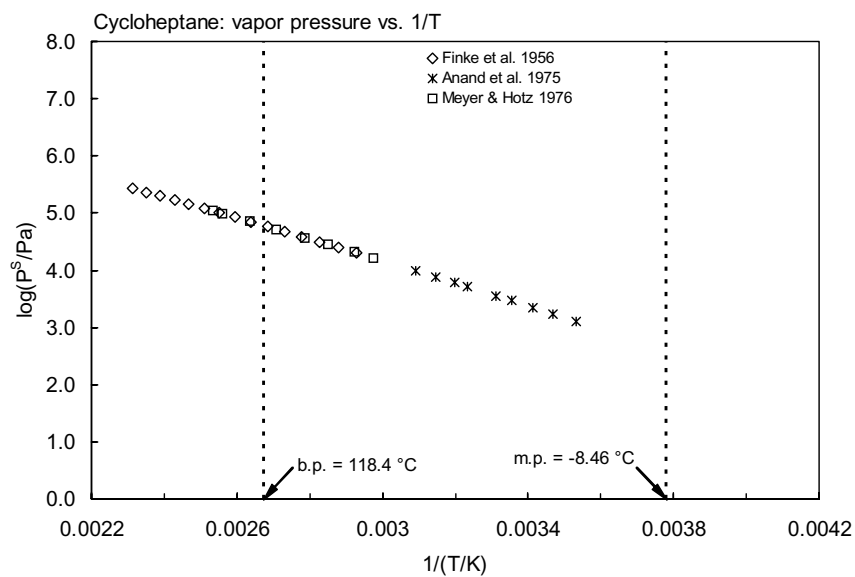


FIGURE 2.1.1.2.12.1 Logarithm of vapor pressure versus reciprocal temperature for cycloheptane.

2.1.1.2.13 Cyclooctane



Common Name: Cyclooctane

Synonym:

Chemical Name: cyclooctane

CAS Registry No: 292-64-8

Molecular Formula: C_8H_{16}

Molecular Weight: 112.213

Melting Point ($^{\circ}C$):

14.59 (Lide 2003)

Boiling Point ($^{\circ}C$): 151

149 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8340 (Weast 1984)

Molar Volume (cm^3/mol):

134.4 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

154.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.32, 0.48, 2.41 (-106.65 , -89.35 , $14.85^{\circ}C$, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

48.89, 51.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

7.90 (shake flask-GC, McAuliffe 1966)

7.48 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

5.80* (generator column-GC, measured range 27.15 – $313.15 K$, Dohányosová et al. 2004)

$\ln x = -55.1375 + 41.2528/\tau + 43.2804 \cdot \ln \tau$; $\tau = T/298.15 K$ (empirical eq., generator column-GC, Dohányosová et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

19920* ($96.7^{\circ}C$, ebulliometry, measured range 96.7 – $194.4^{\circ}C$, Finke et al. 1956)

$\log (P/mmHg) = 6.86173 - 1437.682/(t/^{\circ}C + 210.003)$; temp range 96.7 – $194.4^{\circ}C$ (Antoine eq., ebulliometry, Finke et al. 1956)

748* (static-quartz spiral gauge, measured range 290.961 – $323.326 K$, Anand et al. 1975)

$\log (P/kPa) = 5.97188 - 1447.45/(T/K - 60.67)$; temp range 291 – $323 K$ (static method, vapor-liquid equilibria VLE study, Anand et al. 1975)

22454* ($100.133^{\circ}C$, comparative ebulliometry, measured range 100.1 – $161^{\circ}C$, Meyer & Hotz 1976)

$\log (P/mmHg) = 5.861786 - 1438.455/(t/^{\circ}C + 210.1844)$; temp range 100.1 – $161^{\circ}C$ (Antoine eq., comparative ebulliometry, Meyer & Hotz 1976)

767, 740 (extrapolated-Antoine eq., extrapolated, Boublik et al. 1984)

$\log (P/kPa) = 5.98693 - 1437.751/(210.012 + t/^{\circ}C)$; temp range 96.7 – $194.4^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 6.06524 - 1492.101/(216.413 + t/^{\circ}C)$; temp range 100.1 – $160.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

740 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 6.86187 - 1437.79/(210.02 + t/^{\circ}C)$; temp range 97 – $194^{\circ}C$ (Antoine eq., Dean 1985, 1992)

753 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.98663 - 1437.682/(-63.147 + T/\text{K})$; temp range 369–487 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.9899 - 1440.707/(-62.701 + T/\text{K})$; temp range 369–468 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.20474 - 1564.985/(-50.842 + T/\text{K})$; temp range 289–369 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

10485 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

14526* (derived from solute fugacity and mole fraction solubility, temp range 273.15–313.15 K, Dohányosová et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.28 (calculated- π substituent constant, Hansch et al. 1968)

3.50 (calculated-MCI χ , Murray et al. 1975)

3.28 (Hutchinson et al. 1980; Sangster 1989)

3.28 (calculated-fragment const., Lyman 1982)

4.45 (recommended, Sangster 1989)

3.04 (calculated-molar volume V_M , Wang et al. 1992)

4.47 (calculated-fragment const., Müller & Klein 1992)

3.6117 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 14.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

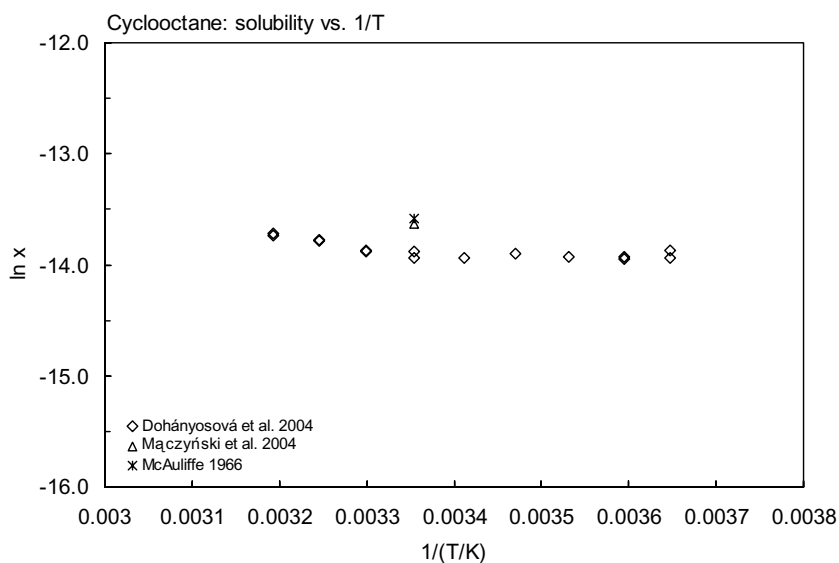
Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.13.1

Reported aqueous solubilities and Henry's law constants of cyclooctane at various temperatures

Aqueous solubility				Henry's law constant	
Dohányosová et al. 2004				Dohányosová et al. 2004	
generator column-GC		smoothed exptl raw data		from solute fugacity f and x	
T/K	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	H/(Pa m ³ /mol)
raw data					
274.15	5.53	273.15	5.73	273.15	2826
274.15	5.885	278.15	5.59	278.15	4158
278.15	5.548	283.15	5.53	283.15	5922
278.15	5.442	288.15	5.55	288.15	8190
283.15	5.548	293.15	5.64	293.15	11052
288.15	5.754	298.15	5.80	298.15	14526
293.15	5.492	303.15	6.02	303.15	18720
298.15	5.848	308.15	6.32	308.15	23400
298.15	5.530	313.15	6.68	313.15	28800
303.15	5.922				
303.15	5.835	$\ln x = A + B/\tau + C \ln \tau$			
308.15	6.483	$\tau = T/298.15$			
308.15	6.421	A	-55.1375		
313.15	6.733	B	41.2528		
313.15	6.858	C	43.2804		

FIGURE 2.1.1.2.13.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cyclooctane.

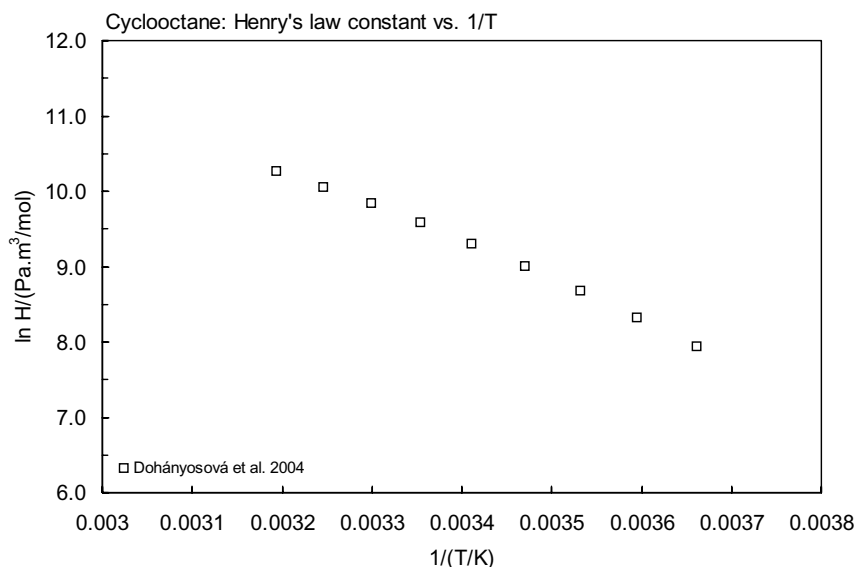


FIGURE 2.1.1.2.13.2 Logarithm of Henry's law constant versus reciprocal temperature for cyclooctane.

TABLE 2.1.1.2.13.2

Reported vapor pressures of cyclooctane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
$\log P = A'[1 - (T_{\text{B}}/K)/(T/K)]$		(5) where $A' = a + bT + cT^2$					
Finke et al. 1956		Anand et al. 1975		Meyer & Hotz 1976		Dohányosová et al. 2004	
ebulliometry		static-quartz spiral gauge		comparative ebulliometry		from Anand et al. 1975	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa
96.711	19920	290.961	488	100.133	22454	273.15	207
103.318	25007	294.376	601	108.375	29598	278.15	292
109.977	31160	298.150	748	118.813	41155	283.15	406
116.694	38457	302.060	944	127.569	53410	288.15	557
123.472	47359	306.922	1244	139.435	74511	293.15	753
130.301	70109	311.678	1605	149.031	95919	303.15	1010
137.190	84525	316.472	2056	157.388	118293	308.15	1330
144.133	101325	323.326	2890	160.911	129263	313.15	1730
151.146	120798						
158.203	143268	Antoine eq.		bp/°C	151.148		
165.321	169052	eq. 3	P/kPa	Antoine eq.			
172.502	198530	A	6.91788	eq. 2	P/cmHg		
187.040	232087	B	1447.45	A	5.861786		
194.397	270110	C	−60.67	B	1438.455		
				C	210.1844		
bp/°C	151.14			temp range 100–161°C			
Antoine eq.							
eq. 2	P/mmHg			Cox equation:			

(Continued)

TABLE 2.1.1.2.13.2 (Continued)

Finke et al. 1956		Anand et al. 1975		Meyer & Hotz 1976		Dohányosová et al. 2004	
ebulliometry		static-quartz spiral gauge		comparative ebulliometry		from Anand et al. 1975	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa
A	686173			eq 5	P/atm		
B	1437.682			a	0.869777		
C	210.003			$-b \times 10^3$	0.775348		
				$c \times 10^6$	0.716695		
Cox equation:							
eq 5	P/atm						
a	0.839609						
$-b \times 10^4$	6.2033						
$c \times 10^7$	5.177						
T_B	424.300						

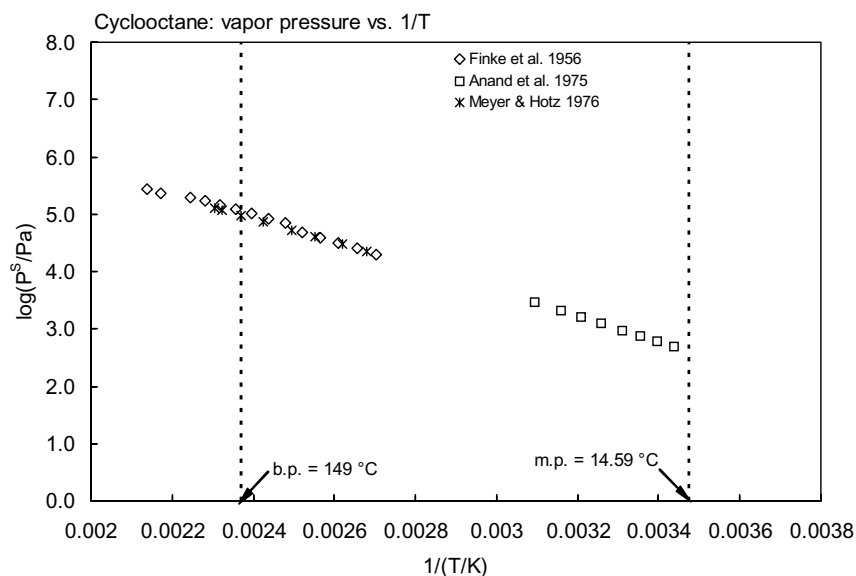
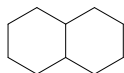


FIGURE 2.1.1.2.13.3 Logarithm of vapor pressure versus reciprocal temperature for cyclooctane.

2.1.1.2.14 Decalin



Common Name: Decalin

Synonym: bicyclo[4.4.0]decane, naphthalane, naphthane

Chemical Name: decahydronaphthalene (mixed isomers)

CAS Registry No: 91-17-8

Molecular Formula: $C_{10}H_{18}$

Molecular Weight: 138.250

Melting Point ($^{\circ}C$):

−42.9 (*cis*-decalin, Lide 2003)

−30.4 (*trans*-decalin, Lide 2003)

Boiling Point ($^{\circ}C$): 191.7

195.774 (*cis*-decalin, Camin & Rossini 1955)

187.273 (*trans*-decalin, Camin & Rossini 1955)

191.7 (Riddick et al. 1986)

Density (g/cm^3 at $20^{\circ}C$):

0.8865, 0.8789 ($20^{\circ}C$, $25^{\circ}C$, mixed isomers, Riddick et al. 1986)

Molar Volume (cm^3/mol):

154.8, 159.6 (*cis*-decalin, *trans*-decalin, calculated-density, Stephenson & Malanowski 1987)

184.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.09 (bp, mixed isomers, Riddick et al. 1986)

51.342, 40.999 (*cis*-decalin, $25^{\circ}C$, bp, Riddick et al. 1986)

49.87, 40.229 (*trans*-decalin, $25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.414, 9.489 (*cis*-decalin, *trans*-decalin, Riddick et al. 1986)

14.43 (*cis*-decalin, Chickos et al. 1999)

2.13, 9.49 (*trans*-decalin, -57.05 , $42.95^{\circ}C$, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

59.45, 52.1 (*cis*-decalin: exptl., calculated-group additivity method, Chickos et al. 1999)

51.1, 52.1 (*trans*-decalin: exptl, calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.889 (shake flask-GC, Price 1976; quoted as more reliable value, Shaw 1989)

6.21 (shake flask-GC, Hutchinson et al. 1980)

1.99 (calculated-QSAR, Passino & Smith 1987)

2.14 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($23.3^{\circ}C$, isomer not specified, ebulliometry, measured range 23.3 – $150.0^{\circ}C$, Gardner & Brewer 1937)

241* ($20^{\circ}C$, *cis*-decalin, manometry, measured range -29.5 to $194.7^{\circ}C$, Seyer & Mann 1945)

381* ($13^{\circ}C$, *trans*-decalin, manometry, measured range -30.0 to $235.3^{\circ}C$, Seyer & Mann 1945)

133.3* ($22.5^{\circ}C$, *cis*-decalin, summary of literature data, temp range 22.5 – $194.6^{\circ}C$, Stull 1947)

666.6* ($30.6^{\circ}C$, *trans*-decalin, summary of literature data, temp range -0.80 to $186.7^{\circ}C$, Stull 1947)

5529* ($99.883^{\circ}C$, *cis*-decalin, ebulliometry, measured range 99.883 – $196.376^{\circ}C$, Camin & Rossini 1955)

5530* ($92.36^{\circ}C$, *trans*-decalin, ebulliometry, measured range 92.36 – $187.867^{\circ}C$, Camin & Rossini 1955)

- log (P/mmHg) = $6.87529 - 1594.460/(203.392 + t/^{\circ}\text{C})$; temp range 99.8–196.4°C (*cis*-decalin, Antoine eq., ebulliometry-manometer measurement, Camin & Rossini 1955)
- log (P/mmHg) = $6.85681 - 1564.683/(206.259 + t/^{\circ}\text{C})$; temp range 92.3–187.0°C (*trans*-decalin, Antoine eq., ebulliometry-manometer measurement, Camin & Rossini 1955)
- 104*, 164* (*cis*-decalin, *trans*-decalin, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
- log (P/mmHg) = $6.87529 - 1594.460/(203.392 + t/^{\circ}\text{C})$; temp range 68.0–277.67°C (*cis*-decalin, Antoine eq., Zwolinski & Wilhoit 1971)
- log (P/mmHg) = $6.85681 - 1564.683/(206.259 + t/^{\circ}\text{C})$; temp range 60.91–218.88°C (*trans*-decalin, Antoine eq., Zwolinski & Wilhoit 1971)
- log (P/mmHg) = $[-0.2185 \times 10515.4/(T/K)] + 7.797540$; temp range 22.5–194.6°C (*cis*-decalin, Antoine eq., Weast 1972–73)
- log (P/mmHg) = $[-0.2185 \times 8749.1/(T/K)] + 6.973042$; temp range –0.80 to 186.7°C (*trans*-decalin, Antoine eq., Weast 1972–73)
- log (P/atm) = $[1 - 468.915/(T/K)] \times 10^{\{0.683577 - 0.900942 \times 10^{-4} \cdot (T/K) + 2.28255 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 295.65–727.59 K (*cis*-decalin, Cox eq., Chao et al. 1983)
- log (P/atm) = $[1 - 460.458/(T/K)] \times 10^{\{0.880979 - 6.38749 \times 10^{-4} \cdot (T/K) + 4.59180 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 365.51–461.02 K, (*trans*-decalin, Cox eq., Chao et al. 1983)
- 178, 104 (*cis*-decalin, calculated-Antoine eq., Boublik et al. 1984)
- log (P/kPa) = $6.96043 - 2358.398/(280.79 + t/^{\circ}\text{C})$; temp range –29.5 to 194.7°C (*cis*-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)
- log (P/kPa) = $6.00042 - 1594.653/(203.415 + t/^{\circ}\text{C})$; temp range 99.88–196.4°C (*cis*-decalin, Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)
- 434, 165 (*trans*-decalin, calculated-Antoine eq., Boublik et al. 1984)
- log (P/kPa) = $7.69594 - 3126.688/(363.012 + t/^{\circ}\text{C})$; temp range –30.0 to 253.3°C (*trans*-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)
- log (P/kPa) = $5.98704 - 1568.642/(206.726 + t/^{\circ}\text{C})$; temp range 92.36–187.9°C (*trans*-decalin, Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)
- 104, 168 (*cis*-, *trans*-decalin, Antoine eq., Dean 1985, 1992)
- log (P/mmHg) = $6.87529 - 1594.81/(203.39 + t/^{\circ}\text{C})$, temp range 68–228°C (*cis*-decalin Antoine eq., Dean 1985, 1992)
- log (P/mmHg) = $6.86581 - 1564.683/(206.26 + t/^{\circ}\text{C})$; temp range 61–219°C (*trans*-decalin Antoine eq., Dean 1985, 1992)
- 130 (mixed isomer, 23.3°C, lit. average, Riddick et al. 1986)
- 100, 164 (selected lit., *cis*-, *trans*-decalin, Riddick et al. 1986)
- log (P/kPa) = $6.00019 - 1594.460/(203.392 + t/^{\circ}\text{C})$, temp range not specified (*cis*-decalin, Antoine eq., Riddick et al. 1986)
- log (P/kPa) = $5.98171 - 1564.683/(206.259 + t/^{\circ}\text{C})$, temp range not specified (*trans*-decalin, Antoine eq., Riddick et al. 1986)
- 105, 168 (*cis*-decalin, *trans*-decalin, extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.00019 - 1595.176/(-69.622 + T/K)$; temp range 371–473 K (*cis*-decalin, Antoine eq., Stephenson & Malanowski 1987)
- log (P_L/kPa) = $5.99363 - 1573.981/(-65.77 + T/K)$; temp range 363–461 K (*trans*-decalin, Antoine eq., Stephenson & Malanowski 1987)
- log (P/mmHg) = $45.6345 - 4.21 \times 10^3/(T/K) - 12.881 \cdot \log (T/K) - 7.8083 \times 10^{-11} \cdot (T/K) + 2.8637 \times 10^{-6} \cdot (T/K)^2$; temp range 230–702 K (*cis*-decalin, vapor pressure eq., Yaws 1994)
- log (P/mmHg) = $76.1002 - 5.03 \times 10^3/(T/K) - 25.078 \cdot \log (T/K) + 9.7608 \times 10^{-3} \cdot (T/K) - 2.5814 \times 10^{-6} \cdot (T/K)^2$; temp range 243–687 K (*trans*-decalin, vapor pressure eq., Yaws 1994)
- 128* (20.42°C, *trans*-decalin, differential pressure gauge, measured range –29.31 to 160.7°C, Mokbel et al. 1995)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 11855* (EPICS-GC/FID, measured range 10–30°C Ashworth et al. 1988)
- ln [H/(atm·m³/mol)] = $11.85 - 4125/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.79 (calculated-fragment const., Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 1.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ of *cis*-decalin and $2.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ of *trans*-decalin at 299 K (Atkinson 1985)

$k_{OH} = 2.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction at 298 K (Atkinson 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 2.1.1.2.14.1

Reported vapor pressures and Henry's law constants of decalin (isomer not specified) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Vapor pressure				Henry's law constant	
Gardner & Brewer 1937				Ashworth et al. 1988	
ebulliometry				EPICS-GC	
$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	H/(Pa m ³ /mol)
23.3	133.3	60.0	987	10	7093
32.8	240	66.1	1293	15	8481
37.3	280	86.8	3520	20	10740
38.4	320	96.0	5186	25	11855
42.5	400	104.5	7293	30	20164
43.0	413	118.8	11652	$\ln H = A - B/(T/K)$	
49.6	587	133.8	20278		
50.6	627	150.0	31997	eq. 4a	H/(atm m ³ /mol)
54.3	747	bp/ $^{\circ}C$	193.8	A	11.85
54.6	800			B	4125
59.8	1027				

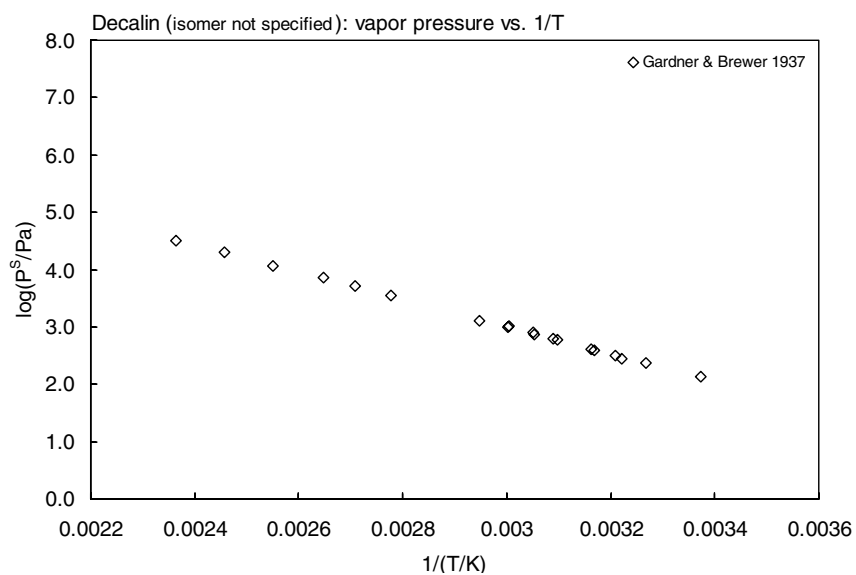


FIGURE 2.1.1.2.14.1 Logarithm of vapor pressure versus reciprocal temperature for decalin.

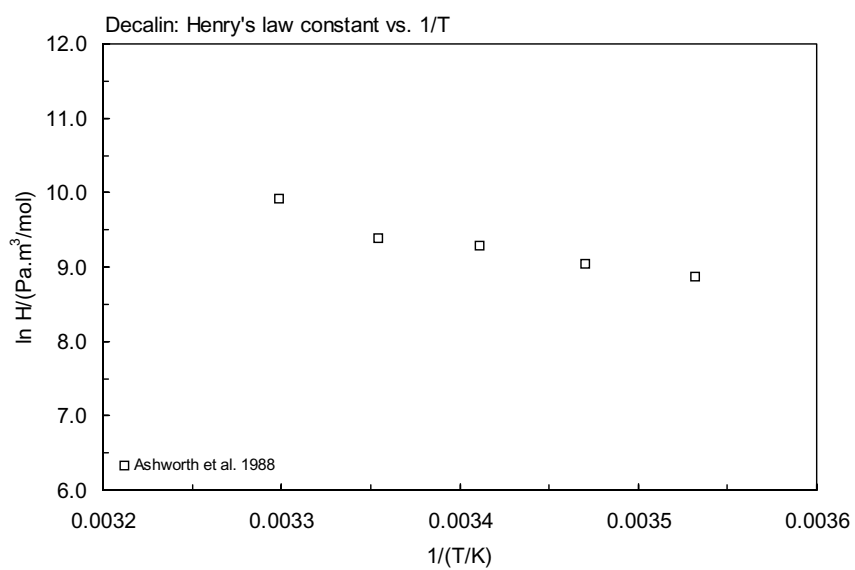


FIGURE 2.1.1.2.14.2 Logarithm of Henry's law constant versus reciprocal temperature for decalin.

TABLE 2.1.1.2.14.2

Reported vapor pressures of *cis*-decalin at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)	ln P = A – B/(T/K) – C·ln (T/K)		(4a)		
Seyer & Mann 1945		Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971	
manometry		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–29.5	51	22.5	133.3	99.883	5529	68.0	1333
–19.2	87	50.1	666.6	105.685	6941	82.64	2666
–10.0	115	64.2	1333	110.490	8331	91.97	4000
0.0	145	79.8	2666	114.152	9523	98.998	5333
12.0	196	97.2	5333	118.004	10943	104.609	6666
20.0	241	108.0	7999	123.132	13008	109.391	7999
38.0	457	123.2	3332	128.731	15827	117.280	10666
43.4	532	145.4	26664	135.021	19433	123.676	13332
49.9	704	169.9	53329	140.176	22881	135.934	19998
50.4	719	194.6	101325	147.456	28546	145.171	26664
52.9	805			154.245	34817	152.718	33331
56.9	971	mp/°C	–43.3	161.885	43164	159.127	39997
10.0	1095			170.056	53773	169.767	53329
70.0	1669			178.629	67068	178.349	66661
80.1	2590			187.823	83031	185.724	79993
92.4	4358			194.370	98080	192.251	93326
105.1	7239			195.055	99658	193.389	95992
109.8	8389			195.635	101001	194.622	98659
112.4	9121			196.376	102727	195.774	101325
124.6	13976						
148.7	29997			bp/°C	195.774		
172.7	57690			eq. 2	P/mmHg	eq. 2	P/mmHg
194.700	101093			A	6.87529	A	6.87529
				B	1594.460	B	1594.460
				C	203.392	C	203.392
eq. 4a	P/cmHg					bp/°C	195.774
A	6.8139					ΔH _v /(kJ mol ^{–1}) = 39.30	
B	1702.20						
C	34.32						at bp
bp/°C	194.5						

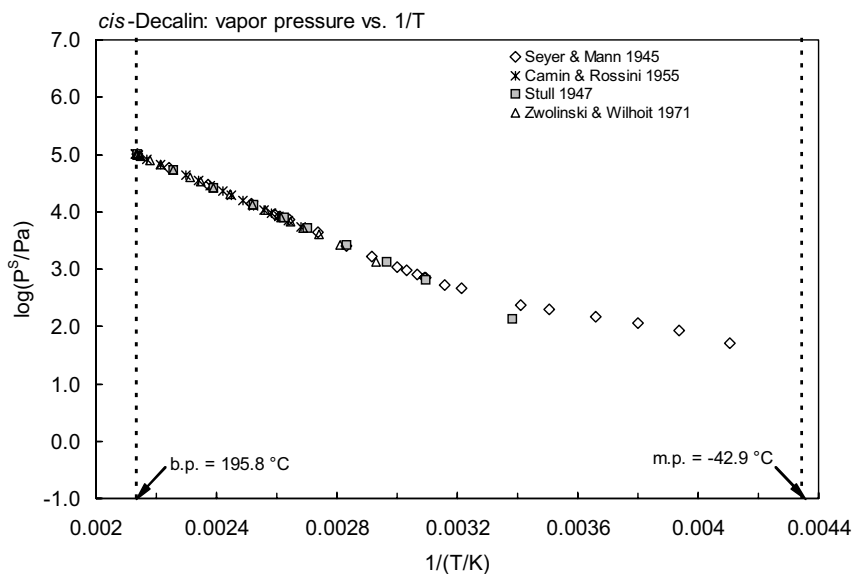


FIGURE 2.1.1.2.14.3 Logarithm of vapor pressure versus reciprocal temperature for *cis*-decalin.

TABLE 2.1.1.2.14.3
Reported vapor pressures of *trans*-decalin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)	$\ln P = A - B/(T/K) - C \cdot \ln (T/K)$	(4a)

1.

Seyer & Mann 1945		Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971	
manometry		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−30.0	59	−0.80	133.3	92.36	5530	60.91	1333
−24.1	80	30.6	666.6	98.129	6942	75.37	2666
−11.1	143	47.2	1333	102.891	8331	84.59	4000
−0.70	229	65.3	2666	106.500	9522	91.527	5333
0.0	241	85.7	5333	110.316	10946	97.072	6666
13.0	381	98.4	7999	115.356	13086	101.800	7999
30.9	801	114.6	13332	120.918	15828	109.599	10666
51.5	1597	136.2	26664	127.140	19434	115.922	13332
59.7	2221	160.1	53329	132.255	22434	128.045	19998
65.3	2657	186.7	101325	146.156	34817	137.182	26664
74.4	3562			153.719	43163	144.649	33331
83.5	5072	mp/°C	−30.7	161.801	53773	150.991	39997
95.5	7307			170.297	67069	161.522	53329
112.4	12635			179.395	84031	170.018	66661
119.4	16087			185.885	98081	177.320	79993
136.7	27478			186.563	99665	183.783	93326
152.3	42595			187.140	101005	184.911	95992
168.0	65024			187.867	102731	186.132	98659

TABLE 2.1.1.2.14.3 (Continued)

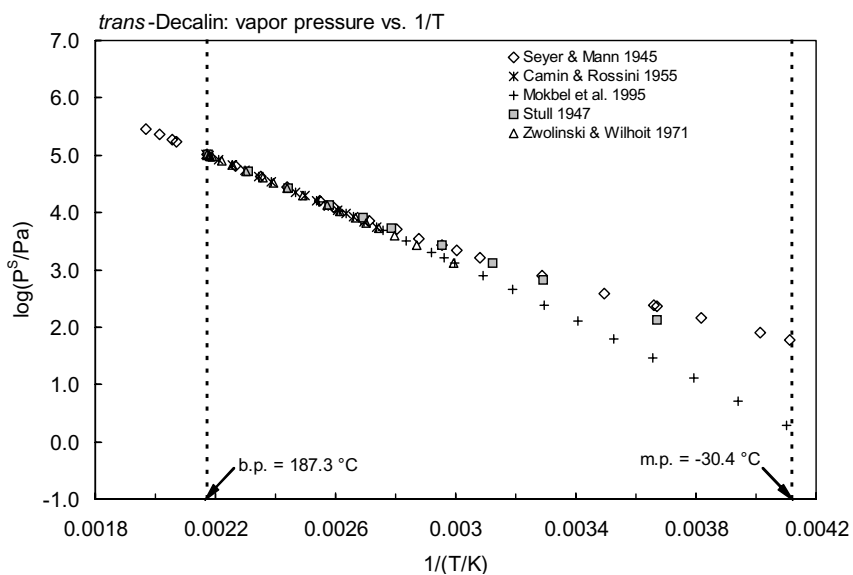
Seyer & Mann 1945		Stull 1947		Camin & Rossini 1955		Zwolinski & Wilhoit 1971	
manometry		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
187.1	103009					187.274	101325
209.8	170060			bp/°C	187.273		
212.9	185496						
223.4	228787			eq. 2	P/mmHg	eq. 2	P/mmHg
235.3	284978			A	6.85681	A	6.83561
				B	1564.683	B	1564.683
				C	206.259	C	206.269
bp/°C	185.8					bp/°C	187.274
eq. 4a	P/cmHg					$\Delta H_v/(\text{kJ mol}^{-1}) = 38.50$	
A	6.8509					at bp	
B	2182.38						
C	32.64						

2.

Mokbel et al. 1995

static method-manometry

t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-29.31	1.91	40.37	448	99.60	7347
-19.37	5.23	50.42	790	109.58	10670
-9.42	13.2	60.41	1329	119.69	15160
0.46	29.4	64.63	1636		
10.44	63.1	69.55	2050	data fitted to Wagner eq.	
20.42	128	79.48	3219		
30.35	245	89.54	4939		

FIGURE 2.1.1.2.14.4 Logarithm of vapor pressure versus reciprocal temperature for *trans*-decalin.

2.1.2 UNSATURATED HYDROCARBONS

2.1.2.1 Alkenes

2.1.2.1.1 2-Methylpropene



Common Name: 2-Methylpropene

Synonym: isobutene, isobutylene

Chemical Name: 2-methylpropene

CAS Registry No: 115-11-7

Molecular Formula: C_4H_8 ; $CH_3C(CH_3)CH_2$

Molecular Weight: 56.107

Melting Point ($^{\circ}C$):

−140.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

−6.9 (Dreisbach 1959; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.5942, 0.5879 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

94.4 ($20^{\circ}C$, calculated-density, McAuliffe 1966)

95.4 ($25^{\circ}C$, calculated-density)

88.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.92 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

44.72, 41.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

263 (shake flask-GC, of liquid at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

131695*, 131855 ($0^{\circ}C$, static method-manometer, measured range -56.75 to $0^{\circ}C$, Lamb & Roper 1940)

101325* ($-6.9^{\circ}C$, summary of literature data, temp range -105.1 to $-6.9^{\circ}C$, Stull 1947)

303700 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.84134 - 923.2/(240.0 + t/^{\circ}C)$; temp range -68 to $39^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

302642* (extrapolated-Antoine eq., temp range -81.95 to $11.88^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.84134 - 923.200/(240.00 + t/^{\circ}C)$; temp range -81.95 to $11.88^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 5742.9/(T/K)] + 7.601563$; temp range -105.1 to $-6.90^{\circ}C$ (Antoine eq., Weast 1972-73)

$\log(P/mmHg) = 6.68466 - 886.25/(234.64 + t/^{\circ}C)$; temp range -82 to $12^{\circ}C$ (Antoine eq., Dean 1985, 1992)

303255 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.96624 - 923.2/(-33.15 + T/K)$; temp range 212-279 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.93211 - 907.644/(-35.082 + T/K)$; temp range 266-313 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.27428 - 1095.288/(-9.441 + T/K)$; temp range 310-376 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.64267 - 2336.466/(160.311 + T/\text{K})$; temp range 371–418 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 39.2295 - 2.1094 \times 10^3/(T/\text{K}) - 12.567 \cdot \log (T/\text{K}) + 7.7304 \times 10^{-3} \cdot (T/\text{K}) - 1.3659 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 133–418 K (vapor pressure eq., Yaws 1994)

607940 (45.44°C, vapor-liquid equilibrium VLE data, Pasanen et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

21600 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

23100, 10800 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

14800 (calculated-P/C, Mackay & Shiu 1981)

35800 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

20994 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.64, 1.32 (quoted, calculated-molar volume V_M , Wang et al. 1992)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O_3} = 6.2 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Hanst et al. 1958)

$k_{O_3} = 2.32 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 30°C (flow system, Bufalini & Altshuller 1965)

$k_{OH} = 6.46 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{O_3} = 13.6 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp (Japar et al. 1974)

$k_{O_3} = 11.7 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Huie & Herron 1975)

$k_{OH} = (3.05 \pm 0.31) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Winer et al. 1976)

$k_{O(3P)} = 1.60 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(^3P)$ atoms (Singleton & Cvetanovic 1976; Atkinson & Pitts Jr. 1977; quoted, Gaffney & Levine 1979)

$k_{OH}^* = 5.07 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297.2 K, measured range 297–425 K (flash photolysis-resonance fluorescence, Atkinson & Pitts 1977)

$k_{O_3} = 11.7 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (chemiluminescence, Adeniji et al. 1981)

$k_{OH} = 5.13 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{OH} = (6.46 \pm 0.13) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Ohta 1984)

$k_{O_3} = 5.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 5.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{O_3} = 1.21 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (review, Atkinson 1990)

$k_{OH} = 5.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 31.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{NO_3} = (3.15 - 3.38) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{OH}^* = 5.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 3.32 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3}^* = 11.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{O(3P)} = 1.69 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $O(^3P)$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric lifetime was estimated to be 5.3 h, based on photooxidation rate constant $k = 5.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radicals in air during summer daylight (Altshuller 1991).

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins and $t_{1/2} = 8.0$ d for substituted olefins, based on rate constant $k = 1 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.1.1

Reported vapor pressures of 2-methylpropene (isobutene) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\log P = A - B/(T/K) - C \cdot (T/K)$	(5)						
Lamb & Roper 1940	Stull 1947	Zwolinski & Wilhoit 1971					
static method-manometer	summary of literature data	selected values					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-56.75	8725	-105.1	133.3	-81.95	1333	-8.983	93326
-25.30	47703	-96.5	666.6	-73.37	2666	-8.274	95992
-20.88	57462	-81.9	1333	-67.90	4000	-7.580	98659
-7.47	99791	-73.4	2666	-63.79	5333	-6.900	101325
-0.67	128789	-63.8	5333	-60.472	6666	25.0	302642
0.0	131695	-57.7	7999	-57.664	7999		
0.0	131855	-49.3	13332	-53.051	10666		
		-36.7	26664	-49.309	13332	eq. 2	P/mmHg
bp/°C	-7.12	-22.2	53329	-42.111	19998	A	6.84134
eq. 5	P/mmHg	-6.9	101325	-36.666	26664	B	923.200
A	9.77465			-32.231	33331	C	240.000
B	1503.866	mp/°C	-140.3	-28.462	39997	bp/°C	-6.90
C	0.0046649			-22.227	53329	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				-17.133	66661	at 25°C	20.59
				-12.789	79993	at bp	22.12

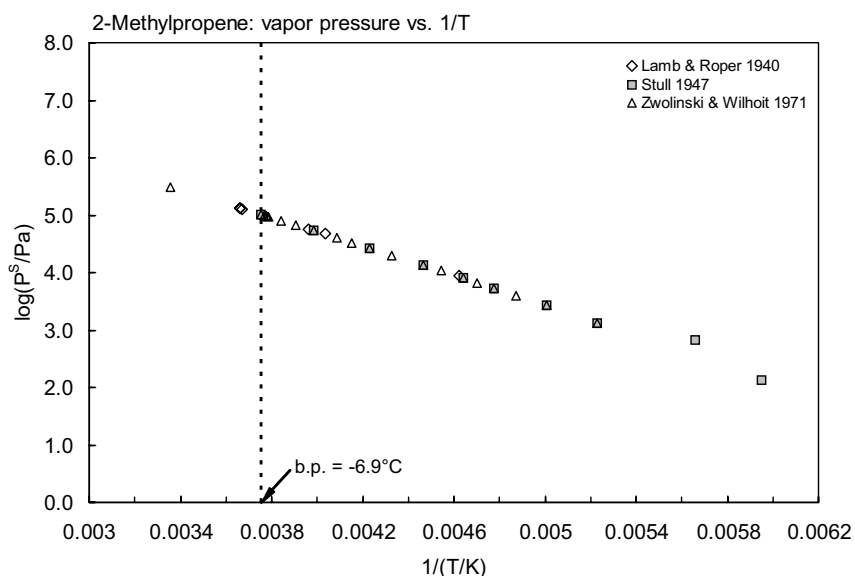


FIGURE 2.1.2.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpropene.

2.1.2.1.2 1-Butene



Common Name: 1-Butene

Synonym: butylene

Chemical Name: 1-butene

CAS Registry No: 106-98-9

Molecular Formula: C_4H_8 ; $CH_3CH_2CHCH_2$

Molecular Weight: 56.107

Melting Point ($^{\circ}C$):

−185.34 (Lide 2003)

Boiling Point ($^{\circ}C$):

−6.26 (Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.5951, 0.5888 ($20^{\circ}C$, $25^{\circ}C$, at saturation pressure, Dreisbach 1959)

Molar Volume (cm^3/mol):

94.3 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)

95.3 ($25^{\circ}C$, calculated-density)

88.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

3.85 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

43.84, 47.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

222 (shake flask-GC, liquid at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

128536* ($0^{\circ}C$, static method-manometer, measured range -56.75 to $0^{\circ}C$, Lamb & Roper 1940)

$\log (P/mmHg) = -1330.977/(T/K) - 0.0017607 \cdot (T/K) + 8.33816$; temp range 195–274 K (static method, Lamb & Roper 1940)

361100* (Antoine eq. regression, temp range -104.8 to $-6.3^{\circ}C$, Stull 1947)

296000 (calculated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.84290 - 926.1/(240.0 + t/^{\circ}C)$; temp range -67 to $40^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

297309* (derived from compiled data, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.84290 - 926.10/(240.00 + t/^{\circ}C)$; temp range -81.5 to $12.6^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = [-0.2185 \times 5996.7/(T/K)] + 7.826754$; temp range -104.8 to $-6.3^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log (P/mmHg) = 6.531 - 810.261/(228.066 + t/^{\circ}C)$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/mmHg) = 6.79290 - 908.80/(238.54 + t/^{\circ}C)$; temp range -82 to $13^{\circ}C$ (Antoine eq., Dean 1985, 1992)

297020, 295800 (interpolated-Antoine eq.-III, V, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.9678 - 926.1/(-33.15 + T/K)$; temp range 200–274 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 8.1706 - 1601.52/(7.059 + T/K)$; temp range 126–192 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.05416 - 970.771/(-27.089 + T/K)$; temp range 267–345 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.77294 - 1482/801/(48.073 + T/K)$; temp range 342–411 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.27411 - 1097.171/(-9.657 + T/K)$; temp range 267–411 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 27.3116 - 1.9235 \times 10^3/(T/K) - 70.2064 \cdot \log (T/K) + 7.4852 \times 10^{-12} \cdot (T/K) + 3.6481 \times 10^{-6} \cdot (T/K)^2$;
temp range 88–420 K (vapor pressure eq., Yaws 1994)
596140 (50.12°C, vapor-liquid equilibrium VLE data, Pasanen et al., 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

25610 (calculated-P/C, Mackay & Shiu 1981)
25370 (calculated- $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
26560, 15280 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
29800 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
24800 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.40; 2.17, 2.26, 2.43 (quoted; calculated-f const., Rekker 1977)
1.59, 1.32 (quoted, calculated-molar volume V_{M} , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{O}_3} = 1.03 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 30°C (flow system, Bufalini & Altshuller 1965)

$k_{\text{OH}} = 4.08 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{\text{O}_3} = 1.23 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp (Japar et al. 1974)

$k_{\text{O}_3} = 1.03 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp (Huie & Herron 1975)

$k_{\text{OH}} = (2.94, 2.96) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{\text{O}_3} = 1.26 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (static system-chemiluminescence, Adeniji et al. 1981)

$k_{\text{O(3P)}} = 4.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O(}^3\text{P)}$ atom (Singleton & Cvetanovic 1976; Atkinson & Pitts Jr. 1977; quoted, Gaffney & Levine 1979)

$k_{\text{OH}}^* = 3.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297.2 K, measured range 297–425 K (flash photolysis-resonance fluorescence, Atkinson & Pitts, Jr. 1977)

$k_{\text{OH}} = 3.13 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{\text{OH}} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.10 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.23 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{\text{OH}} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated lifetime of 5.5 h during summer daylight hours (Altshuller 1991)

$k_{\text{OH}}^* = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}^* = 1.35 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}_3}^* = 9.64 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O(3P)}} = 4.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O(}^3\text{P)}$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric lifetime was estimated to be 5.5 h, based on the reaction rate constant $k = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radicals during summer daylight in the gas phase (Altshuller 1991).

Surface water: $t_{1/2} = 320$ h and 9×10^4 d for reaction with OH and RO_2 radicals of olefins in aquatic system, and $t_{1/2} = 7.3$ d, based on oxidation reaction rate constant $k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ with singlet O_2 for unsubstituted olefins in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.2.1

Reported vapor pressures of 1-butene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot (T/K)$	(5)		
Lamb & Roper 1940		Zwolinski & Wilhoit 1971	
static method-manometer		summary of literature data	
selected values			
t/°C	P/Pa	t/°C	P/Pa
-56.75	8549	-104.8	133.3
-25.3	45423	-89.4	666.6
-22.91	50436	-81.6	1333
-10.60	85513	-73.0	2666
-7.47	96992	-63.4	5333
-0.67	125549	-57.2	7999
0.0	128536	-48.9	13332
		-36.2	26664
bp/°C	-6.30	-21.7	53329
eq. 5	P/mmHg	-6.3	101325
A	6.33816		
B	1330.977	mp/°C	-130
C	0.0017607		

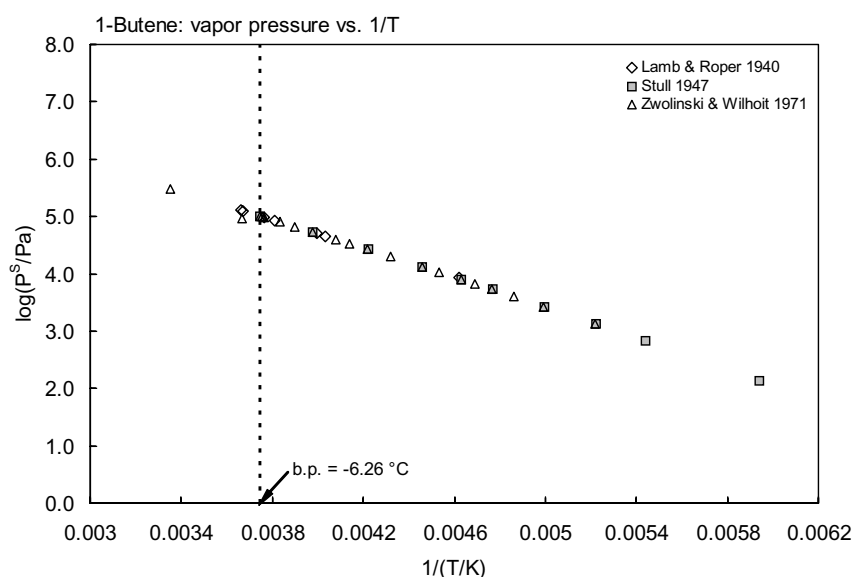


FIGURE 2.1.2.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 1-butene.

2.1.2.1.3 2-Methyl-1-butene



Common Name: 2-Methyl-1-butene

Synonym:

Chemical Name: 2-methyl-1-butene

CAS Registry No: 563-46-2

Molecular Formula: C_5H_{10} , $CH_3CH_2C(CH_3)=CH_2$

Molecular Weight: 70.133

Melting Point ($^{\circ}C$):

-137.53 (Lide 2003)

Boiling Point ($^{\circ}C$):

31.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6504, 0.6451 ($20^{\circ}C$, $25^{\circ}C$, at saturation pressure, Dreisbach 1959; Dean 1985)

Molar Volume (cm^3/mol):

107.8, 108.7 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.91 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

58.34, 48.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

215* ($20^{\circ}C$, shake flask-GC, measured range 20 – $60^{\circ}C$, Pavlova et al. 1966)

155 (estimated-nomograph of Kabadi & Danner 1979; Brookman et al. 1985)

130 (misquoted from 3-methyl-1-butene, Wakita et al. 1986)

168 (calculated-fragment solubility constants, Wakita et al. 1986)

260 (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)

137 (calculated-molar volume V_M , Wang et al. 1992)

128, 198 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

135540* (interpolated-Antoine eq. regression, temp range -89.1 to $20.2^{\circ}C$, Stull 1947)

70242* ($20.996^{\circ}C$, ebulliometry, measured range 1.155 – $62.675^{\circ}C$, Scott et al. 1949)

$\log(P/mmHg) = 6.87314 - 1053.780/(232.768 + t/^{\circ}C)$; temp range 1.155 to $62.675^{\circ}C$ (Antoine eq., ebulliometry, Scott et al. 1949)

81320 (calculated from determined data, Dreisbach 1959)

$\log(P/mmHg) = 6.87314 - 1053.8/(233.0 + t/^{\circ}C)$; temp range -38 to $75^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

81327*, 81330 (derived from compiled data, interpolated-Antoine eq., temp range -53.4 to $52.24^{\circ}C$ Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.87314 - 1053.780/(232.788 + t/^{\circ}C)$; temp range -53.4 to $52.24^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 6474.6/(T/K)] + 7.751419$; temp range -89.1 to $20.2^{\circ}C$ (Antoine eq., Weast 1972–73)

82830 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.98834 - 1046.771/(232.181 + t/^{\circ}C)$ temp range 1.115 – $63.68^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

99500 (interpolated-Antoine eq., temp range -53 to $52^{\circ}C$, Dean 1985, 1992)

$\log(P/mmHg) = 6.84637 - 1039.69/(236.65 + t/^{\circ}C)$; temp range -53 to $52^{\circ}C$ (Antoine eq., Dean 1985, 1992)

81360 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.99292 - 1050.937/(-40.727 + T/\text{K})$; temp range 240–336 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 30.2418 - 2.2723 \times 10^3/(T/\text{K}) - 8.1482 \cdot \log (T/\text{K}) + 5.2331 \times 10^{-11} \cdot (T/\text{K}) + 3.6802 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 136–465 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

43080 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.07 (calculated-regression of Lyman et al. 1982, Wang et al. 1992)

1.89 (calculated-molar volume V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = 9.01 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{\text{OH}} = (6.37 \pm 0.16) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (relative rate method, Ohta 1984)

$k_{\text{OH}} = 9.01 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to $6.07 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Atkinson 1985)

$k_{\text{OH}} = (60.7 - 90.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Atkinson 1989)

$k_{\text{OH}} = 6.10 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated atmospheric lifetime of 2.3 h during summer daylight hours (Altshuller 1991)

$k_{\text{OH}} = 6.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}_3} = 16.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric lifetime $\tau \sim 2.3$ h, based on the photooxidation rate constant $k = 6.10 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radical in air during summer daylight (Altshuller 1991).

Surface water: $t_{1/2} = 320$ h and 9×10^4 d for reaction with OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 7.3$ d, based on oxidation reaction rate constant of $3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ with singlet oxygen for unsubstituted olefins in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.3.1
Reported aqueous solubilities of 2-methyl-1-butene at various temperatures

Pavlova et al. 1966

Shake flask-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
20	215
40	326
50	250
60	267

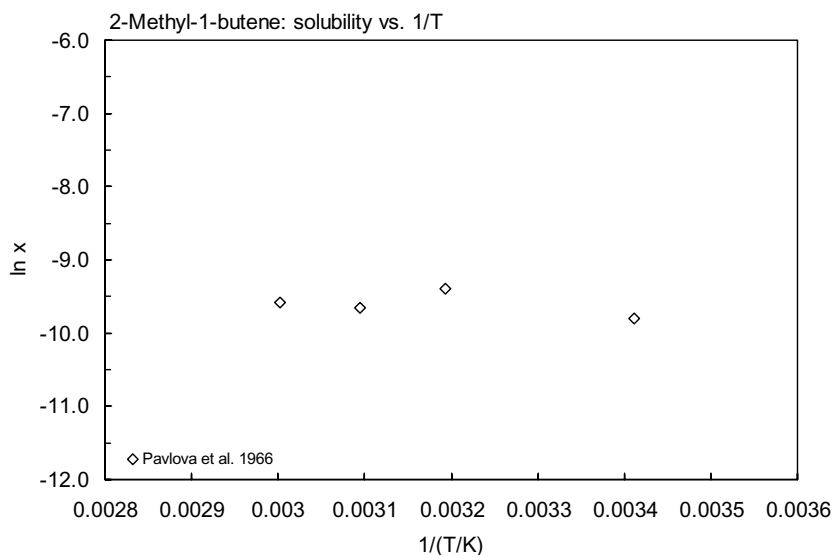


FIGURE 2.1.2.1.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-methyl-1-butene.

TABLE 2.1.2.1.3.2

Reported vapor pressures of 2-methyl-1-butene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Scott et al. 1949		Zwolinski & Wilhoit 1971			
summary of literature data		ebulliometry		selected values			
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
−89.1	133.3	1.155	31163	−53.4	1333	eq. 2	P/mmHg
−72.8	666.6	6.054	38547	−43.7	2666	A	6.87314
−64.3	1333	10.993	47357	−37.5	4000	B	1053.780
−54.8	2666	15.973	57800	−32.87	5333	C	232.788
−44.1	5333	20.996	70242	−29.13	6666	bp/ $^{\circ}\text{C}$	31.163
−37.3	7999	26.062	84534	−25.96	7999	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
−28.0	13332	31.162	101319	−20.76	10666	at 25 $^{\circ}\text{C}$	25.86
−13.8	26664	36.308	120792	−16.54	13332	at bp	25.50
2.5	53329	41.500	143281	−8.44	19998		
20.2	101325	46.728	169952	−2.308	26664		
		52.005	198556	2.683	33331		
mp/ $^{\circ}\text{C}$	−135	57.320	232100	6.924	39997		
		62.675	270083	13.936	53329		
				19.865	66661		
		bp/ $^{\circ}\text{C}$	31.16	24.546	79993		
		Antoine eq.		28.623	93326		
		eq. 2	P/mmHg	29.620	95992		
		A	6.87314	30.400	98659		
		B	1052.780	31.163	101325		
		C	232.788	25.0	81327		

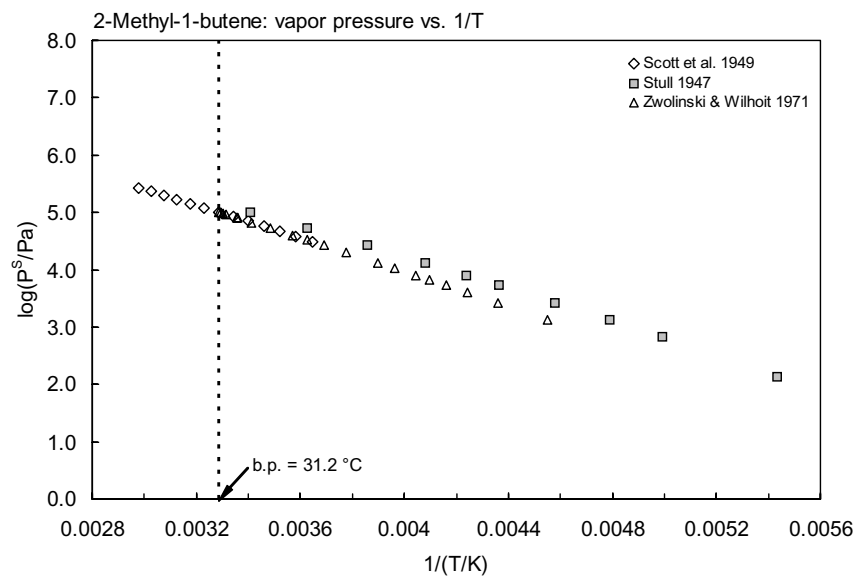


FIGURE 2.1.2.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-1-butene.

2.1.2.1.4 3-Methyl-1-butene



Common Name: 3-Methyl-1-butene

Synonym:

Chemical Name: 3-methyl-1-butene

CAS Registry No: 563-45-1

Molecular Formula: C_5H_{10} , $(CH_3)_2CCHCH=CH_2$

Molecular Weight: 70.133

Melting Point ($^{\circ}C$):

-168.43 (Lide 2003)

Boiling Point ($^{\circ}C$):

20.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.6272, 0.6219 ($20^{\circ}C$, $25^{\circ}C$, at saturation pressure, Dreisbach 1959)Molar Volume (cm^3/mol):111.8 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.36 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

51.19, 41.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

130 (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):101325 ($20.2^{\circ}C$, summary of literature data, temp range -89.1 to $20.2^{\circ}C$, Stull 1947)120790* ($25.128^{\circ}C$, ebulliometry, measured range 0.218 – $51.139^{\circ}C$, Scott & Waddington 1950) $\log(P/mmHg) = 6.82618 - 1013.474/(236.816 + t/^{\circ}C)$; temp range 0.219 – $51.139^{\circ}C$ (Antoine eq., ebulliometric method, Scott & Waddington 1950)

120260 (calculated-Antoine eq., Dreisbach 1959)

 $\log(P/mmHg) = 6.82618 - 1013.474/(237.0 + t/^{\circ}C)$; temp range -47 to $60^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

120000 (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

120270* (derived from compiled data, temp range -62.9 to $40.84^{\circ}C$, Zwolinski & Wilhoit 1971) $\log(P/mmHg) = 6.82618 - 1013.474/(236.816 + t/^{\circ}C)$; temp range -62.9 to $40.84^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)120180 (interpolated-Antoine eq., temp range -63 to $41^{\circ}C$, Dean 1985, 1992) $\log(P/mmHg) = 6.82455 - 1012.37/(236.65 + t/^{\circ}C)$; temp range -63 to $41^{\circ}C$ (Antoine eq., Dean 1985, 1992)

120300 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

 $\log(P_L/kPa) = 5.94656 - 1010.866/(-36.694 + T/K)$; temp range 237 – 324 K (Antoine eq., Stephenson & Malanowski 1987) $\log(P/mmHg) = 31.1486 - 2.1764 \times 10^3/(T/K) - 8.6146 \cdot \log(T/K) + 5.9672 \times 10^{-11} \cdot (T/K) + 4.7555 \times 10^{-6} \cdot (T/K)^2$; temp range 105 – 450 K (vapor pressure eq., Yaws 1994)Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):54230 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

63715, 22610 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

54700 (calculated-P/C, Mackay & Shiu 1981)

43080 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

52940 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.07 (calculated-regression of Lyman et al. 1982, Wang et al. 1992)

2.05 (calculated-molar volume V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = (3.10 \pm 0.31) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299.2 K, measured range 299–433 K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)

$k_{O(3P)} = 4.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(^3P)$ atom (Singleton & Cvetanovic 1976; quoted, Gaffney & Levine 1979)

$k_{OH} = 3.18 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{OH} = 9.01 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $6.07 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985)

$k_{OH}^* = 3.18 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{NO_3} = 9.8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1991)

$k_{OH}^* = 3.18 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = 11.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O(3P)} = 4.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $O(^3P)$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} = 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for reaction with OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 7.3 \text{ d}$, based on oxidation reaction rate constant $k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ with singlet oxygen for (unsubstituted olefins in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.4.1

Reported vapor pressures of 3-methyl-1-butene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log(T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Scott & Waddington 1950				Zwolinski & Wilhoit 1971			
ebulliometry				selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0.210	47363	bp/°C	20.06	-62.9	1333	17.757	93326
5.112	57799	Antoine eq.		-53.4	2666	18.541	95992
10.053	70109	eq. 2	P/mmHg	-47.3	4000	19.309	98659
15.033	84158	A	6.82618	-42.6	5333	20.061	101325
20.061	101325	B	1913.474	-39.2	6666	25.0	120270
25.128	120790	C	236.816	-36.05	7999		
30.245	143268			-30.96	10666	eq. 2	P/mmHg
35.402	169066			-26.82	13332	A	6.82618
40.602	198543			-18.87	19998	B	1013.474
45.847	232073			-12.85	26664	C	236.816
51.139	280097			-7.95	33331	bp/°C	20.061
				-3.783	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				3.109	53329	at 25°C	23.85
				8.743	66661	at bp	24.06
				13.546	79993		

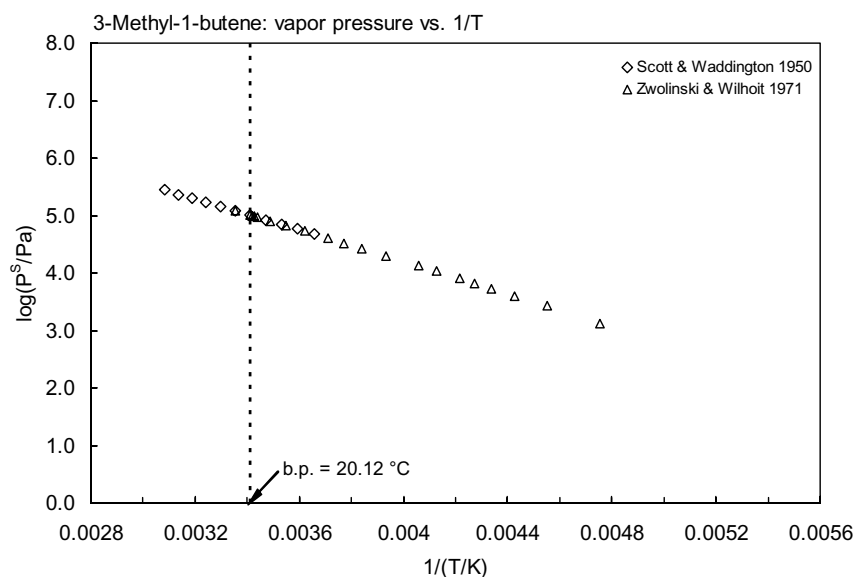


FIGURE 2.1.2.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for 3-methyl-1-butene.

2.1.2.1.5 2-Methyl-2-butene



Common Name: 2-Methyl-2-butene

Synonym:

Chemical Name: 2-methyl-2-butene

CAS Registry No: 513-35-9

Molecular Formula: C_5H_{10} , $CH_3CH=C(CH_3)CH_3$

Molecular Weight: 70.133

Melting Point ($^{\circ}C$):

−133.72 (Lide 2003)

Boiling Point ($^{\circ}C$):

38.56 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6623, 0.6570 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

105.9, 106.8 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.60 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

54.47, 59.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

215* ($20^{\circ}C$, shake flask-GC, measured range 20 – $60^{\circ}C$, Pavlova et al. 1966)

325* (calculated-liquid-liquid equilibrium LLE data, temp range 288 – $333.2 K$, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

47876* ($18.07^{\circ}C$, static method, measured range -78.85 to $18.07^{\circ}C$, Lamb & Roper 1940)

$\log(P/mmHg) = 9.86840 - 1773.506/(T/K) + 0.0035747 \cdot \log(T/K)$; temp range -78.85 to $18.07^{\circ}C$ (static method, Lamb & Roper 1940)

53329* (21.6 , summary of literature data, temp range -75.4 to $38.5^{\circ}C$, Stull 1947)

57798* (ebulliometry, measured range 3.042 to $70.59^{\circ}C$, Scott et al. 1949)

$\log(P/mmHg) = 6.91562 - 1095.088/(232.842 + t/^{\circ}C)$; temp range 3.042 to $70.59^{\circ}C$ (Antoine eq., ebulliometry, Scott et al. 1949)

62140 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.91562 - 1095.088/(233.0 + t/^{\circ}C)$; temp range -31 to $85^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

62142*, 62140 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.91562 - 1095.088/(232.842 + t/^{\circ}C)$; temp range -47.7 to $60.0^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

62890, 62140 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.15017 - 1146.28/(238.416 + t/^{\circ}C)$; temp range -78.85 to $18.07^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.04808 - 1099.054/(233.314 + t/^{\circ}C)$; temp range 3.04 – $70.59^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

62240 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.96659 - 1124.33/(236.63 + t/^{\circ}C)$; temp range -48 to $60^{\circ}C$ (Antoine eq., Dean 1985, 1992)

62170 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.04475 - 1097.501/(-39.985 + T/\text{K})$; temp range 271–343 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 33.7539 - 2.426 \times 10^3/(T/\text{K}) - 9.4429 \cdot \log (T/\text{K}) + 9.8488 \times 10^{-11} \cdot (T/\text{K}) + 4.7156 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 139–471 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

24650 (calculated-P/C from selected data)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k ; for gas-phase second-order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O_3} = 7.47 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 30°C (flow system, Bufalini & Altshuller 1965)

$k_{OH} = 11.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{O(3P)} = 5.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $O(3P)$ (Herron & Huie 1973; Furuyama et al. 1974; Atkinson & Pitts Jr. 1978; quoted, Gaffney & Levine 1979)

$k_{O_3} = 4.93 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (Japar et al. 1974)

$k_{OH} = 4.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with atmospheric $t_{1/2} < 0.24 \text{ h}$ (Darnall et al. 1976, Lloyd et al. 1976)

$k_{OH} = 8.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)

$k_{OH} = 8.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{O(3P)} = 54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (LFE correlation, Gaffney & Levine 1979)

$k_{OH} = (87.1 \pm 2.6) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ (relative rate method, Ohta 1984)

$k_{NO_3} = (5.5 \pm 1.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 295 K (relative rate method, Atkinson et al. 1984a)

$k_{O_3} = 4.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetimes $\tau = 55 \text{ min}$ and 17 min in clean and moderately polluted atmosphere respectively, $k_{OH} = 8.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetimes $\tau = 3.2 \text{ h}$ and 1.6 h in clean and moderately polluted atmosphere, respectively; $k_{NO_3} = 5.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetimes $\tau = 13 \text{ min}$ and 1.3 min in clean and moderately polluted atmosphere, respectively (Atkinson et al. 1984a)

$k_{NO_2} < 0.5 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson et al. 1984b)

$k_{O_3} = 4.5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH} = 8.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{NO_3} = 5.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{O(3P)} = 47.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $O(3P)$ atom at room temp. (Atkinson et al. 1984b)

$k_{OH} = 8.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate method, Atkinson & Aschmann 1984)

$k_{O_3} = (6.79\text{--}7.97) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, 296–299 K (Atkinson & Carter 1984)

$k_{O_3} = 4.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 25 d^{-1} ; $k_{OH} = 8.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 8 d^{-1} , and $k_{NO_3} = 9.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 205 d^{-1} (Atkinson & Carter 1984)

$k_{OH} = 7.7 \times 10^{-11}$ to $1.19 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ between 297.7–299.5 K (Atkinson 1985)

$k_{O_3} = 4.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 25 d^{-1} ; $k_{OH} = 8.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 3.8 d^{-1} , and $k_{NO_3} = 9.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 205 d^{-1} at room temp (Atkinson 1985)

$k_{NO_3} = (9.33 \pm 1.18) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ $296 \pm 2 \text{ K}$ (relative rate method, Atkinson 1988)

$k_{OH} = 8.69 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 6.89 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = 4.23 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 198 K (Atkinson 1990)

$k_{OH} = 8.69 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 9.33 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{\text{NO}_3} = 9.37 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{\text{OH}}^* = 8.69 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 9.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3}^* = 4.03 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}(^3\text{P})} = 5.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O}(^3\text{P})$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} < 0.24 \text{ h}$, based on the photooxidation rate constant $k = 4.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with hydroxyl radical in air (Darnall et al. 1976; Lloyd et al. 1976);

atmospheric lifetimes, $\tau(\text{calc}) = 0.95 \text{ h}$ for the reaction with O_3 , $\tau = 3.2 \text{ h}$ with OH radical and $\tau = 0.12 \text{ h}$ with NO_3 radical, based on the rate constants and environmental concentrations of OH, O_3 and NO_3 in the gas phase (Atkinson & Carter 1984);

calculated lifetimes: $\tau = 55 \text{ min}$ due to reaction with O_3 in 24-h period, $\tau = 3.2 \text{ h}$ with OH radical during daytime, and $\tau = 13 \text{ min}$ for NO_3 radical during nighttime for “clean” atmosphere; $\tau = 17 \text{ min}$ for reaction with O_3 in 24-h period, $\tau = 1.6 \text{ h}$ with OH radical during daytime, and $\tau = 1.3 \text{ min}$ with NO_3 radical during nighttime in “moderately” polluted atmosphere (Atkinson et al. 1984a);

atmospheric lifetimes $\tau(\text{calc}) = 6.38 \text{ h}$ for the reaction with OH radical, $\tau(\text{calc}) = 0.92 \text{ h}$ with O_3 and $\tau(\text{calc}) = 0.12 \text{ h}$ with NO_3 radical in the gas phase (Atkinson 1985).

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for reaction with OH and RO_2 radicals respectively in aquatic system, and $t_{1/2} = 8.0 \text{ d}$, based on rate constant of $10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.5.1

Reported aqueous solubilities of 2-methyl-2-butene at various temperatures

Pavlova et al. 1966		Góral et al. 2004	
shake flask-GC		calc-recommended LLE data	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	215	15	343
40	236	20	334
50	250	25	325
60	267	40	325
		50	338
		60	361

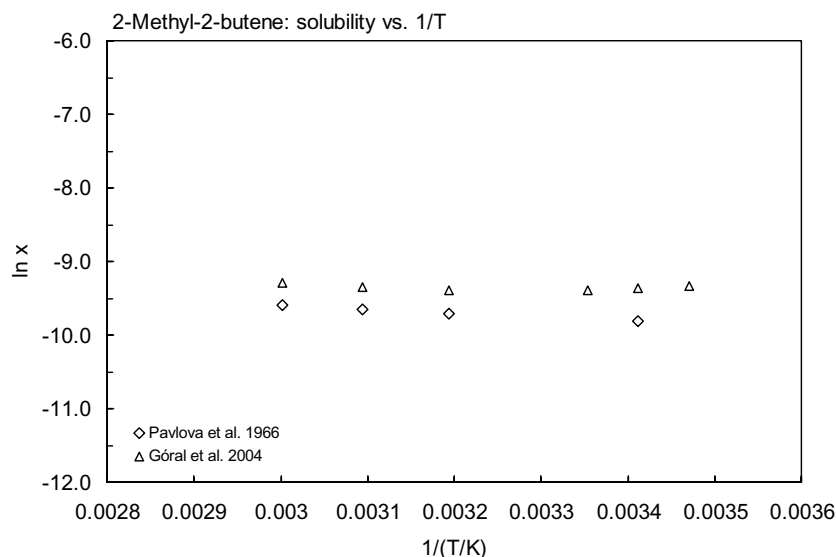


FIGURE 2.1.2.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methyl-2-butene.

TABLE 2.1.2.1.5.2
Reported vapor pressures of 2-methyl-2-butene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)
log P = A – B/(C + T/K)		(3)			
log P = A – B/(T/K) – C·log (T/K)		(4)			
log P = A – B/(T/K) – C·(T/K)		(5)			

Lamb & Roper 1940		Stull 1947		Scott et al. 1949		Zwolinski & Wilhoit 1971	
Static method-manometer		Summary of literature data		Ebulliometry		Selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–78.85	97	–75.4	133.3	3.042	25007	–47.7	1333
–54.78	811	–57.0	666.6	8.008	31172	–37.8	2666
–37.98	2696	–47.0	1333	12.987	38534	–31.46	4000
–29.84	4517	–37.9	2666	18.033	47364	–26.75	5333
–21.06	7537	–26.7	5333	23.103	57798	–22.92	6666
–12.14	11767	–19.4	7999	28.220	70110	–19.68	7999
–3.98	18238	–9.9	13332	33.373	84522	–14.37	10666
0.0	21918	4.0	26664	38.567	101319	–10.06	13332
0.0	22025	21.6	53329	43.806	120810	–1.786	19998
2.44	24625	38.5	101325	49.078	143268	4.486	26664
4.51	27024			54.399	169079	9.559	33331
16.31	44783	mp/°C	–133	59.753	198543	13.883	39997
18.07	47876			65.151	232087	21.029	53329
				70.590	272230	26.864	66661
bp/°C	38.43					31.834	79993
eq. 5	P/mmHg					36.187	93326
A	9.68640					36.998	95992
B	1773.506					37.791	98659
C	0.0035747					38.568	101325

TABLE 2.1.2.1.5.2 (Continued)

Lamb & Roper 1940		Stull 1947		Scott et al. 1949		Zwolinski & Wilhoit 1971	
Static method-manometer		Summary of literature data		Ebulliometry		Selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						25.0	62142
						eq. 2	P/mmHg
						A	6.91562
						B	1095.088
						C	232.842
						bp/°C	38.568
						ΔH_v /(kJ mol ⁻¹) =	
						at 25°C	27.06
						at bp	26.30

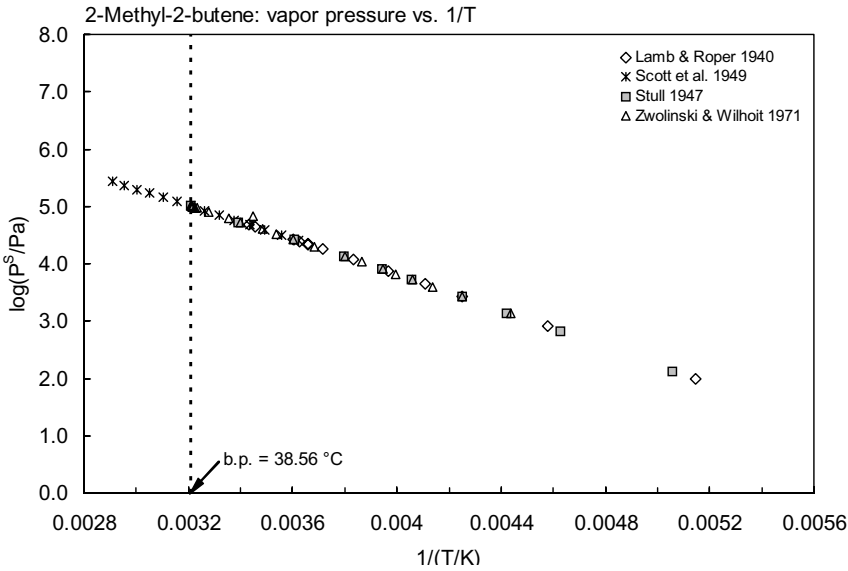


FIGURE 2.1.2.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-2-butene.

2.1.2.1.6 1-Pentene



Common Name: 1-Pentene

Synonym: amylene, α -*n*-amylene, propylethylene

Chemical Name: 1-pentene

CAS Registry No: 109-67-1

Molecular Formula: C₅H₁₀

Molecular Weight: 70.133

Melting Point (°C):

−165.12 (Lide 2003)

Boiling Point (°C):

29.96 (Lide 2003)

Density (g/cm³):

0.6405, 0.63533 (20°C, 25°C, Forziati et al. 1950, Dreisbach 1959)

0.6353 (20°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

109.5 (20°C, calculated-density, Stephenson & Malanowski 1987)

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

25.47, 25.20 (25 °, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.998 (Riddick et al. 1986)

5.81 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

53.82, 54.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

148 (shake flask-GC, McAuliffe 1966)

191 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

91420* (interpolated-Antoine eq. regression, temp range −80.4 to 30.1°C, Stull 1947)

70834 (20°C, static method, measured range 0–200°C, Day et al. 1948)

$\log (P/\text{mmHg}) = 7.40607 - 1372.194/(T/K)$; temp range 0–30°C (static method, Day et al. 1948)

$\log (P/\text{mmHg}) = 7.31561 - 1342.407/(T/K)$; temp range 40–95°C (static method, Day et al. 1948)

84508* (ebulliometry, measured range −0.159 to 61.64°C, Scott et al. 1949)

$\log (P/\text{mmHg}) = 6.85487 - 1049.00/(233.994 + t/^\circ\text{C})$; temp range −0.159 to 61.64°C (Antoine eq., ebulliometry, Scott et al. 1949)

83750* (24.6°C, ebulliometry-manometer, measured range 12.8–30.7°C, Forziati et al. 1950)

$\log (P/\text{mmHg}) = 6.78568 - 1014.293/(229.783 + t/^\circ\text{C})$; temp range 12.8–30.7°C (Antoine eq., ebulliometry measurements, Forziati et al. 1950)

86500 (calculated from determined data, Dreisbach 1959)

$\log (P/\text{mmHg}) = 6.84650 - 1044.9/(234.0 + t/^\circ\text{C})$; temp range −39 to 73°C (Antoine eq. for liquid state, Dreisbach 1959)

85000* (interpolated-Antoine eq., temp range −63 to 41°C, Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 6.84650 - 1044.895/(233.516 + t/^\circ\text{C})$; temp range −63 to 41°C (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 6931.2/(T/K)] + 7.914969$; temp range −80.4 to 30.1°C (Antoine eq., Weast 1972–73)

85020 (interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.9716 - 1045.212/(233.598 + t/^{\circ}\text{C})$; temp range 12.84–30.7°C (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)

85200 (interpolated-Antoine eq., temp range –55 to 51°C, Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.84424 - 1044.015/(233.50 + t/^{\circ}\text{C})$; temp range –55 to 51°C (Antoine eq., Dean 1985, 1992)

85100 (literature average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 5.96914 - 1044.01/(233.49 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

85040 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.96999 - 1043.962/(-39.767 + T/\text{K})$; temp range 218–311 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 36.2741 - 2.4452 \times 10^3/(T/\text{K}) - 10.405 \cdot \log (T/\text{K}) - 7.4629 \times 10^{-11} \cdot (T/\text{K}) + 5.4070 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 110–465 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

40330 (calculated-P/C, Mackay & Shiu 1975; selected, Mills et al. 1982)

41140 (calculated as $1/K_{AW} \cdot C_W/C_A$, reported as exptl., Hine & Mookerjee 1975)

37520, 22610 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

40300 (calculated-P/C, Mackay & Shiu 1981)

37520 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

40405 (calculated-P/C, Eastcott et al. 1988)

40280 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.20 (calculated- π substituent constant, Hansch et al. 1968)

2.69 (calculated-f const., Yalkowsky & Morozowich 1980)

2.20 (calculated-MCI χ , Murray et al. 1975)

2.80 (selected, Müller & Klein 1992)

2.3970 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.0* (20.29°C, from GC determined γ^{∞} in octanol, measured range 20.29–50.2°C, Gruber et al. 1997)

1.93 (calculated-measured γ^{∞} in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 4.25 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{O_3} = 1.07 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Japar et al. 1974)

$k_{O_3} = 5.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $7.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $1.07 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (review, Atkinson & Carter 1984)

$k_{OH} = 3.13 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = 1.10 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{O_3} = 1.00 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1994)

$k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3}^* = 10.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O(3P)} = 4.65 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $O(3P)$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for olefins in aquatic system by oxidation with OH and RO_2 radicals; while $t_{1/2} = 7.3$ d based on rate constant $k = 3 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for the oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.6.1

Reported vapor pressures of 1-pentene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Scott et al. 1949		Forziati et al. 1950		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−80.4	133.3	−0.159	31168	12.834	53703	−54.8	1333
−63.3	666.6	4.751	38545	18.468	66797	−45.1	2666
−54.5	1333	9.706	47348	24.584	63754	−38.91	4000
−46.0	2666	14.706	57789	28.900	97645	−34.28	5333
−34.1	5333	19.750	70094	29.362	99227	−30.53	6666
−27.1	7999	24.834	84508	29.796	100727	−27.36	7999
−17.7	13332	29.967	101322	30.289	102453	−22.14	10666
−3.40	26664	35.142	120813	30.723	103988	−17.92	13332
12.8	53329	40.359	143295			−9.789	19998
30.1	101325	45.614	169079	bp/°C	29.968	−3.640	26664
mp/°C		50.914	198557			1.368	33331
		56.253	232061	eq. 2	P/mmHg	5.624	39997
		61.641	270071	A	6.78568	12.664	53329
				B	1014.294	18.416	66661
		bp/°C	29.97	C	229.783	23.319	79993
		Antoine eq.				27.616	93326
		eq. 2	P/mmHg			28.417	95992
		A	6.85487			29.201	98659
		B	1049.00			29.968	101325
		C	233.994			25.0	85020
						eq. 2	P/mmHg
						A	6.84650
					B	1044.895	
					C	233.516	
					bp/°C	29.968	
					$\Delta H_v/(\text{kJ mol}^{-1}) =$		
					at 25°C	25.47	
					at bp	25.20	

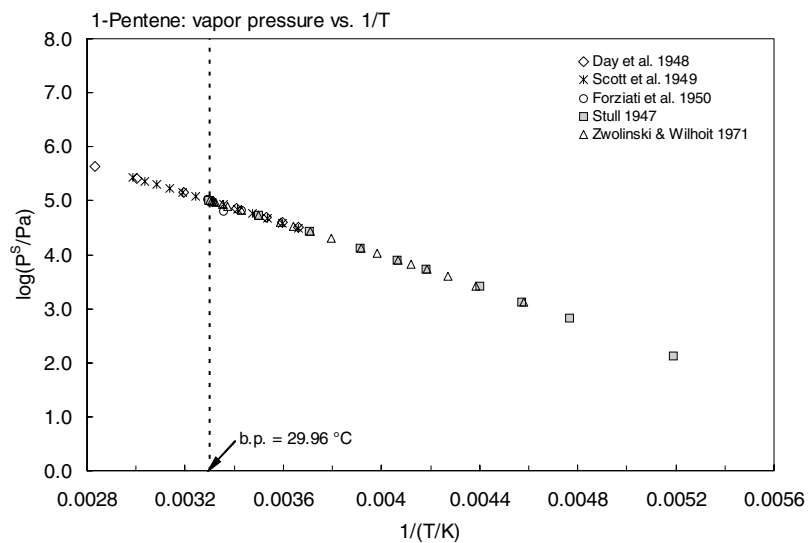


FIGURE 2.1.2.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for 1-pentene.

TABLE 2.1.2.1.6.2

Reported octanol-air partition coefficients of 1-pentene at various temperatures and temperature dependence equations

Gruber et al. 1997

GC det'd activity coefficient

t/°C	log K_{OA}
20.29	1.995
30.3	1.852
40.4	1.740
50.28	1.630

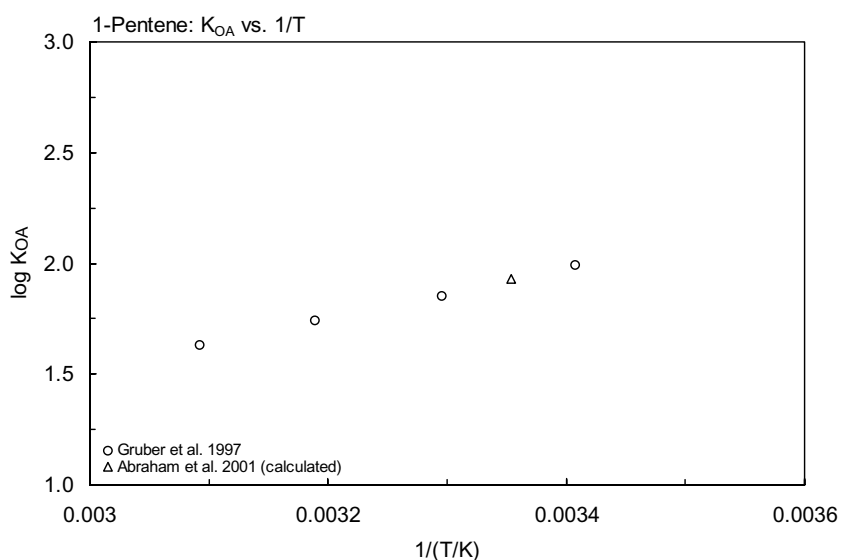
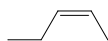


FIGURE 2.1.2.1.6.2 Logarithm of K_{OA} versus reciprocal temperature for 1-pentene.

2.1.2.1.7 *cis*-2-Pentene

Common Name: *cis*-2-Pentene

Synonym: (Z)-2-pentene

Chemical Name: *cis*-2-pentene

CAS Registry No: 627-20-3

Molecular Formula: C₅H₁₀

Molecular Weight: 70.133

Melting Point (°C):

−151.36 (Lide 2003)

Boiling Point (°C):

36.93 (Lide 2003)

Density (g/cm³ at 20°C):

0.6556, 0.6504 (20°C, 25°C, Dreisbach 1959)

Molar Volume (cm³/mol):

107.0, 107.8 (20°C, 25°C, calculated-density)

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.112 (Riddick et al. 1986)

7.11 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

58.39, 52.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

203 (shake flask-GC, *cis-trans* form not specified, McAuliffe 1966)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

57795* (21.541°C, ebulliometry, measured range 1.595–68.842°C, Scott & Waddington 1950)

log (P/mmHg) = 6.87540 – 1069.460/(240.786 + t/°C); temp range 1.595–68.842°C (Antoine eq., ebulliometric method, Scott & Waddington 1950)

65940 (calculated-Antoine eq., Dreisbach 1959)

log (P/mmHg) = 6.87274 – 1068.0/(231.0 + t/°C); temp range −33 to 82°C (Antoine eq. for liquid state, Dreisbach 1959)

66000, 65941 (interpolated-Antoine eq., derived from compiled data, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.87274 – 1067.951/(230.585 + t/°C); temp range −48.7 to 58.31°C (Antoine eq., Zwolinski & Wilhoit 1971)

65950 (interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.99984 – 1069.227/(230.757 + t/°C); temp range 1.595–68.88°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

66640 (interpolated-Antoine eq., Dean 1985, 1992)

66000 (quoted lit., Riddick et al. 1986)

log (P/kPa) = 5.96798 – 1052.44/(228.693 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/mmHg) = 6.84308 – 1052.44/(228.69 + t/°C); temp range −49 to 58°C (Antoine eq., Dean 1985, 1992)

65970 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.99069 – 1064.178/(−43.035 + T/K); temp range 234–318 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 34.0427 – 2.4524 × 10³/(T/K) – 9.5014 · log (T/K) – 5.0816 × 10^{−11} · (T/K) + 4.3638 × 10^{−6} · (T/K)²; temp range 122–476 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

22800	(calculated-P/C, Mackay & Shiu 1981)
22770	(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.20	(calculated- π substituent constant, Hansch et al. 1968)
2.20	(calculated-MCI χ , <i>cis-trans</i> form not specified, Murray et al. 1975)
2.3772	(calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{O}(^3\text{P})} = 1.80 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom (Herron & Huie 1973; quoted, Gaffney & Levine 1979)

$k_{\text{OH}} = 6.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)

$k_{\text{OH}} = (6.23 \pm 0.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Ohta 1984)

$k_{\text{OH}} = (65.4 - 65.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298-303 \text{ K}$ (Atkinson 1989)

$k_{\text{OH}} = 6.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}} = 6.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated atmospheric lifetime of 2.29 h in summer daylight (Altshuller 1991)

$k_{\text{OH}} = 6.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}(^3\text{P})} = 1.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O}(^3\text{P})$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

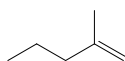
Air: photooxidation reaction rate constant $k = 6.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with hydroxyl radical in air (Atkinson 1990, Altshuller 1991) with an estimated atmospheric lifetime of 2.29 h in summer daylight (Altshuller 1991).

Surface water: $t_{1/2} \sim 320 \text{ h}$ for oxidation by OH radicals, $t_{1/2} = 9 \times 10^4 \text{ d}$ for olefins in aquatic system, and $t_{1/2} = 7.3 \text{ d}$ based on rate constant $k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of unsubstituted olefins by singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.7.1
Reported vapor pressures of *cis*-2-pentene at various temperatures

Scott & Waddington 1950			
ebulliometric method			
t/°C	P/Pa	t/°C	P/Pa
1.595	25009	58.070	198556
6.522	31163	63.456	232087
11.486	38546	68.882	270057
16.494	47357		
21.541	57795	$\log P = A - B/(C + t/^{\circ}\text{C})$	
26.633	70102	bp/°C	36.94
31.766	84518		P/mmHg
36.944	101329	A	6.87540
42.161	120804	B	1069.460
47.423	143281	C	240.786
52.724	169066		

2.1.2.1.8 2-Methyl-1-pentene



Common Name: 2-Methyl-1-pentene

Synonym:

Chemical Name: 2-methyl-1-pentene

CAS Registry No: 763-29-1

Molecular Formula: C_6H_{12} ; $CH_3(CH_2)_2C(CH_3)CH_2$

Molecular Weight: 84.159

Melting Point ($^{\circ}C$):

−135.7 (Dreisbach 1959; Lide 2003)

Boiling Point ($^{\circ}C$):

60.7 (Dreisbach 1959)

62.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6799, 0.6751 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

123.8, 124.7 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

133.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

78.0 (shake flask-GC, McAuliffe 1966)

98.2 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

27464 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.88772 - 1154.7/(227.0 + t/^{\circ}C)$; temp range -14 to $100^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

26000, 26051 (interpolated-Antoine eq., derived from compiled data, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.85030 - 1138.516/(224.764 + t/^{\circ}C)$; temp range -30.1 to $85.16^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.85030 - 1138.516/(224.70 + t/^{\circ}C)$; temp range -30 to $85^{\circ}C$ (Antoine eq., Dean 1985, 1992)

26060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.89056 - 1091.679/(-46.306 + T/K)$; temp range 265–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.99434 - 1148.616/(-49.853 + T/K)$; temp range: 275–344 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 32.9509 - 2.8171 \times 10^3/(T/K) - 8.9572 \cdot \log(T/K) - 8.7635 \times 10^{-11} \cdot (T/K) + 3.1710 \times 10^{-6} \cdot (T/K)^2$; temp range 137–507 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

28100 (calculated-P/C, Mackay & Shiu 1981)

28093 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = 1.05 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ under atmospheric conditions (Atkinson & Carter 1984)

$k_{OH} = (8.76 \pm 0.14) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Ohta 1984)

$k_{OH} = 62.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985, Atkinson 1989)

$k_{OH} = 6.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = 15.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

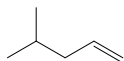
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 8.0 \text{ d}$, based on rate constant $k = 1.0 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of substituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.1.9 4-Methyl-1-pentene



Common Name: 4-Methyl-1-pentene

Synonym:

Chemical Name: 4-methyl-1-pentene

CAS Registry No: 691-37-2

Molecular Formula: C₆H₁₂

Molecular Weight: 84.159

Melting Point (°C):

−153.6 (Dreisbach 1959; Lide 2003)

Boiling Point (°C):

53.88 (Dreisbach 1959)

53.9 (Lide 2003)

Density (g/cm³ at 20°C):

0.6642, 0.6594 (20°C, 25°C, Dreisbach 1059)

Molar Volume (cm³/mol):

126.7 (20°C, calculated-density, McAuliffe 1966, Ruelle & Kesselring 1997)

127.6 (25°C, calculated-density)

133.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

48.0 (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

35600 (calculated-Antoine eq., Dreisbach 1959)

log (P/mmHg) = 6.87757 − 1130.0/(229.0 + t/°C); temp range −20 to 91°C (Antoine eq. for liquid state, Dreisbach 1959)

36104, 36100 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.83529 − 1121.302/(229.687 + t/°C); temp range −37.5 to 76.75°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.83529 − 1121.302/(229.687 + t/°C); temp range −38 to 77°C (Antoine eq., Dean 1985, 1992)

36110 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 5.94694 − 1114.082/(−44.332 + T/K); temp range 265–333 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 44.7746 − 2.7364 × 10³/(T/K) − 14.283·log (T/K) + 7.31 × 10^{−3}·(T/K) + 4.8402 × 10^{−14}·(T/K)²; temp range 120–496 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

62270 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

65200, 34220 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

63200 (calculated-P/C, Mackay & Shiu 1981)

63270 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.50 (calculated-π constant, Hansch et al. 1968)

2.51 (calculated-MCI χ, Murray et al. 1975)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = 1.06 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson & Carter 1984)

$k_{O_3} = 9.2 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

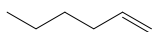
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 8.0 \text{ d}$, based on rate constant $k = 1.0 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of substituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.1.10 1-Hexene



Common Name: 1-Hexene

Synonym: α -hexene

Chemical Name: 1-hexene

CAS Registry No: 646-04-8

Molecular Formula: C_6H_{12} ; $CH_3(CH_2)_3CHCH_2$

Molecular Weight: 84.159

Melting Point ($^{\circ}C$):

−139.76 (Lide 2003)

Boiling Point ($^{\circ}C$):

63.48 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6732, 0.6685 ($20^{\circ}C$, $25^{\circ}C$, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

125.0 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Wang et al. 1992; Ruelle & Kesselring 1997)

125.9 ($25^{\circ}C$, calculated-density)

133.2 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.347 (Riddick et al. 1986)

9.35 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

70.1, 61.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

50.0 (shake flask-GC, McAuliffe 1966)

65.5 (shake flask-titration, Natarajan & Venkatachalam 1972)

65.5, 54.12, 42.16 (25 , 30 , $35^{\circ}C$, shake flask-titration, in $0.001M HNO_3$ solution, Natarajan & Venkatachalam 1972)

55.4 (shake flask-GC, Leinonen & Mackay 1973)

60.0 ($20^{\circ}C$, shake flask-GC, Budantseva et al. 1976)

69.7 (generate column-GC, Tewari et al. 1982a)

100, 53 ($20^{\circ}C$, $25^{\circ}C$, “best” values, IUPAC Solubility Data Series, Shaw 1989a)

$\ln x = -268.791 + 11353.70/(T/K) + 38.4871 \cdot \ln (T/K)$; temp range 290 – 400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 2001)

$\ln x = -276.423 + 11833.54/(T/K) + 39.5126 \cdot \ln (T/K)$; temp range 290 – 400 K (eq. derived from direct fit of solubility data, Tsionopoulos 2001)

51.43* (calculated-liquid-liquid equilibrium LLE data, temp range 293.2 – 494.3 K, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

22300* (Antoine eq. regression, temp range -57.5 to $66^{\circ}C$, Stull 1947)

23500* ($23.7^{\circ}C$, ebulliometry-manometer, measured range 15.9 – $64.3^{\circ}C$, Forziati et al. 1950)

$\log (P/mmHg) = 6.86573 - 1152.971/(225.849 + t/^{\circ}C)$; temp range 15.9 – $64.3^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)

25000 (calculated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.86572 - 1152.971/(226.0 + t/^{\circ}C)$; temp range -12 to $79^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

24800*, 24798 (interpolated-Antoine eq., derived from compiled data, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.86573 - 1152.971/(225.849 + t/^{\circ}C)$; temp range -29.3 to $86.64^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 7787.6/(T/K)] + 7.930324$; temp range -57.5 to 66°C (Antoine eq., Weast 1972–73)
 24800 (interpolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 5.99426 - 1154.952/(226.002 + t/^\circ\text{C})$; temp range 15.89 – 64.311°C (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)
 24800 (interpolated-Antoine eq., temp range -16 to 64°C , Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 6.85770 - 1148.62/(225.25 + t/^\circ\text{C})$; temp range -16 to 64°C (Antoine eq., Dean 1985, 1992)
 24800 (selected lit., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 5.98260 - 1148.62/(225.346 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 24800 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.98336 - 1149.029/(-47.755 + T/K)$; temp range 273 – 343 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 33.4486 - 2.6221 \times 10^3/(T/K) - 9.1784 \cdot \log (T/K) + 3.093 \times 10^{-12} \cdot (T/K) + 3.678 \times 10^{-6} \cdot (T/K)^2$;
 temp range 133 – 504 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

41750 (calculated-P/C, Mackay & Shiu 1975)
 44080 (calculated- $1/K_{\text{AW}}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 51790, 34220 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 41800 (calculated-P/C, Mackay & Shiu 1981)
 47230 (calculated- χ , Nirmalakhandan & Speece 1988)
 41640 (calculated-P/C, Eastcott et al. 1988)
 29940 (calculated-vapor–liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.39 (generator column-GC, Tewari et al. 1982a,b)
 3.47 (calculated-activity coeff. γ , Wasik et al. 1981)
 3.48 (calculated-activity coeff. γ , Wasik et al. 1982)
 3.39, 3.40 (generator column-GC, calculated-activity coeff. γ , Schantz & Martire 1987)
 3.40 (recommended, Sangster 1989)
 3.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.50* (20.29°C , from GC-determined γ^∞ in octanol, measured range 20.29 – 50.28°C , Gruber et al. 1997)
 2.41 (calculated-measured γ^∞ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{O}_3} = 0.90 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Cadle & Schadt 1952)
 $k_{\text{O}_3} = 1.00 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Hanst et al. 1958)
 $k_{\text{O}_3} = 1.10 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 30°C (flow system, Bufalini & Altshuller 1965)
 $k_{\text{O}_3} = 1.40 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (static system-chemiluminescence, Cox & Penkett 1972)
 $k_{\text{O}_3} = 1.10 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (static system-chemiluminescence, Stedman et al. 1973)
 $k_{\text{O}_3} = 1.11 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (static system-chemiluminescence, Japar et al. 1974)
 $k_{\text{O}_3} = 1.08 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 ± 2 K (static system-chemiluminescence, Adeniji et al. 1981)
 $k_{\text{O}_3} = 1.21 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (static system-chemiluminescence, Atkinson et al. 1982)
 $k_{\text{O}_3} = (0.91 \text{ to } 1.36) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 – 303 K (Atkinson & Carter 1984)
 $k_{\text{OH}} = 3.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{\text{OH}} = (3.75 - 3.25) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295–303 K (Atkinson 1985)

$k_{\text{OH}} = (32.9 - 37.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295–303 K (Atkinson 1989)

$k_{\text{OH}} = 3.18 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3} = 1.17 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{O}_3} = 1.10 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

$k_{\text{OH}} = 3.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3^*} = 11.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}(^3\text{P})} = 4.65 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O}(^3\text{P})$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 7.3 \text{ d}$, based on rate constant $k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.10.1
Reported aqueous solubilities of 1-hexene at various temperatures

Góral et al. 2004

Calc-recommended LLE data

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
20	56.11
25	51.43
36.8	51.43
93.3	102.9
148.8	392.8
204.4	2151
221.1	3740

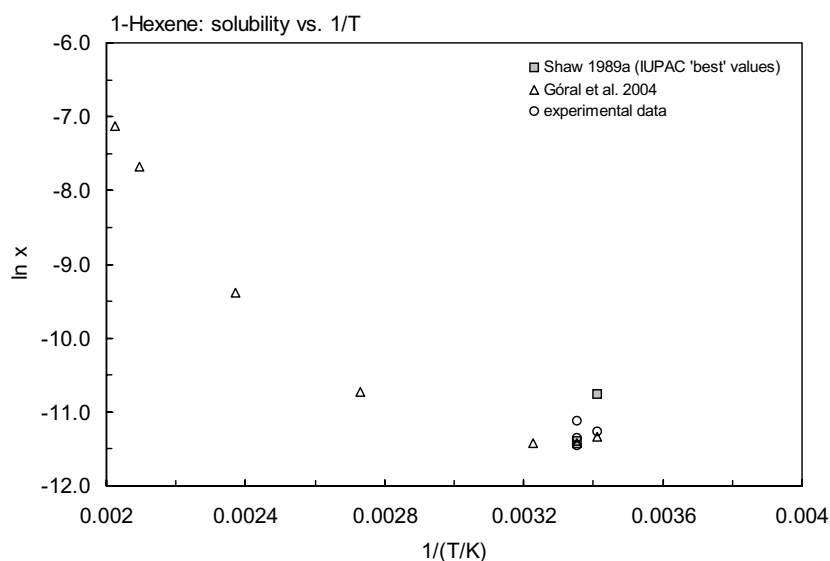


FIGURE 2.1.2.1.10.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-hexene.

TABLE 2.1.2.1.10.2

Reported vapor pressures and octanol-air partition coefficients of 1-hexene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Vapor pressure						log K _{OA}	
Stull 1947		Forziati et al. 1950		Zwolinski & Wilhoit 1971		Gruber et al. 1997	
Summary of literature data		Ebulliometry		Selected values		GC det'd activity coefficient	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	log K _{OA}
–57.5	133.3	15.890	16645	–29.30	1333	20.29	2.503
–38.0	666.6	19.950	19946	–18.65	2666	30.3	2.331
–28.1	1333	23.720	23485	–11.88	4000	40.4	2.20
–17.2	2666	28.762	28990	–6.81	5333	50.28	2.068
–5.0	5333	33.399	34936	–2.70	6666		
2.8	7999	38.993	43366	0.776	7999		
13.0	13332	44.763	53705	8.482	10666		
29.0	26664	50.914	66798	11.109	13332		
46.8	53329	62.323	97648	20.006	19998		
66.0	101325	62.827	99230	26.736	26664		
mp/°C		63.299	100730	32.215	33331		
		62.837	102457	38.871	39997		
		64.311	103995	44.569	53329		
				50.859	66661		
		eq. 2	P/mmHg	56.219	79993		
		A	6.86573	60.915	93326		
		B	1152.971	61.790	95992		
		C	225.849	62.647	98659		
		bp/°C	63.485	63.585	101325		
				25.0	24798		
				eq. 2	P/mmHg		
				A	6.86572		
				B	1152.971		
				C	225.849		
				bp/°C	63.485		
			ΔH _v /(kJ mol ^{–1}) =				
			at 25°C		28.28		
			at bp		30.63		

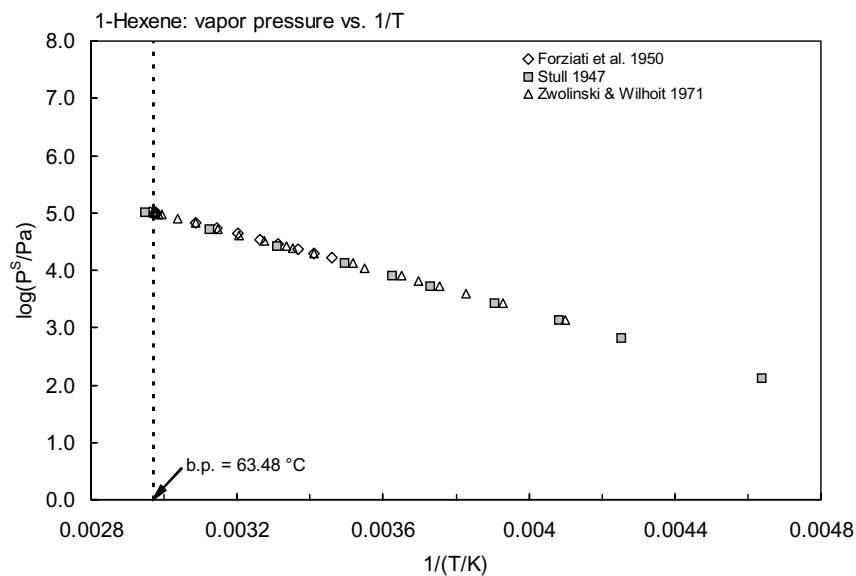


FIGURE 2.1.2.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-hexene.

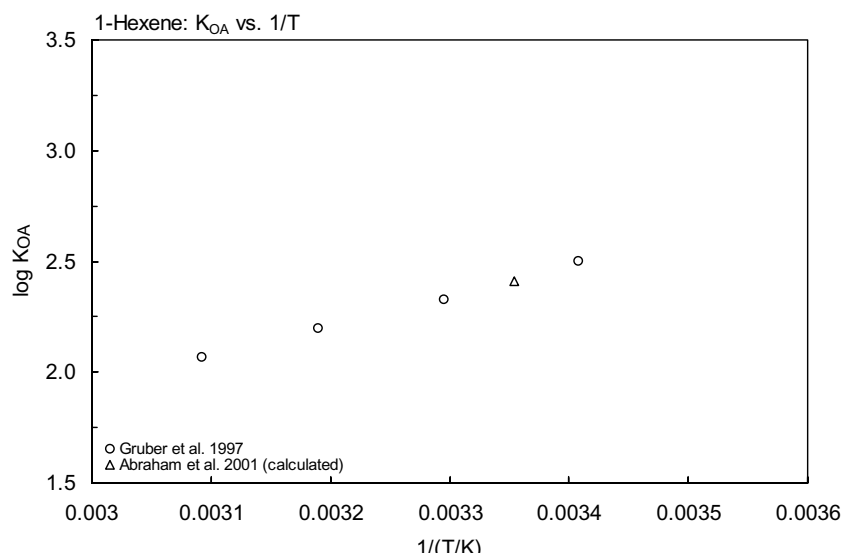
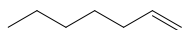


FIGURE 2.1.2.1.10.3 Logarithm of K_{OA} versus reciprocal temperature for 1-hexene.

2.1.2.1.11 1-Heptene



Common Name: 1-Heptene

Synonym: 1-heptylene, α -heptene

Chemical Name: 1-heptene

CAS Registry No: 592-76-7

Molecular Formula: C_7H_{14} , $CH_3(CH_2)_4CH=CH_2$

Molecular Weight: 98.186

Melting Point ($^{\circ}C$):

-118.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

93.64 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6970, 0.6927 ($20^{\circ}C$, $25^{\circ}C$, Forziati et al. 1950; Dreisbach 1959)

Molar Volume (cm^3/mol):

140.9 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

141.8 ($25^{\circ}C$, calculated-density)

155.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.65, 31.09 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.401 (Riddick et al. 1986)

12.66 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

82.5, 77.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

31.03, 27.6, 24.06 ($20^{\circ}C$, $25^{\circ}C$, $30^{\circ}C$, shake flask-titration, in 0.001M HNO_3 solution, Natarajan & Venkatachalam 1972)

18.16 (generator column-GC, Tewari et al. 1982a)

23.6 (calculated-activity coeff. γ and K_{ow} , Tewari et al. 1982b)

19, 25, 32, 38 (10, 20, 24, $30^{\circ}C$, "best values", IUPAC Solubility Data Series, Shaw 1989a)

15.27, 13.6, 13.1 (10, 20, $30^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

7690* ($25.5^{\circ}C$, ebulliometry-manometer, measured range 21.6 – $94.5^{\circ}C$, Forziati et al. 1950)

$\log(P/mmHg) = 6.90069 - 1257.505/(219.179 + t/^{\circ}C)$; temp range 21.6 – $94.5^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)

7510 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.90069 - 1257.505/(219.18 + t/^{\circ}C)$; temp range 10 – $128^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

26663* ($53.17^{\circ}C$, temp range 53.17 – $93.61^{\circ}C$, Eisen & Orav 1970; quoted, Boublik et al. 1984)

7506*, 7510 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.90069 - 1257.505/(219.179 + t/^{\circ}C)$; temp range -6.07 to $118.44^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 8643.2/(T/K)] + 7.991519$; temp range -35.8 to $98.5^{\circ}C$ (Antoine eq., Weast 1972–73)

7520, 7530 (interpolated-Antoine equations., Boublik et al. 1984)

$\log(P/kPa) = 6.04107 - 1266.473/(220.202 + t/^{\circ}C)$; temp range 21.6 – $94.53^{\circ}C$ (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.03512 - 1263.343/(219.922 + t/^{\circ}\text{C})$; temp range 54.17–93.61°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

7515 (interpolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.91087 - 1258.345/(219.30 + t/^{\circ}\text{C})$; temp range –6 to 118°C (Antoine eq., Dean 1985, 1992)

7500 (quoted lit., Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.02677 - 1258.34/(219.299 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

7500 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.99079 - 1237.44/(-56.26 + T/\text{K})$; temp range 311–368 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 38.1255 - 3.064 \times 10^3/(T/\text{K}) - 10.679 \cdot \log (T/\text{K}) + 1.2244 \times 10^{-10} \cdot (T/\text{K}) + 3.668 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 154–537 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

40580 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.99 (generator column-concn. ratio-GC, Tewari et al. 1982a,b)

4.09 (calculated-activity coeff. γ , Wasik et al. 1982)

4.06 (generator column-GC, Schantz & Martire 1987)

3.99 (recommended, Sangster 1989, 1993)

3.99 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{O}_3} = 8.1 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Cadle & Schadt 1952)

$k_{\text{O}_3} = 1.73 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (static system-chemiluminescence, Atkinson et al. 1982)

$k_{\text{OH}} = 3.97 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{\text{OH}} = 40.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $36.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and 305 K respectively (Atkinson 1989)

$k_{\text{OH}} = 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3} = 1.73 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}} = 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3} = 12.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 7.3 \text{ d}$, based on rate constant $k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.11.1

Reported vapor pressures of 1-heptene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Forziati et al. 1950		Eisen & Orav 1970		Zwolinski & Wilhoit 1971			
Ebulliometry		in Boublik et al. 1984		Selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
21.609	6485	53.17	26663	–6.07	1333	eq. 2	P/mmHg
25.492	7691	65.06	39997	5.39	2666	A	6.90069
28.768	8991	73.32	53329	12.68	4000	B	1257.505
34.525	11700	80.07	66661	18.15	5333	C	219.179
38.281	13845	85.82	79993	22.569	6666	bp/°C	93.643
42.564	16644	90.86	93325	26.306	7999		
46.923	19945	91.33	94659	32.443	10666	ΔH _v /(kJ mol ^{–1}) =	
50.970	23482	91.79	95992	37.418	13332	at 25°C	31.09
56.384	28988	92.25	97325	46.982	19998	at bp	35.65
67.366	43366	92.71	98658	54.212	26664		
73.563	53705	93.16	99991	60.096	33331		
80.179	66801	93.61	101325	65.095	39997		
92.391	97650			73.357	53329		
92.941	99233			80.104	66661		
93.444	100733			84.853	79993		
94.022	102462			90.888	93326		
94.531	104002			91.826	95992		
				92.744	98659		
eq. 2	P/mmHg			93.643	101325		
A	6.90069			25.0	7506		
B	1257.505						
C	219.179						
bp/°C	93.643						

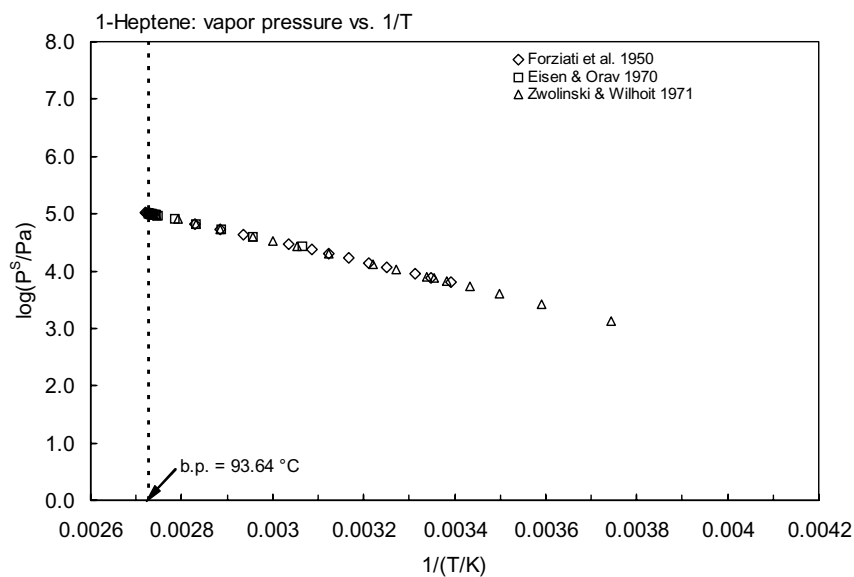
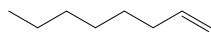


FIGURE 2.1.2.11.1 Logarithm of vapor pressure versus reciprocal temperature for 1-heptene.

2.1.2.1.12 1-Octene



Common Name: 1-Octene

Synonym: α -octene, caprylene, α -octylene

Chemical Name: 1-octene

CAS Registry No: 111-66-0

Molecular Formula: C_8H_{16} ; $CH_3(CH_2)_5CH=CH_2$

Molecular Weight: 112.213

Melting Point ($^{\circ}C$):

−101.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

121.29 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7149, 0.7109 ($20^{\circ}C$, $25^{\circ}C$, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

154.9 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

177.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.35, 33.95 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.569 (Riddick et al. 1986)

15.31 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

89.29, 86.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2.70 (shake flask-GC, McAuliffe 1966)

4.10 (generator column-GC, Tewari et al. 1982a)

6.82 (calculated-activity coeff. γ and K_{ow} , Tewari et al. 1982b)

2.70, 22.2 (quoted, IUPAC Solubility Data Series, Shaw 1989)

2.93, 2.93 (25 , $37.78^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6382* ($44.893^{\circ}C$, ebulliometry, measured range 44.893 – $122.223^{\circ}C$, Forziati et al. 1950)

$\log(P/mmHg) = 6.93262 - 1353.486/(212.765 + t/^{\circ}C)$; temp range 44.8 – $122.2^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)

2317 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.93263 - 1253.5/(212.764 + t/^{\circ}C)$; temp range 0 – $151^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

2320* (interpolated-Antoine eq., temp range 15.38 – $147.54^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.93263 - 1253.486/(212.764 + t/^{\circ}C)$; temp range 15.38 – $147.54^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

2320 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.06421 - 1356.472/(213.099 + t/^{\circ}C)$; temp range 44.89 – $122.2^{\circ}C$ (Antoine eq. from reported exptl. data Forziati et al. 1950, Boublik et al. 1984)

2320 (interpolated-Antoine eq., temp range 15 – $147^{\circ}C$, Dean 1985, 1992)

$\log(P/mmHg) = 6.93495 - 1355.46/(213.05 + t/^{\circ}C)$; temp range 15 – $147^{\circ}C$ (Antoine eq., Dean 1985, 1992)

2300 (quoted lit., Riddick et al. 1986)

$\log(P/kPa) = 6.05985 - 1355.46/(213.054 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

2320 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.05178 - 1350.245/(-60.716 + T/\text{K})$; temp range 317–400 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 56.1183 - 3.7657 \times 10^3/(T/\text{K}) - 10.006 \cdot \log (T/\text{K}) + 7.7387 \times 10^{-3} \cdot (T/\text{K}) - 1.3036 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 171–567 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

91700 (calculated-P/C, Mackay & Shiu 1975; selected, Mills et al. 1982)
 96440 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 101000, 75000 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 96400 (calculated-P/C, Mackay et al. 1981; Eastcott et al. 1988)
 74860 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 63500 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.57 (generator column-GC, Tewari et al. 1982a)
 4.76 (calculated-activity coeff. γ , Wasik et al. 1981, 1982)
 4.56, 4.72 (generator column-GC, calculated-activity coeff. γ , Schantz & Martire 1987)
 4.57 (recommended, Sangster 1989)
 4.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.53 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k ; for gas-phase second-order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = 8.1 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with ozone in air (Atkinson & Carter 1984)

$k_{OH} = 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = 1.70 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O(3P)} = 1.10 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(^3P)$ atom in gas phase (Paulson & Seinfeld 1992)

$k_{O_3} = 14.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 7.3 \text{ d}$, based on rate constant $k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.12.1
Reported vapor pressures of 1-octene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Forziati et al. 1950		Zwolinski & Wilhoit 1971					
ebulliometry		selected values					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
44.893	6382	121.075	100743	15.38	1333	118.362	93326
48.975	7690	121.685	102474	27.57	2666	119.355	95992
52.140	8994	122.223	102019	35.33	4000	120.328	98659
55.581	10330			41.15	5333	121.2880	101325
58.557	11720	eq. 2	P/mmHg	45.848	6666	25.0	2320
62.557	13844	A	6.93262	49.820	7999		
67.096	16644	B	1353.486	56.343	10666	eq. 2	P/mmHg
71.736	19945	C	212.764	61.630	13332	A	6.93263
76.022	23482	bp/°C	121.280	71.789	19998	B	1353.486
81.779	2890			79.645	26664	C	212.764
87.053	34934			85.710	33331	bp/°C	121.280
93.428	43366			91.014	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
106.997	66806			99.778	53329	at 25°C	37.95
119.967	97658			106.932	66661	at bp	33.76
120.539	99242			113.026	79993		

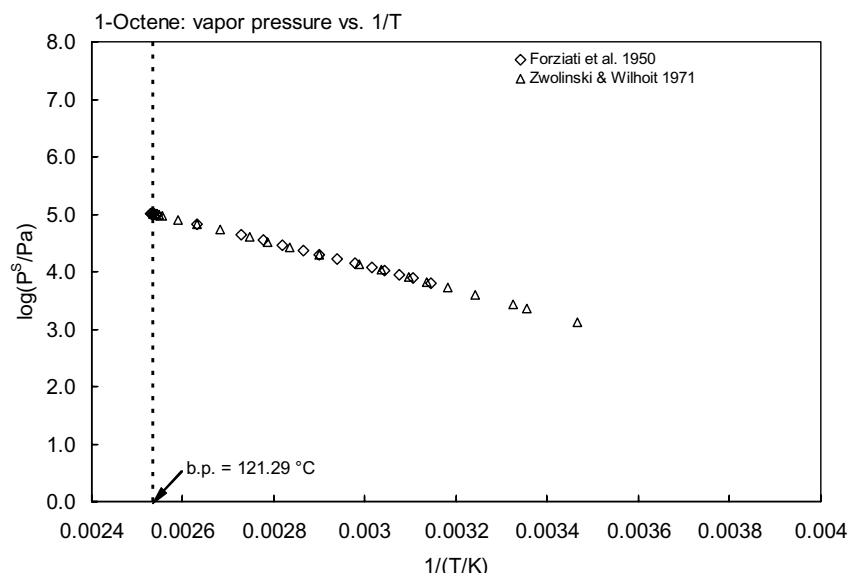


FIGURE 2.1.2.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for 1-octene.

2.1.2.1.13 1-Nonene



Common Name: 1-Nonene

Synonym: α -nonene, *n*-heptylethylene, 1-nonylene

Chemical Name: 1-nonene

CAS Registry No: 124-11-8

Molecular Formula: C_9H_{18} ; $CH_3(CH_2)_6CH=CH_2$

Molecular Weight: 126.239

Melting Point ($^{\circ}C$):

−81.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

146.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7292, 0.7235 ($20^{\circ}C$, $25^{\circ}C$, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm^3/mol):

173.1, 174.1 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

199.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.52, 36.31 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.075 (Riddick et al. 1986)

19.37 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

104.23, 96.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.63 (estimated-nomograph, Brookman et al. 1986)

1.12 (generator column-GC, Tewari et al. 1982a)

2.09 (calculated-activity coeff. γ and K_{ow} , Tewari et al. 1982b)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6385* ($66.607^{\circ}C$, ebulliometry, measured range 66.607 – $147.860^{\circ}C$, Forziati et al. 1950)

$\log (P/mmHg) = 6.95389 - 1435.359/(205.535 + t/^{\circ}C)$; temp range 66.6 – $147.9^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)

712 (calculated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.95387 - 1435.295/(205.535 + t/^{\circ}C)$; temp range 25 – $173^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

707*, 712 (derived from compiled data, extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.95430 - 1436.20/(205.69 + t/^{\circ}C)$; temp range 35 – $175^{\circ}C$ (Antoine eq., Dean 1985, 1992)

710 (quoted lit., Riddick et al. 1986)

$\log (P/kPa) = 6.07920 - 1436.20/(205.690 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

712 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.07341 - 1432.435/(-67.884 + T/K)$; temp range 339 – $423\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 60.6089 - 4.2023 \times 10^3/(T/K) - 19.446 \cdot \log (T/K) + 7.8308 \times 10^{-3} \cdot (T/K) + 1.591 \times 10^{-13} \cdot (T/K)^2$; temp range 192 – $593\ K$ (vapor pressure eq., Yaws 1994)

650.4 ($23.25^{\circ}C$, transpiration method, Verevkin et al. 2000)

$\ln (P/Pa) = 24.60 - 5379/(T/K)$; temp range 278.5 – $318.3\ K$ (transpiration method, Verevkin et al. 2000)

Henry's Law Constant (Pa m³/mol at 25°C):

80450 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

5.15 (generator column-GC, Tewari et al. 1982a,b)
 5.34 (calculated-activity coeff. γ , Wasik et al. 1981, 1982)
 5.31 (calculated-activity coeff. γ , Schantz & Martire 1987)
 5.15 (recommended, Sangster 1989)
 5.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

3.83 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

Surface water: t_{1/2} ~ 320 h and 9 × 10⁴ d for oxidation by OH and RO₂ radicals for olefins in aquatic system, and t_{1/2} = 7.3 d, based on rate constant k = 3 × 10³ M⁻¹ s⁻¹ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.13.1

Reported vapor pressures of 1-nonene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$ (1)				$\ln P = A - B/(T/K)$ (1a)			
$\log P = A - B/(C + t/^\circ\text{C})$ (2)				$\ln P = A - B/(C + t/^\circ\text{C})$ (2a)			
$\log P = A - B/(C + T/K)$ (3)							
$\log P = A - B/(T/K) - C \cdot \log (T/K)$ (4)							
Forziati et al. 1950				Zwolinski & Wilhoit 1971			
ebulliometry				selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
66.607	6385	146.091	99242	35.55	1333	143.805	93326
70.874	7691	146.653	100742	48.38	2666	144.848	95992
74.517	8994	147.289	102474	56.55	4000	145.869	98659
77.861	10331	147.860	104020	62.67	5333	146.868	101325
81.001	11722			67.612	6666	25.0	706.6
85.202	13805	bp/°C	146.868	71.790	7999		
89.942	16644			78.651	10666	eq. 2	P/mmHg
94.829	19945	eq. 2	P/mmHg	84.210	13332	A	6.95387
99.341	23482	A	6.95389	94.889	19998	B	1435.359
110.935	34934	B	1435.359	102.956	26664	C	205.535
117.622	43364	C	146.868	109.518	33331	bp/°C	146.868
124.521	53707			115.090	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
131.881	66806			124.295	53329	at 25°C	36.32
139.859	83770			131.808	66661	at bp	45.52
145.488	97658			138.204	79993		

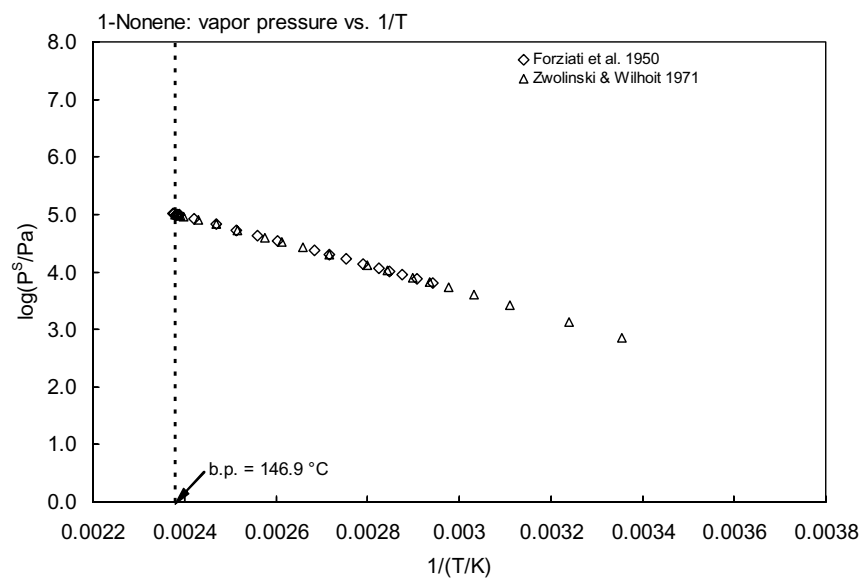
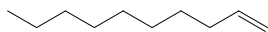


FIGURE 2.1.2.13.1 Logarithm of vapor pressure versus reciprocal temperature for 1-nonene.

2.1.2.1.14 1-Decene



Common Name: 1-Decene

Synonym: α -decene

Chemical Name: 1-decene

CAS Registry No: 872-05-9

Molecular Formula: $C_{10}H_{20}$

Molecular Weight: 140.266

Melting Point ($^{\circ}C$):

-66.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

170.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7408, 0.7369 ($20^{\circ}C$, $25^{\circ}C$, Forziati et al. 1950; Dreisbach 1959)

Molar Volume (cm^3/mol):

189.3 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

190.3 ($25^{\circ}C$, calculated-density)

222.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

50.43, 38.66 (25° , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.75 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

106.8, 105.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

5.70 (shake flask-titration with bromine, Natarajan & Venkatachalam 1972; quoted Shaw 1989)

11.0, 8.50, 5.70 (15, 20, $25^{\circ}C$, shake flask-titration, in 0.001M HNO_3 solution, Natarajan & Venkatachalam 1972)

0.161 (calculated- K_{ow} , Wang et al. 1992)

0.433 (calculated-molar volume V_M , Wang et al. 1992)

0.222, 0.344 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.429, 4.29, 70.13 (101, 151.5, $202^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($14.7^{\circ}C$, summary of literature data, temp range 14.7 – $192.0^{\circ}C$, Stull 1947)

6397* ($86.774^{\circ}C$, ebulliometry, measured range 86.774 – $171.605^{\circ}C$, Forziati et al. 1950)

$\log(P/mmHg) = 6.96036 - 1501.812/(197.578 + t/^{\circ}C)$; temp range 86.7 – $171.6^{\circ}C$ (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)

218 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.96034 - 1501.872/(197.58 + t/^{\circ}C)$; temp range 25 – $253^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

218* (extrapolated-Antoine eq., temp range 54.4 – $199.3^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.96034 - 1501.872/(197.578 + t/^{\circ}C)$; temp range 54.4 – $199.3^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.07985 - 1497.943/(197.102 + t/^{\circ}C)$; temp range 86.77 – $171.6^{\circ}C$ (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)

215 (extrapolated-Antoine eq., temp range: 54 – $199^{\circ}C$, Dean 1985, 1992)

$\log(P/mmHg) = 6.93477 - 1484.98/(195.707 + t/^{\circ}C)$, temp range: 54 – $199^{\circ}C$ (Antoine eq., Dean 1985, 1992)

210 (quoted lit., Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.05967 - 1484.98/(195.707 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
223 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.12458 - 1528.811/(-72.566 + T/\text{K})$; temp range 383–445 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 2.2678 - 3.1244 \times 10^3/(T/\text{K}) + 5.432 \cdot \log (T/\text{K}) - 2.0137 \times 10^{-2} \cdot (T/\text{K}) + 1.1221 \times 10^{-5} \cdot (T/\text{K})^2$;
temp range 207–617 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.78 (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)

5.18 (calculated-molar volume V_M , Wang et al. 1992)

4.7037 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{O}_3} = 1.08 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with ozone in the gas phase (Atkinson & Carter 1984)

$k_{\text{O}_3} = 9.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 7.3 \text{ d}$, based on rate constant $k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.1.14.1

Reported vapor pressures of 1-decene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/\text{K})$		(1)	$\ln P = A - B/(T/\text{K})$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/\text{K})$		(3)			
$\log P = A - B/(T/\text{K}) - C \cdot \log (T/\text{K})$		(4)			
Stull 1947		Forziati et al. 1950		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
14.7	133.3	86.774	6397	54.40	1333
40.3	666.6	91.308	7694	67.80	2666
53.7	1333	95.134	8997	76.33	4000
67.8	2666	98.604	10334	82.71	5333
83.3	5333	101.844	11723	87.875	6666

(Continued)

TABLE 2.1.2.1.14.1 (Continued)

Stull 1947		Forziati et al. 1950		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
93.5	7999	106.223	13848	92.236	7999
14.7	133.3	86.774	6397	54.40	1333
106.5	13332	111.213	16647	99.396	10666
126.7	26664	116.283	19950	105.198	13332
149.2	53329	120.995	23463	116.342	19998
192.0	101325	127.265	28990	124.760	26664
mp/°C		140.063	43759	131.607	33331
		147.265	53710	137.421	39997
		154.939	66810	147.024	53329
		169.134	97662	154.861	66661
		169.762	99247	161.533	79993
		170.345	100747	163.376	93326
		171.012	102487	168.464	95992
		171.605	104026	170.052	98659
				170.570	101325
		eq. 2	P/mmHg	eq. 2	P/mmHg
	A	6.96036	A	6.96034	
	B	1501.872	B	1501.872	
	C	197.578	C	197.578	
	bp/°C	170.570	C	197.578	
			bp/°C	170.570	
			ΔH _v /(kJ mol ⁻¹) =		
			at 25°C	38.66	
			at bp	50.46	

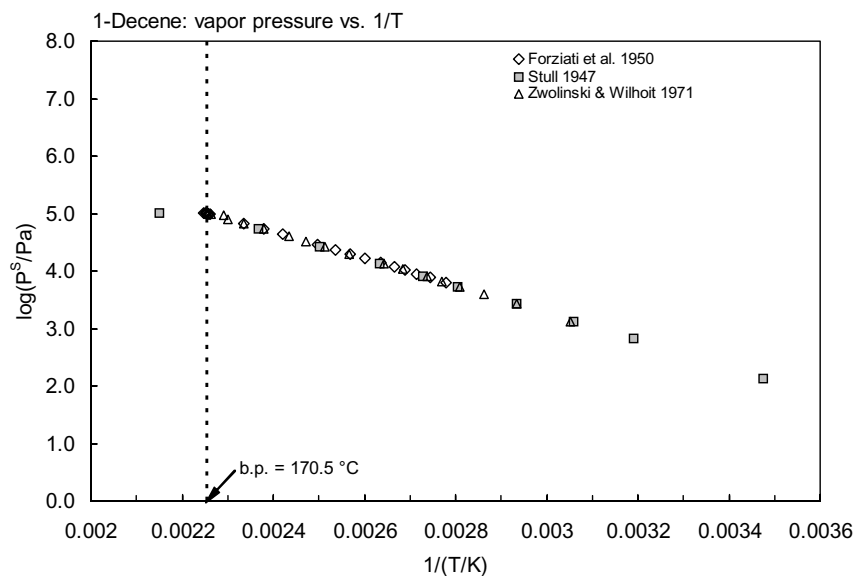


FIGURE 2.1.2.1.14.1 Logarithm of vapor pressure versus reciprocal temperature for 1-decene.

2.1.2.2 Dienes

2.1.2.2.1 1,3-Butadiene



Common Name: 1,3-Butadiene

Synonym: α,γ -butadiene, bivinyl, divinyl, erythrene, vinylethylene, biethylene, pyrrolylene

Chemical Name: 1,3-butadiene

CAS Registry No: 106-99-0

Molecular Formula: C_4H_6 ; $CH_2=CHCH=CH_2$

Molecular Weight: 54.091

Melting Point ($^{\circ}C$):

−108.91 (Lide 2003)

Boiling Point ($^{\circ}C$):

−4.41 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6211, 0.6149 ($20^{\circ}C$, $25^{\circ}C$, at saturation pressure, Dreisbach 1959)

Molar Volume (cm^3/mol):

87.1 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987; Wang et al. 1992 Ruelle & Kesseling 1997)

81.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.98 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

48.62, 45.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

735 (shake flask-GC, at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

113857* ($-1.50^{\circ}C$, static method-manometer, measured range -75.5 to $-1.50^{\circ}C$, Heisig 1933)

336200* (calculated-Antoine eq. regression, temp range -102.8 to $4.6^{\circ}C$, Stull 1947)

280600 (calculated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.85941 - 935.53/(239.55 + t/^{\circ}C)$; temp range -66 to $46^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

281000* (extrapolated-Antoine eq., temp range -58.201 to $14.43^{\circ}C$, Zwolinski & Wilhoit 1971)

280644 (derived from compiled data, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.84999 - 930.546/(238.854 + t/^{\circ}C)$; temp range -58.201 to $14.43^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

61295* ($20.211^{\circ}C$, temp range -16.204 to $33.257^{\circ}C$, Boublikova 1972; quoted, Boublik et al. 1984)

247700 (extrapolated-Antoine eq., temp range -82.5 to $9.7^{\circ}C$, Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 7761.0/(T/K)] + 8.997505$; temp range -82.5 to $9.7^{\circ}C$ (Antoine eq., Weast 1972–73)

281650, 281510* (static method quartz manometer, measured range 15 – $55^{\circ}C$, Flebbe et al. 1982)

281230, 310400 (extrapolated-Antoine equations, Boublik et al. 1984)

$\log (P/kPa) = 6.86369 - 1313.687/(275.492 + t/^{\circ}C)$; temp range -81 to $-24^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 5.97484 - 931.996/(239.329 + t/^{\circ}C)$; temp range -75 to $-1.5^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/mmHg) = 7.03555 - 998.106/(245.233 + t/^{\circ}C)$; temp range -87 to $-62^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 6.84999 - 930.546/(238.854 + t/^{\circ}C)$; temp range -58 to $15^{\circ}C$ (Antoine eq., Dean 1985, 1992)

281000 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.16045 - 998.106/(-27.916 + T/\text{K})$; temp range 193–213 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.97489 - 930.546/(-34.306 + T/\text{K})$; temp range 213–276 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.99667 - 940.687/(-33.017 + T/\text{K})$; temp range 270–318 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.31615 - 1130.927/(-5.606 + T/\text{K})$; temp range 315–382 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 8.86984 - 3877.451/(315.612 + T/\text{K})$; temp range 380–425 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 30.0572 - 1.9891 \times 10^3/(T/\text{K}) - 8.2922 \cdot \log (T/\text{K}) + 2.5664 \times 10^{-10} \cdot (T/\text{K}) + 5.1334 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 164–425 K (vapor pressure eq., Yaws 1994)

$\ln (P/\text{atm}) = 9.16107 - 2154.139/(T/\text{K} - 33.596)$; temp range 207–319 K (Antoine eq., Oliveira & Uller 1996)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

7460 (calculated-P/C, Mackay & Shiu 1981)

6370 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975; quoted, Howard 1989)

7150, 6230 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

10820 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

7720 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.99 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979)

1.87, 1.68, 1.90 (calculated-fragment const., Rekker 1977)

2.22 (calculated-UNIFAC, Banerjee & Howard 1988)

1.99 (recommended, Sangster 1989)

1.56 (calculated- V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.28 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

1.86–2.36 (soils and sediments, calculated- K_{OW} and S , Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: volatilizes rapidly from water and land (Howard 1989).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O_3} = 8.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (Japer et al. 1974)

$k_{OH} = (46.4 \pm 9.3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Lloyd et al. 1976)

$k_{OH} = 4.64 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$, $t_{1/2} = 0.25 \text{ h}$ for reaction with OH radical only, $t_{1/2} = 0.24 \text{ h}$ with an average concn of 0.1 ppm of O_3 at 300 K (Darnall et al. 1976)

$k_{O(3P)} = 1.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $O(^3P)$ atom at room temp. (Atkinson & Pitts, Jr. 1977)

$k_{OH}^* = (6.85 \pm 0.69) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299.5 K, measured range 299.9–424 K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)

$k_{OH} = 6.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)

$k_{O_3}^* = (1.17 \pm 0.19) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 276–324 K with atmospheric lifetime $\tau \sim 24 \text{ h}$ due to reaction with O_3 and $\tau \sim 4 \text{ h}$ with OH radical (Atkinson et al. 1982)

$k_{\text{OH}} = 6.85 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm \text{K}$, $k_{\text{OH}}(\text{calc}) = 6.22 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (relative rate method, Ohta 1983)

$k_{\text{O}_3} = (6.1 - 8.4) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. to 299 K (Atkinson & Carter 1984)

$k_{\text{NO}_3} = (5.34 \pm 0.62) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson et al. 1984a)

$k_{\text{NO}_2} = (3.1 \pm 0.3) \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with NO_2 at $295 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1984b)

$k_{\text{OH}} = 6.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 0.053 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3} = 8.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{O}(3\text{P})} = 6.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{NO}_2} = 3.1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with NO_2 , at room temp. (Atkinson et al. 1984b)

$k_{\text{OH}} = 6.65 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{\text{NO}_3} = 2.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (fast flow system/MS, Benter & Schindler 1988)

$k_{\text{OH}}^* = 6.66 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{NO}_3} = (4.4 \pm 0.8) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 1 \text{ K}$ (FTIR, Andersson & Ljungström 1989)

$k_{\text{OH}} = 66.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 7.5 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1990)

$k_{\text{NO}_3} = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{\text{OH}} = 6.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 7.5 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljić & Gusten 1990)

$k_{\text{OH}} = 2.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3}^* = 6.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}(3\text{P})} = 1.98 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O}(^3\text{P})$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis: will hydrolyze appreciably (Howard 1989).

Biodegradation: $t_{1/2}(\text{aerobic}) = 7 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: estimated photooxidation $t_{1/2} = 0.24\text{--}24 \text{ h}$ (Darnall et al 1976) for the reaction with hydroxyl radical; photooxidation with OH radicals with an estimated $t_{1/2} \sim 3.1 \text{ h}$ (Lyman et al. 1982; quoted, Howard 1989); completely degraded within 6 h in a smog chamber irradiated by sunlight (Kopczynski et al 1972; quoted, Howard 1989);

$t_{1/2} = 15 \text{ h}$ in air for the reaction with nitrate radical (Atkinson et al. 1984a; quoted, Howard 1989);

$t_{1/2} = 0.76\text{--}7.8 \text{ h}$, based on measured photooxidation rate constants in air (Howard et al. 1991).

Surface water: $t_{1/2} = 1200$ to 48000 h , based on measured photooxidation rate constants with OH radicals in water (Güsten et al. 1981; quoted, Howard et al. 1991);

estimated $t_{1/2} = 3.8 \text{ h}$ for evaporation from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} \sim 320 \text{ h}$ and $t_{1/2} = 9 \times 10^4$ for oxidation by OH and RO_2 radicals and $t_{1/2} = 9 \times 10^4 \text{ d}$ for olefins in aquatic system, and $t_{1/2} = 19 \text{ h}$, based on rate constant of $1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of dienes with singlet oxygen in aquatic system (Mill & Mabey 1985);

volatilizes rapidly with a half-life estimated to be several hours (Howard 1989);

$t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 7 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2} = 336\text{--}1344 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biota:

TABLE 2.1.2.2.1.1

Reported vapor pressures of 1,3-butadiene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)				
$\log P = A - B/(C + T/K)$		(3)							
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)							
$\log P = A[1 - \Phi/(T/K)]$		(5)	where $\log A = a + bT + cT^2$						
Heisig 1933		Stull 1947		Zwolinski & Wilhoit 1971		Flebbe et al. 1982			
static method-manometer		summary of literature data		selected values		static-quartz manometer			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa		
-75.5	1946	-102.8	133.3	-79.86	1333	15	144720		
-63.4	4720	-87.6	666.6	-71.18	2666	15	144700		
-51.6	10279	-79.7	1333	-65.676	4000	25	281650		
-39.4	20452	-71.0	2666	-61.44	5333	25	281510		
-38.6	21558	-61.3	5333	-58.201	6666	35	499680		
-32.7	29197	-55.1	7999	-55.381	7999	35	499250		
-26.1	40183	-46.8	13332	-50.747	10666	55	824250		
-19.9	53395	-33.9	26664	-46.989	13332	55	823810		
-15.5	64554	-19.3	53329	-39.760	19998	vapor pressure eq. given in reference			
-10.4	79980	-4.60	101325	-34.292	26664				
-5.60	97285	mp/°C	-108.0	-29.839	33331				
-1.50	113857			-26.054	39997				
				-19.796	53329				
				-14.681	66661				
				-10.322	79993				
				-6.502	93326				
				-5.979	95992				
				-5.093	98659				
				-4.411	101325				
				25.0	280644				
				eq. 2	P/mmHg				
				A	6.84999				
				B	930.546				
				C	238.854				
				temp range	-58 to 14.4°C				
				bp/°C	-4.411				
				$\Delta H_v/(\text{kJ mol}^{-1}) =$					
				at 25°C	21.05				
				at bp	22.68				

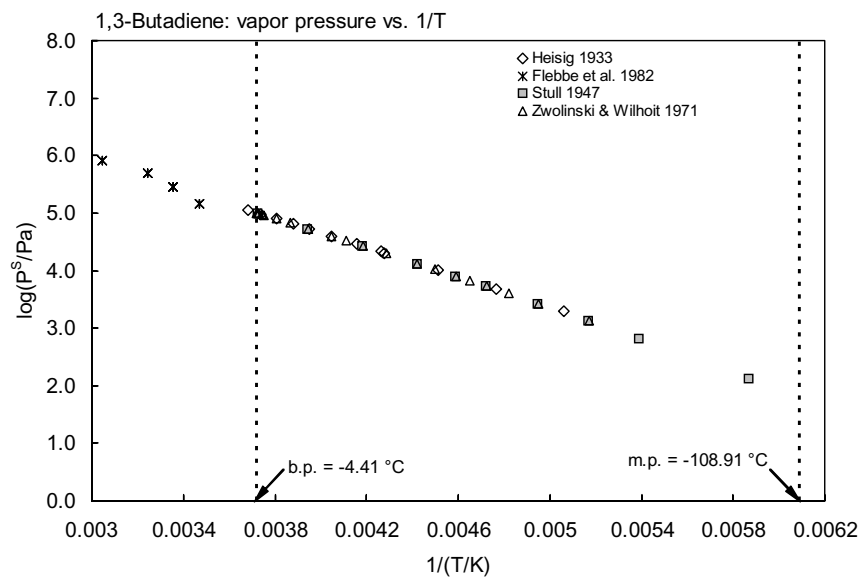


FIGURE 2.1.2.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3-butadiene.

2.1.2.2.2 2-Methyl-1,3-butadiene (Isoprene)



Common Name: 2-Methyl-1,3-butadiene

Synonym: isoprene

Chemical Name: 2-methyl-1,3-butadiene

CAS Registry No: 78-79-5

Molecular Formula: C_5H_8 ; $CH_2=C(CH_3)CH=CH_2$

Molecular Weight: 68.118

Melting Point ($^{\circ}C$):

−145.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

34 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6809, 0.6759 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

100.4 ($20^{\circ}C$, calculated-density)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.92 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

38.68, 34.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

642 (shake flask-GC, McAuliffe 1966)

545* ($20^{\circ}C$, shake flask-GC, measured range 20 – $60^{\circ}C$, Pavlova et al. 1966)

610* (recommended best value, IUPAC Solubility Data Series, temp range 20 – $60^{\circ}C$, Shaw 1989a)

530* (calculated-liquid-liquid equilibrium LLE data, temp range 293.2 – $313.2 K$, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

53329* ($15.4^{\circ}C$, summary of literature data, temp range -79.8 to $32.6^{\circ}C$, Stull 1947)

66816* ($22.5^{\circ}C$, ebulliometry, measured range 16.8 – $34.8^{\circ}C$, Forziati et al. 1950)

$\log (P/mmHg) = 6.90335 - 1080.996/(234.668 + t/^{\circ}C)$; temp range 16.8 – $34.8^{\circ}C$ (Antoine eq., ebulliometry measurements, Forziati et al. 1950)

3349* ($-38.227^{\circ}C$, inclined-piston manometer, measured range -57.598 to $-38.227^{\circ}C$, Osborn & Douslin 1969)

73330 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)

$\log (P/mmHg) = 6.90334 - 1080.996/(234.67 + t/^{\circ}C)$; temp range -35 to $84^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

73300 (interpolated-Antoine eq., temp range -18.477 to $55.36^{\circ}C$, Zwolinski & Wilhoit 1971)

73340* (derived from compiled data, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.88564 - 1071.578/(233.513 + t/^{\circ}C)$; temp range -18.477 to $55.36^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

73000, 78380 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.05468 - 1095.41/(236.322 + t/^{\circ}C)$; temp range -58 to $-38.2^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 6.05329 - 1092.997/(236.002 + t/^{\circ}C)$; temp range -16 to $33^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- 73350 (interpolated-Antoine eq., temp range -52 to -24°C , Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 7.01187 - 1126.159/(238.88 + t/^{\circ}\text{C})$; temp range -52 to -24°C (Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.88564 - 1071.518/(233.51 + t/^{\circ}\text{C})$; temp range -19 to 55°C (Antoine eq., Dean 1985, 1992)
 73350 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.13677 - 1126.159/(-34.266 + T/\text{K})$; temp range 221–254 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.01-54 - 1071.578/(-39.637 + T/\text{K})$; temp range 254–316 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 73330, 10770 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 7840 (calculated- $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
 6230, 6520 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 7780 (calculated-P/C, Mackay & Shiu 1981)
 14940 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 7780 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.05 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
 1.91 (calculated-molar volume V_{M} , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 2.06 (calculated-measured γ^{∞} in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{O}_3} = 16.5 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (chemiluminescence, Adeniji et al. 1981)

$k_{\text{O}_3}^* = 1.25 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with ozone in air at 296 K, measured range 278–323 K (static system-chemiluminescence, Atkinson et al. 1982)

$k_{\text{OH}}^* = (9.26 \pm 1.5) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K, measured range 299–422 K (flash photolysis-resonance fluorescence, Kleindienst et al. 1982)

$k_{\text{OH}} = 10.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm \text{K}$, $k_{\text{OH}}(\text{calc}) = 9.40 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (relative rate method, Ohta 1983)

$k_{\text{O}_3}^* = (0.58 - 1.25) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ between 260–296 K (Atkinson & Carter 1984)

$k_{\text{O}_3} = 1.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.8 d^{-1} , $k_{\text{OH}} = 9.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 8 d^{-1} , and $k_{\text{NO}_3} = 5.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 12 d^{-1} (Atkinson & Carter 1984)

$k_{\text{NO}_3} = (3.23 \pm 0.38) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate method, Atkinson et al. 1984a)

$k_{\text{NO}_2} = (10.3 \pm 0.3) \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with NO_2 at $295 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1984b)

$k_{\text{O}_3} = 1.2 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} = 9.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 3.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1984b)

$k_{\text{OH}} = 10.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)

$k_{\text{OH}} = 9.98 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $9.26 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (Atkinson 1985)

$k_{\text{OH}} = (101 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $23.7 \pm 0.5^\circ\text{C}$ (Edney et al. 1986)

$k_{\text{NO}_3} = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Benter & Schindler 1988)

$k_{\text{OH}}^* = 1.01 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 1.01 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3} = 1.43 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}} = 5.91 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.01 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{\text{NO}_3}^* = 6.78 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{\text{OH}}^* = 1.01 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}^* = 6.78 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3}^* = 12.8 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}(^3\text{P})} = 3.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: calculated atmospheric lifetimes: 32 h due to reaction with O_3 in 24-h period, 2.9 h with OH radical during daytime, and 3.6 h for NO_3 radical during nighttime for “clean atmosphere”; 10 h for reaction with O_3 in 24-h period, 1.4 h with OH radical during daytime, and 22 min with NO_3 radical during nighttime in “moderately polluted atmosphere” (Atkinson et al. 1984a, Winer et al. 1984); atmospheric lifetimes are calculated to be 28.3 h for the reaction with O_3 , 2.9 h with OH radicals and 0.083 h with NO_3 radicals, all based on the reaction rate constants with O_3 , OH and NO_3 radicals in the gas phase (Atkinson & Carter 1984)

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 19$ h, based on rate constant of $1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of dienes with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.2.1

Reported aqueous solubilities of 2-methyl-1,3-butadiene (isoprene) at various temperatures

Pavlova et al. 1966		Shaw 1989a		Góral et al. 2004	
shake flask-GC		IUPAC tentative values		calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	544.8	20	540	20	530
40	664.6	25	610	25	530
50	760.9	40	660	40	530
60	867.1	50	760		
		60	870		

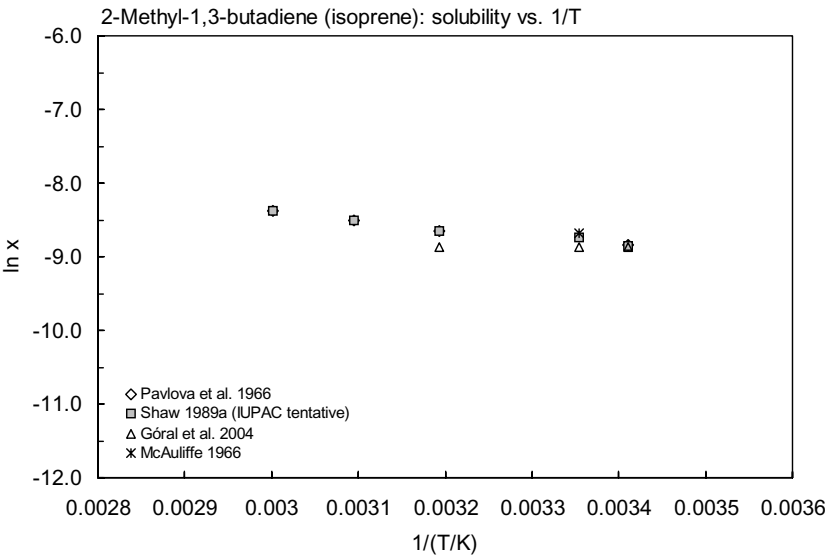


FIGURE 2.1.2.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methyl-1,3-butadiene.

TABLE 2.1.2.2.2
Reported vapor pressures of 2-methyl-1,3-butadiene (isoprene) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$
 $\log P = A - B/(C + t/^{\circ}C)$
 $\log P = A - B/(C + T/K)$
 $\log P = A - B/(T/K) - C \cdot \log (T/K)$
 $\log P = A[1 - \Phi/(T/K)]$

(1)

(2)

(3)

(4)

(5) where $\log A = a + bT + cT^2$

$\ln P = A - B/(T/K)$
 $\ln P = A - B/(C + t/^{\circ}C)$

(1a)

(2a)

1.

Stull 1947		Forziati et al. 1950		Osborn & Douslin 1969		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		inclined-piston manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-79.8	133.3	16.836	53718	-57.598	842.86	-51.561	liquid
-62.3	666.6	22.506	66816	-55.186	1017	-41.587	1333
-53.3	1333	28.061	83780	-52.77	1221	-35.413	2666
-43.5	2666	33.006	97665	-50.35	1460	-30.714	4000
-32.6	5333	33.469	99260	-47.93	1738	-26.917	5333
-25.4	7999	33.903	100757	-45.507	2060	-23.710	6666
-16.0	13332	34.399	102484	-43.083	2432		7999
-1.2	26664	34.834	104030	-40.656	2860	-18.447	liquid
15.4	53329			-38.227	3349	-14.181	10666
32.6	101325	Antoine eq.				-5.98	13332
		eq. 2	P/mmHg	Cox eq.		0.221	19998
mp/°C	-146.7	A	6.90335	eq. 5	P/atm	5.268	26664
		B	1080.996	Φ	307.217	9.557	33331
		C	234.668	a	0.820543	16.646	39997
							53329

(Continued)

TABLE 2.1.2.2.2.2 (Continued)

Stull 1947		Forziati et al. 1950		Osborn & Douslin 1969		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		inclined-piston manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				$-b \times 10^{-4}$	8.31178	22.437	66661
		bp/°C	34.067	$c \times 10^{-7}$	10.32622	27.371	79993
						31.693	93326
						32.499	95992
						33.287	98659
						34.059	101325
						bp/°C	34.059
						eq. 2	P/mmHg
						A	6.88654
						B	1071.578
						C	233.513
						for temp range -18 – 55°C	
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	26.44
						at bp	26.07

2.

Boublikova 1972 (thesis)

in Boublik et al. 1984

t/°C	P/Pa
–16.204	12046
–12.508	14549
–8.291	17921
–4.649	21314
–0.541	25780
2.793	29923
6.725	35493
10.416	41470
14.852	49704
20.211	61295
26.339	77125
33.257	98578
bp/°C	34.036
eq. 2	P/kPa
A	6.05329
B	1092.997
C	236.002

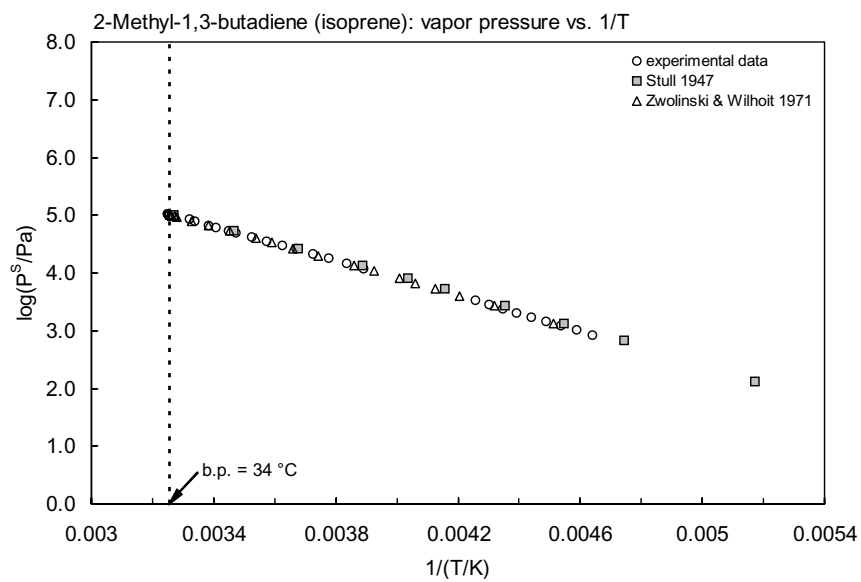


FIGURE 2.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-1,3-butadiene.

2.1.2.2.3 2,3-Dimethyl-1,3-butadiene



Common Name: 2,3-Dimethyl-1,3-butadiene

Synonym:

Chemical Name: 2,3-dimethyl-1,3-butadiene

CAS Registry No: 513-81-5

Molecular Formula: C_6H_{10} ; $CH_2 = (CH_3)C(CH_3)=CH_2$

Molecular Weight: 82.143

Melting Point ($^{\circ}C$):

-76 (Lide 2003)

Boiling Point ($^{\circ}C$):

68.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7267, 0.7222 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

113.0, 113.7 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

125.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

327 (quoted, Hine & Mookerjee 1975)

226 (calculated-fragment solubility constants, Wakita et al. 1986)

94.3, 226 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

19200 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 7.02388 - 1220.88/(225.9 + t/^{\circ}C)$; temp range -6 to $116^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

20160 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.25005 - 1302.766/(238.42 + t/^{\circ}C)$; temp range 0.04 – $68.6^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

20160 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.1197 - 1299.69/(238.09 + t/^{\circ}C)$; temp range 0 – $68.5^{\circ}C$ (Antoine eq., Dean 1985, 1992)

20150 (interpolated-Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.3266 - 1346.0/(-30.15 + T/K)$; temp range 273 – $342 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 29.9755 - 2.5677 \times 10^3/(T/K) - 7.8544 \cdot \log(T/K) + 2.2361 \times 10^{-10} \cdot (T/K) + 2.4591 \times 10^{-6} \cdot (T/K)^2$; temp range 197 – $526 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$) :

4830 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

5420, 6990 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

21100 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.25 \pm 0.05) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$; $k_{OH}(\text{calc}) = 1.26 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (relative rate method, Ohta 1983)

$k_{OH} = 1.22 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (Atkinson 1985, 1989)

$k_{NO_3} = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Benter & Shindler 1988)

$k_{OH} = 1.22 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 1.052 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{NO_3} = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{OH} = 1.22 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 2.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O_3}^* = 26.5 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

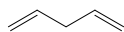
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 19 \text{ h}$, based on rate constant $k = 1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.2.4 1,4-Pentadiene



Common Name: 1,4-Pentadiene

Synonym:

Chemical Name: 1,4-pentadiene

CAS Registry No: 591-93-5

Molecular Formula: C_5H_8 ; $CH_2=CHCH_2CH=CH_2$

Molecular Weight: 68.118

Melting Point ($^{\circ}C$):

−148.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

26 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6608, 0.6557 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

103.1, 103.9 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.14 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

49.41, 52/3 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

558 (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

105100* (interpolated-Antoine eq. regression, temp range -83.5 to $26.1^{\circ}C$, Stull 1947)

63774* ($20.669^{\circ}C$, ebulliometry, measured range 14.7 – $26.7^{\circ}C$ (Forziati et al. 1950)

$\log(P/mmHg) = 6.84880 - 1025.016/(232.354 + t/^{\circ}C)$; temp range 14.7 – $26.7^{\circ}C$ (Antoine eq., ebulliometry measurements, Forziati et al. 1950)

97900 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)

$\log(P/mmHg) = 6.84880 - 1025.016/(232.354 + t/^{\circ}C)$; temp range -41 to $72^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

3611* ($-43.083^{\circ}C$, inclined-piston manometer, measured range -60.01 to $-43.083^{\circ}C$, Osborn & Douslin 1969)

98000 (interpolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981)

97940* (derived from compiled data, temp range -57.16 to $26^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.83543 - 1017.995/(231.461 + t/^{\circ}C)$; temp range -33.271 to $46.73^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 6826.6/(T/K)] + 7.899113$; temp range -83.5 to $26.1^{\circ}C$ (Antoine eq., Weast 1972–73)

98300, 99400 (extrapolated-Antoine equations, Boublik et al. 1984)

$\log(P/kPa) = 6.06018 - 1063.485/(236.447 + t/^{\circ}C)$; temp range -78.84 to $-18.08^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.34694 - 1239.949/(238.278 + t/^{\circ}C)$; temp range -60.0 to $-26.05^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

97930 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.17401 - 1155.378/(244.30 + t/^{\circ}C)$; temp range -57 to $-37^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.83543 - 1017.995/(231.46 + t/^{\circ}C)$; temp range -33 to $47^{\circ}C$ (Antoine eq., Dean 1985, 1992)

97900 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.29891 - 1155.378/(-28.852 + T/\text{K})$; temp range 216–234 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.96033 - 1017.995/(-41.698 + T/\text{K})$; temp range 236–307 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 23.7408 - 2.0505 \times 10^3/(T/\text{K}) - 5.679 \cdot \log (T/\text{K}) - 5.9671 \times 10^{-11} \cdot (T/\text{K}) + 1.1242 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 125–479 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

12140 (calculated $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

15640 (calculated-bond contribution, Hine & Mookerjee 1975)

12000 (calculated-P/C, Mackay & Shiu 1981)

13620 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

11946 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.48 (shake flask, Log P Database, Hansch & Leo 1987)

2.48 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (50.6 \pm 1.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$; $k_{\text{OH}}(\text{calc}) = 50.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (relative rate method, Ohta 1983)

$k_{\text{OH}} = 5.33 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (Atkinson 1985, Atkinson 1989)

$k_{\text{OH}} = 5.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp (Atkinson et al. 1984b)

$k_{\text{NO}_3} = 7.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (fast flow system, Benter & Shindler 1988)

$k_{\text{OH}} = 5.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 19 \text{ h}$, based on rate constant $k = 1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of dienes with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.2.4.1

Reported vapor pressures of 1,4-pentadiene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
$\log P = A[1 - \Phi /(T/K)]$		(5)	where $\log A = a + bT + cT^2$				
Stull 1947		Forziati et al. 1950		Osborn & Douslin 1969		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		inclined-piston manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−83.5	133.3	14.706	66811	−60.01	1071.4	−57.162	1333
−66.2	666.6	20.699	83774	−57.598	1291	−47.57	2666
−57.1	1333	24.931	97660	−55.186	1550	−41.49	4000
−47.7	2666	25.384	99253	−52.77	1851	−36.492	5333
−37.0	5333	25.806	100752	−50.35	2201	−33.271	6666
−30.0	7999	26.287	102480	−47.93	2605	−30.168	7999
−20.0	13332	26.714	104026	−45.507	3072	−25.069	10666
−6.70	26664			−43.083	3611	−20.933	13332
8.30	53329	bp/°C	25.967			−12.976	19998
26.1	101325					−6.956	26664
		Antoine eq.		Cox eq.		−2.053	33331
mp/°C		eq. 2	P/mmHg	eq. 5	P/atm	2.115	39997
		A	6.84880	Φ	299.117	9.009	53329
		B	1025.016	a	0.812446	14.642	66661
		C	232.354	$-b \times 10^{-4}$	7.52279	19.445	79993
				$c \times 10^{-7}$	8.34048	23.654	93326
						24.439	95992
						25.206	98659
						25.958	101325
						eq. for temp−33−46.7°C:	
						eq. 2	P/mmHg
						A	6.83543
						B	1017.995
						C	231.461
						bp/°C	25.958
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	25.15
						at bp	25.15

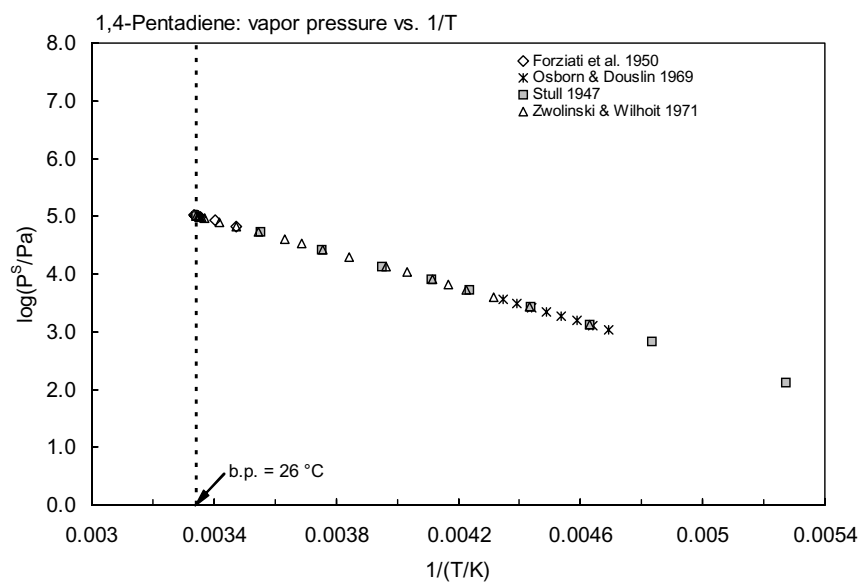
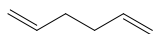


FIGURE 2.1.2.2.4.1 Logarithm of vapor pressure versus reciprocal temperature for 1,4-pentadiene.

2.1.2.2.5 1,5-Hexadiene



Common Name: 1,5-Hexadiene

Synonym:

Chemical Name: 1,5-Hexadiene

CAS Registry No: 592-42-7

Molecular Formula: C_6H_{10} ; $CH_2=CH(CH_2)_2CH=CH_2$

Molecular Weight: 82.143

Melting Point ($^{\circ}C$):

-140.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

59.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6920 (Weast 1984)

0.6923, 0.6878 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

119.0 ($20^{\circ}C$, calculated-density, Wang et al. 1992)

125.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

169 (shake flask-GC, McAuliffe 1966)

320 ($14^{\circ}C$, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

27730 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 7.00740 - 1184.99/(227.7 + t/^{\circ}C)$; temp range -13 to $102^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

32077* ($26.95^{\circ}C$, static method-Hg manometer, measured range 26.95 – $46.13^{\circ}C$, Letcher & Marsicano 1974)

29690 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.5741 - 1013.5/(214.8 + t/^{\circ}C)$; temp range 0 – $59^{\circ}C$ (Antoine eq., Dean 1985, 1992)

29670, 29690 (interpolated-Antoine eq.-I, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.7368 - 1032.0/(-56.15 + T/K)$; temp range 273 – $333 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.98314 - 1159.908/(-40.998 + T/K)$; temp range 299 – $333 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 10.5886 - 2.0106 \times 10^3/(T/K) + 0.28813 \cdot \log(T/K) - 9.562 \times 10^{-3} \cdot (T/K) + 7.164 \times 10^{-6} \cdot (T/K)^2$; temp range 132 – $507 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

13620 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

17550, 23130 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

17150 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.40 (calculated- π substituent constant, Hansch et al. 1968)

2.29 (calculated-MCI χ , Murray et al. 1975)

2.45 (calculated-fragment const., Yalkowsky & Morozowich 1980)

2.68 (calculated-hydrophobicity const., Iwase et al. 1985)

2.80	(recommended, Sangster 1989)
2.8208	(calculated-UNIFAC group contribution, Chen et al. 1993)
2.78	(calculated-f const., Müller & Klein 1992)
2.43	(calculated-molar volume V_M , Wang et al. 1992)
2.75	(recommended, Sangster 1993)
2.73	(selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 6.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ (relative rate method, Ohta 1983)

$k_{OH} = 6.35 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $5.85 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with 1,3-butadiene and propylene as standard substances respectively at $297 \pm 2 \text{ K}$ (relative rate method, Ohta 1983)

$k_{OH} = 6.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 19 \text{ h}$, based on rate constant of $1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.2.5.1
Reported vapor pressures of 1,5-hexadiene at various temperatures

Letcher & Marsicano 1974	
static method-Hg manometer	
$t/^\circ\text{C}$	P/Pa
26.95	32077
28.93	34690
31.62	38530
34.54	43036
36.94	47169
39.96	52622
41.77	56022
43.04	58622
46.13	65221
Antoine eq.	
$\log P = A - B/(C + T/K)$	
	P/mmHg
A	6.6228
B	1037.35
C	-55.52

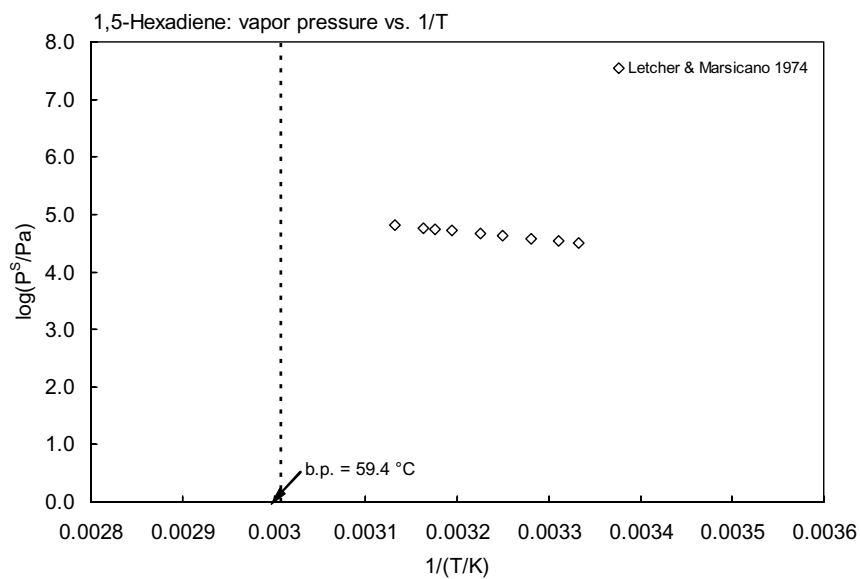
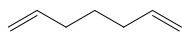


FIGURE 2.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for 1,5-hexadiene.

2.1.2.2.6 1,6-Heptadiene



Common Name: 1,6-Heptadiene

Synonym:

Chemical Name: 1,6-heptadiene

CAS Registry No: 3070-53-9

Molecular Formula: C_7H_{12}

Molecular Weight: 96.170

Melting Point ($^{\circ}C$):

-129 (Lide 2003)

Boiling Point ($^{\circ}C$):

90 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$): 0.714

Molar Volume (cm^3/mol):

134.0 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Wang et al. 1992)

148.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

44.0 (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.90 (calculated- π substituent constants, Hansch et al. 1968)

2.73 (calculated-MCI χ , Murray et al. 1975)

3.31 (calculated-fragment const., Müller & Klein 1992)

2.85 (calculated-molar volume V_M , Wang et al. 1992)

3.2189 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and 9×10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 19$ h, based on rate constant of $1.0 \times 10^7\ M^{-1}\ s^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.3 Alkynes

2.1.2.3.1 1-Butyne



Common Name: 1-Butyne

Synonym: ethyl acetylene, but-1-yne

Chemical Name: 1-butyne

CAS Registry No: 107-00-6

Molecular Formula: C_4H_6 , $CH_3CH_2C\equiv CH$

Molecular Weight: 54.091

Melting Point ($^{\circ}C$):

-125.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

8.08 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.650, 0.65 ($20^{\circ}C$, $25^{\circ}C$, at saturation pressure, Dreisbach 1959)

Molar Volume (cm^3/mol):

83.22 ($20^{\circ}C$, calculated-density)

81.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.03 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

40.9, 36.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2870 (shake flask-GC, at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/mmHg) = 6.97497 - 986.46/(232.85 + t/^{\circ}C)$; temp range -67 to $43^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

188251 (derived from compiled data, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 7.07338 - 1101.71/(235.81 + t/^{\circ}C)$; temp range -30.8 to $26.8^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = [-0.2185 \times 6596.9/(T/K)] + 8.032581$; temp range -92.5 to $8.7^{\circ}C$ (Antoine eq., Weast 1972-73)

$\log (P/mmHg) = 6.98198 - 988.75/(233.01 + t/^{\circ}C)$; temp range -68 to $27^{\circ}C$ (Antoine eq., Dean 1985, 1992)

188220 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.10688 - 988.75/(-40.14 + T/K)$; temp range $205-289 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 43.8278 - 2.4255 \times 10^3/(T/K) - 14.141 \cdot \log (T/K) + 8.2138 \times 10^{-3} \cdot (T/K) + 7.4889 \times 10^{-14} \cdot (T/K)^2$; temp range $147-443 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

1880 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

2210, 1800 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1910 (calculated-P/C, Mackay & Shiu 1981)

2820 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

1846 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.44, 1.48 (quoted, calculated-molar volume V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = 1.79 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (static system-IR, Dillemath et al. 1963)

$k_{O_3} = (33 \pm 5) \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 1 \text{ K}$ (static system-UV, DeMore 1971)

$k_{O_3} = (19.7 \pm 2.6) \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1984b)

$k_{OH}^* = (10.42 \pm 1.38) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K, measured range 253–343 K (discharge flow-resonance fluorescence, Boodaghians et al. 1987)

$k_{OH} = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = 2.0 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{O_3} = 1.79 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K; and $1.79 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $4.0 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (literature review, Atkinson 1991)

Hydrolysis:

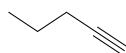
Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.2.3.2 1-Pentyne



Common Name: 1-Pentyne

Synonym: pent-1-yne

Chemical Name: 1-pentyne

CAS Registry No: 627-19-0

Molecular Formula: C_5H_8 ; $CH\equiv C(CH_2)_2CH_3$

Molecular Weight: 68.118

Melting Point ($^{\circ}C$):

-90 (Lide 2003)

Boiling Point ($^{\circ}C$):

40.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.6901, 0.6849 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)Molar Volume (cm^3/mol):98.71, 99.46 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} ($J/mol K$):Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1570 (shake flask-GC, McAuliffe 1966)

1049 (generator column-GC, Tewari et al. 1982a,b)

1363 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

57520 (calculated from determined data, Dreisbach 1959)

 $\log(P/mmHg) = 6.97263 - 1095.42/(227.53 + t/^{\circ}C)$; temp range -50 to $70^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)57600 (interpolated-Antoine eq., temp range -33 to $61^{\circ}C$ Zwolinski & Wilhoit 1971)

57462 (derived from compiled data, Zwolinski & Wilhoit 1971)

 $\log(P/mmHg) = 7.04614 - 1092.52/(227.18 + t/^{\circ}C)$; temp range -33 to $61^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)57540 (interpolated-Antoine eq., temp range -44 to $61^{\circ}C$, Dean 1985) $\log(P/mmHg) = 6.96734 - 1092.52/(227.18 + t/^{\circ}C)$; temp range -44 to $61^{\circ}C$ (Antoine eq., Dean 1985, 1992)

57540 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

 $\log(P_L/kPa) = 6.09224 - 1092.52/(-45.97 + T/K)$; temp range 229–315 K (Antoine eq., Stephenson & Malanowski 1987) $\log(P/mmHg) = 33.8369 - 2.4684 \times 10^3/(T/K) - 9.4301 \cdot \log(T/K) + 6.1345 \times 10^{-10} \cdot (T/K) + 4.676 \times 10^{-6} \cdot (T/K)^2$; temp range 167–481 K (vapor pressure eq., Yaws 1994)Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):2536 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

2980, 2660 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2500 (calculated-P/C, Mackay & Shiu 1981)

3422 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

4983 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.98 (shake flask-UV, Hansch et al. 1968, Hansch & Anderson 1967)

2.12 (generator column-GC, Tewari et al. 1982a,b)

1.98 (recommended, Sangster 1989, 1993)

1.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^* = (11.17 \pm 0.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 253–343 K (discharge flow-resonance fluorescence, Boodaghians et al. 1987, quoted, Atkinson 1989)

$k_{NO_3} = 7.54 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1991)

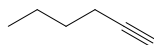
Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

2.1.2.3.3 1-Hexyne



Common Name: 1-Hexyne

Synonym: hex-1-yne

Chemical Name: 1-hexyne

CAS Registry No: 693-02-7

Molecular Formula: C_6H_{10} ; $C_4H_9C\equiv CH$

Molecular Weight: 82.143

Melting Point ($^{\circ}C$):

-131.9 (Dreisbach 1959; Lide 2003)

Boiling Point ($^{\circ}C$):

71.33 (Dreisbach 1959)

71.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.7155, 0.7155 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)Molar Volume (cm^3/mol):114.8 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

125.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

360 (shake flask-GC, McAuliffe 1966)

686 (generator column-GC, Tewari et al. 1982a,b)

688 (generator column-GC, Miller et al. 1985)

392 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$):

18140 (calculated-Antoine eq., Dreisbach 1959)

 $\log(P/mmHg) = 6.91212 - 1194.6/(225.0 + t/^{\circ}C)$; temp range -8 to $118^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

18145 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

 $\log(P_L/kPa) = 6.03702 - 1194.6/(-48.15 + T/K)$; temp range 265–391 K (Antoine eq., Stephenson & Malanowski 1987) $\log(P/mmHg) = 55.7231 - 3.2541 \times 10^3/(T/K) - 18.405 \cdot \log(T/K) + 9.5814 \times 10^{-3} \cdot (T/K) + 9.2278 \times 10^{-14} \cdot (T/K)^2$; temp range 141–516 K (vapor pressure eq., Yaws 1994)Henry's Law Constant ($Pa\ m^3/mol$):4020 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

4210, 4020 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

4310 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

2166 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:2.48 (calculated- π substituent constants, Hansch et al. 1968)

2.73 (generator column-GC, Tewari et al. 1982a,b)

2.73 (recommended, Sangster 1989, 1993)

2.73 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^* = (12.6 \pm 0.04) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 253–343 K (discharge flow-resonance fluorescence, Boodaghians et al. 1987; quoted, Atkinson 1989)

$k_{NO_3} = 1.60 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1991)

Hydrolysis:

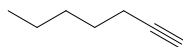
Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

2.1.2.3.4 1-Heptyne



Common Name: 1-Heptyne

Synonym:

Chemical Name: 1-heptyne

CAS Registry No: 628-71-7

Molecular Formula: C_7H_{12}

Molecular Weight: 96.170

Melting Point ($^{\circ}C$):

-81 (Lide 2003)

Boiling Point ($^{\circ}C$):

99.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7330 (Weast 1984)

0.7328, 0.7283 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)Molar Volume (cm^3/mol):131.2 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

148.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

94.0 (shake flask-GC, McAuliffe 1966)

107 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7000 (Antoine eq., Dreisbach 1959)

4298 (extrapolated-Antoine eq., Boublik et al. 1984)

 $\log(P/kPa) = 6.27249 - 1314.492/(208.097 + t/^{\circ}C)$; temp range 63.1 – $99.98^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

7500 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

 $\log(P_L/kPa) = 6.4039 - 1392.4/(-56.55 + T/K)$; temp range 336 – $373\ K$ (Antoine eq., Stephenson & Malanowski 1987) $\log(P/mmHg) = 38.1255 - 3.064 \times 10^3/(T/K) - 10.679 \cdot \log(T/K) + 1.2244 \times 10^{-10} \cdot (T/K) + 3.668 \times 10^{-6} \cdot (T/K)^2$; temp range 154 – $537\ K$ (vapor pressure eq., Yaws 1994)Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):6830 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

5950, 6090 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

5420 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

7160 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:2.98 (calculated- π substituent constants, Hansch et al. 1968)2.93 (calculated-MCI χ , Murray et al. 1975)2.98 (calculated-molar volume V_M , Wang et al. 1992)

2.99 (calculated-fragment const., Müller & Klein 1992)

3.18 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

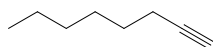
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

2.1.2.3.5 1-Octyne



Common Name: 1-Octyne

Synonym:

Chemical Name: 1-octyne

CAS Registry No: 629-05-0

Molecular Formula: C_8H_{14} ; $C_6H_{13}C\equiv CH$

Molecular Weight: 110.197

Melting Point ($^{\circ}C$):

-79.3 (Dreisbach 1959; Lide 2003)

Boiling Point ($^{\circ}C$): 127–128

126.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7461, 0.7419 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

147.7 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

170.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

24.0 (shake flask-GC, McAuliffe 1966)

25.4 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1813 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 7.02447 - 1413.8/(215.0 + t/^{\circ}C)$; temp range 25 – $170^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

1723 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.36895 - 1997.558/(202.608 + t/^{\circ}C)$; temp range 69.2 – $271.1^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1715 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.19321 - 1427.434/(-214.625 + T/K)$; temp range 84.8 – $126.26 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

8208 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

8208, 9000 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

6827 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

8325 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.48 (calculated- π substituent constants, Hansch et al. 1968)

3.37 (calculated-MCI χ , Murray et al. 1975)

3.49 (calculated-molar volume V_M , Wang et al. 1992)

3.52 (calculated-f const., Müller & Klein 1992)

3.84 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

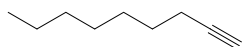
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

2.1.2.3.6 1-Nonyne



Common Name: 1-Nonyne

Synonym:

Chemical Name: 1-nonyne

CAS Registry No: 3452-09-3

Molecular Formula: C_9H_{16} ; $C_7H_{15}C\equiv CH$

Molecular Weight: 124.223

Melting Point ($^{\circ}C$):

−50 (Dreisbach 1959; Lide 2003)

Boiling Point ($^{\circ}C$): 150–151

150.8 (Dreisbach 1959; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7570 (Weast 1984)

0.7568, 0.7527 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

164.1 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)

192.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

7.20 (shake flask-GC, McAuliffe 1966)

6.30 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$):

835 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)

$\log(P/mmHg) = 6.77410 - 1404.7/(210.0 + t/^{\circ}C)$; temp range 50 – $223^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

Henry's Law Constant (Pa m^3/mol):

14600 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

11600, 13010 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

8700 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

14400 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.98 (calculated- π substituent constants, Hansch et al. 1968)

3.81 (calculated-MCI χ , Murray et al. 1975)

3.98 (calculated-molar volume V_M , Wang et al. 1992)

4.05 (calculated-fragment const., Müller & Klein 1992)

4.50 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

2.1.2.4 Cycloalkenes

2.1.2.4.1 Cyclopentene



Common Name: Cyclopentene

Synonym:

Chemical Name: cyclopentene

CAS Registry No: 142-29-0

Molecular Formula: C_5H_8

Molecular Weight: 68.118

Melting Point ($^{\circ}C$):

−135.0 (Lide 2003)

Boiling Point ($^{\circ}C$):

44.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7720, 0.7665 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

Molar Volume (cm^3/mol):

88.2 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

92.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.92, 26.96 ($25^{\circ}C$, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

0.48, 3.36; 3.84(−186.08, −135.05 $^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

29.83, 37.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

535 (shake flask-GC, McAuliffe 1966)

611 (shake flask-titration with bromine, Natarajan & Venkatachalam 1972)

1645 (shake flask-GC, Pierotti & Liabastre 1972)

540 (suggested “tentative” value, IUPAC Solubility Data Series, Shaw 1989a)

719 (calculated-liquid-recommended liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

39890* ($19.77^{\circ}C$, static method-quartz spiral gauge, measured range −42.75 to $19.77^{\circ}C$, Lister 1941)

43375* ($21.028^{\circ}C$, ebulliometry, measured range 11.3–45.024 $^{\circ}C$, Forziati et al. 1950)

$\log(P/mmHg) = 6.92066 - 1121.818/(233.446 + t/^{\circ}C)$; temp range 11.3–45.0 $^{\circ}C$ (Antoine eq., ebulliometry, Forziati et al. 1950)

50690 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.92066 - 1121.818/(233.446 + t/^{\circ}C)$; temp range −30 to $105^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [1 - 317.520/(T/K)] \times 10^{0.814441 - 7.42372 \times 10^{-4} \cdot (T/K) + 8.49035 \times 10^{-7} \cdot (T/K)^2}$; temp range: 223.2–393.2 K (Cox eq., Chao et al. 1983)

$\log(P/mmHg) = 6.92066 - 1121.818/(223.45 + t/^{\circ}C)$; temp range not specified (Antoine eq., Dean 1985, 1992)

50710 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.01617 - 1105.926/(-41.615 + T/K)$; temp range 249–318 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 30.1132 - 2.3537 \times 10^3/(T/K) - 8.0609 \cdot \log(T/K) - 5.7786 \times 10^{-11} \cdot (T/K) + 3.4591 \times 10^{-6} \cdot (T/K)^2$; temp range 138–507 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

- 6370 (calculated- $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
 3580, 9650 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 6460 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 2957, 3408, 3863, 4372* (10, 15, 20, 25°C , headspace-GC, measured range $10\text{--}25^\circ\text{C}$, Bakierowska & Trzeszczyński 2003)
 $\ln(1/K_{\text{AW}}) = 6.989 - 1915/(T/\text{K})$; temp range $10\text{--}25^\circ\text{C}$, headspace-GC, Bakierowska & Trzeszczyński 2003)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.75 (calculated- π substituent const., Hansch et al. 1968)
 1.76 (calculated-molar volume V_{M} , Wang et al. 1992)
 2.25 (calculated-fragment const., Müller & Klein 1992)
 2.1791 (calculated-UNIFAC group contribution, Chen et al. 1993)
 2.80 (calculated-UNIFAC activity coeff., Dallos et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{O}_3} = 8.13 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Japar et al. 1974; quoted, Adeniji et al. 1981)

$k_{\text{O}_3} = 9.69 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (chemiluminescence, Adeniji et al. 1981)

$k_{\text{O}_3} = (2.75 \pm 0.33) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 1 \text{ K}$ (Atkinson et al. 1983a)

$k_{\text{OH}} = (6.39 \pm 0.23) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1983b)

$k_{\text{O}_3} = 4.97 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 291.5 K in synthetic air (Bennett et al. 1987)

$k_{\text{O}_3} = (62.4 \pm 3.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ in a smog chamber (Nolting et al. 1988)

$k_{\text{OH}} = 4.99 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 3 \text{ K}$, and $k_{\text{OH}} = 5.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative to propene (relative rate method, Rogers 1989)

$k_{\text{OH}} = (5.02 - 6.73) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (literature review, Atkinson 1989)

$k_{\text{OH}} = 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 4.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}} = 6.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 5.81 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{\text{OH}} = 6.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 5.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3}^* = 5.7 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}(^3\text{P})} = 2.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation rate constant of $4.97 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with O_3 in synthetic air was determined at atmospheric pressure at 291.5 K (Bennett et al. 1987);

rate constant $k = 4.99 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radicals in air at 298 K (Rogers 1989).

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals in aquatic system, and $t_{1/2} = 40 \text{ d}$, based on rate constant $k = 2 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for the oxidation of cyclic olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.4.1.1

Reported vapor pressures and Henry's law constants of cyclopentene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot \log (T/K) + D \cdot [P/(T/K)^2]$	(5)		
$\log (P/\text{atm}) = A'[1 - (T_B/T)]$	(6)	where $\log A' = a + bT + cT^2$	

Vapor pressure				Henry's law constant	
Lister 1941		Forziati et al. 1950		Bakierowska & Trzeszczyński 2003	
static-quartz spiral gauge		ebulliometry		headspace-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	Pa m ³ mol ⁻¹
-42.75	1447	11.325	28994	10	2957
-24.18	4742	15.718	34940	15	3408
0	17292	21.028	43375	20	3863
19.77	39890	26.506	53710	25	4372
		32.34	66807		
		39.678	93760		
		43.146	97653		
		43.624	99247		
		44.071	100744		
		44.576	102469		
		45.024	104009		
		bp/°C	44.242		
		Antoine eq.			
		eq. 2	P/mmHg		
		A	6.92066		
		B	1121.818		
		C	233.446		

$$\ln (1/K_{AW}) = 6.989 - 1915/(T/K)$$

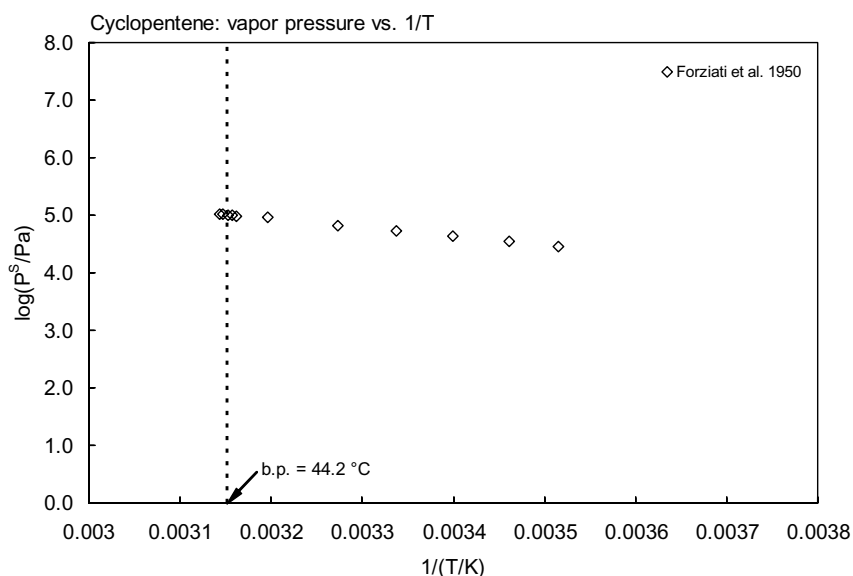


FIGURE 2.1.2.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for cyclopentene.

2.1.2.4.2 Cyclohexene



Common Name: Cyclohexene

Synonym: 1,2,3,4-tetrahydrobenzene, tetrahydrobenzene

Chemical Name: cyclohexene

CAS Registry No: 110-83-8

Molecular Formula: C₆H₁₀

Molecular Weight: 82.143

Melting Point (°C):

−103.5 (Weast 1982–83; Lide 2003)

Boiling Point (°C):

82.98 (Lide 2003)

Density (g/cm³ at 20°C):

0.8110, 0.8061 (20°C, 25°C, Dreisbach 1959)

0.8102 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):

101.4 (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

33.142, 30.485 (25°C, bp, Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

29.125, 27.276 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

3.28 (Riddick et al. 1986)

4.23, 3.28; 7.51(−134.45, −104.45°C; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

49.85, 41.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

130 (shake flask-cloud point, McBain & Lissant 1951)

160 (Farkas 1964)

213 (shake flask-GC, McAuliffe 1966)

299* (25.11°C, shake flask-GC, measured 5.11–45.21°C, Pierotti & Liabastre 1972)

281, 286 (23.5°C, elution chromatography, Schwarz 1980)

160 (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)

246* (calculated-liquid-liquid equilibrium LLE data, temp range 278.2–318.2 K, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

160, 752, 3345, 8723* (−44.42, −24.85, 0, 18.45°C, static method-quartz spiral gauge, Lister 1941)

11734* (24.794°C, ebulliometry, measured range 12.2–83.9°C (Forziati et al. 1950)

log (P/mmHg) = 6.888617 − 1229.973/(224.104 + t/°C); temp range 12.2–83.9°C (Antoine eq., ebulliometry measurements, Forziati et al. 1950)

11840 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.88617 − 1229.973/(224.104 + t/°C); temp range 3.0–146°C (Antoine eq. for liquid state, Dreisbach 1955)

19885* (36.875°C, comparative ebulliometry, measured range 36.875–91.378°C, Meyer & Hotz 1973)

log (P/mmHg) = [1 − 356.172/(T/K)] × 10⁴{0.873674 − 9.73841 × 10^{−4}·(T/K) + 10.9078 × 10^{−7}·(T/K)²}; temp range 213.2–364.53 K (Cox eq., Chao et al. 1983)

11800 (selected lit., Riddick et al. 1986)

$\log(P/\text{kPa}) = 7.109 - 2289.0/(T/\text{K})$; temp range: not specified (Antoine eq., Riddick et al. 1986)

11850 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.997323 - 1221.899/(-49.978 + T/\text{K})$; temp range 309–385 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 52.1749 - 3.238 \times 10^3/(T/\text{K}) - 16.878 \cdot \log(T/\text{K}) + 8.0388 \times 10^{-3} \cdot (T/\text{K}) + 1.3259 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 170–560 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

4020 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

4946, 13310 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

4568 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

3960 (23°C , batch air stripping-IR, Nielsen et al. 1994)

2069, 2467, 2618, 2965 (10, 15, 20, 25°C , headspace-GC, Bakierowska & Trzeszczyński 2003)

$\ln(1/K_{AW}) = 5.860 - 1691/(T/\text{K})$; temp range 10 – 25°C , headspace-GC, Bakierowska & Trzeszczyński 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.16 (calculated- π substituent constants, Hansch et al. 1968)

2.86 (shake flask-GC, Leo et al. 1975)

1.90 (shake flask-GC, Canton & Wegman 1983)

2.86 (recommended, Sangster 1989, 1993)

2.86 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.92* (20.29°C , from GC-determined γ^∞ in octanol, measured range 20.29 – 50.28°C , Gruber et al. 1997)

2.83 (calculated-measured γ^∞ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O(3P)} = 2.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom (Herron & Huie 1973)

$k_{OH} = 6.77 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Atkinson et al. 1979)

$k_{O_3} = 1.69 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Japar et al. 1974)

$k_{O_3} = 2.04 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (chemiluminescence, Adeniji et al. 1981)

$k_{O_3} = (1.04 \pm 0.14) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 1 \text{ K}$ (Atkinson et al. 1983a)

$k_{OH} = (6.43 \pm 0.17) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1983b)

$k_{OH} = (64.1 \pm 2.5) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ (relative rate method, Ohta 1983)

$k_{O_3} = 1.04 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (Atkinson & Carter 1984)

$k_{O_3} = 1.04 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = 6.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 0.29 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O(3P)} = 21 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\text{O}(^3\text{P})$ atom and $k_{NO_2} < 0.2 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with NO_2 (Atkinson & Aschmann 1984)

$k_{O_3} = 1.51 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in synthetic air at 295 K (Bennett et al. 1987)

$k_{O_3} = (7.8 \pm 0.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ in a smog chamber (Nolting et al. 1988)

$k_{OH} = 5.40 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and $k_{OH} = 6.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative to propene (relative rate method, Rogers 1989)

$k_{OH} = 6.77 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 6.77 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 5.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{OH} = 6.75 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 5.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{\text{NO}_3} = 5.28 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (quoted, Atkinson 1991)

$k_{\text{OH}} = 6.77 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}^* = 5.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}_3}^* = 81.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}(^3\text{P})} = 2.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals in aquatic system, and $t_{1/2} = 40 \text{ d}$, based on rate constant $k = 2 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.4.2.1

Reported aqueous solubilities of cyclohexene at various temperatures

Pierotti & Liabastre 1972		Shaw 1989a		Góral et al. 2004	
shake flask-GC/FID		IUPAC "tentative" values		calc-recommended LLE data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
5.11	280	5	—	5.1	265
15.21	298.5	15	—	15.2	251
25.11	299	20	—	20	246
35.21	302.5	25	160	23.5	246
45.21	310.5	35	—	25	246
		45	—	25.1	246
				35.2	251
				45.2	265

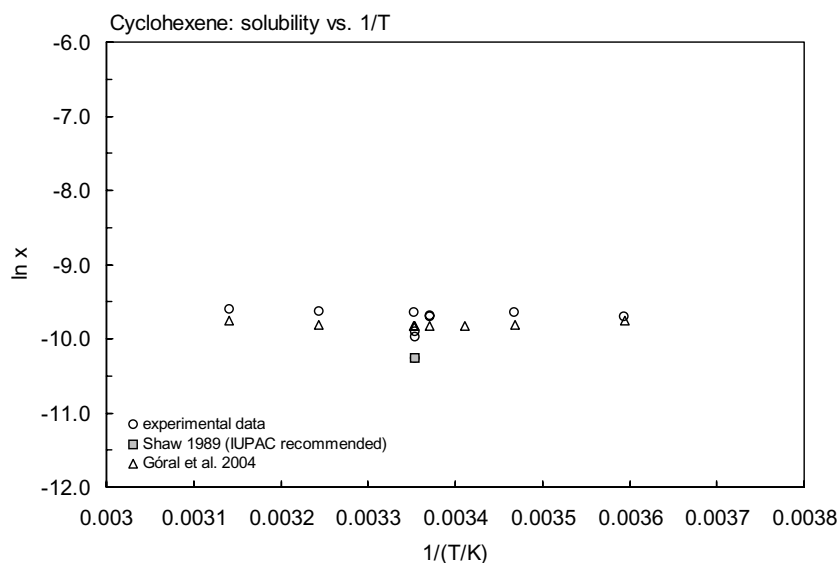


FIGURE 2.1.2.4.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cyclohexene.

TABLE 2.1.2.4.2.2

Reported vapor pressures and octanol-air partition coefficients of cyclohexene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot \log (T/K) + D \cdot [P/(T/K)^2]$	(5)		
$\log (P/\text{atm}) = A'[1 - (T_B/T)]$	(6)	where $\log A' = a + bT + cT^2$	

Vapor pressure						log K _{OA}	
Lister 1941		Forziati et al. 1950		Meyer & Hotz 1973		Gruber et al. 1997	
static-quartz spiral gauge		ebulliometry		comparative ebulliometry		GC det'd activity coeff.	
t/ ^o C	P/Pa	t/ ^o C	P/Pa	t/ ^o C	P/Pa	t/ ^o C	P/Pa
-44.42	160	12.236	6417	36.875	19885	20.29	2.926
-24.85	752	15.920	7709	43.560	26084	30.3	2.762
0	3345	19.137	9006	49.795	33189	40.4	2.594
18.45	8723	22.063	10344	55.785	41404	50.28	2.447
		24.794	11734	62.537	52551		
$\Delta H_v/(\text{kJ mol}^{-1}) = 32.59$ at 27°C		28.490	13858	68.815	64943		
		32.702	16651	75.354	80213		
		36.996	19958	81.075	95764		
		40.976	23358	86.112	111325		
		46.302	28995	91.378	129633		
		51.191	35060				
		57.107	43376	bp/ ^o C	82.945		
		63.200	53712				
		69.708	66808	Antoine eq.			
		76.766	83761	eq. 3	P/cmHg		
		81.757	97648	A	5.872420		
		82.292	99248	B	1221.899		
		82.791	100746	C	223.1720		
		83.353	102470				
		83.852	104010	Cox eq.			
				eq. 6	P/atm		
		eq. 2	P/mmHg	a	0.833958		
		A	6.88617	-b × 10 ³	0.742586		
		B	1229.973	c × 10 ⁶	0.767278		
		C	224.104	T _B /K	356.0954		
		bp/ ^o C	82.979				

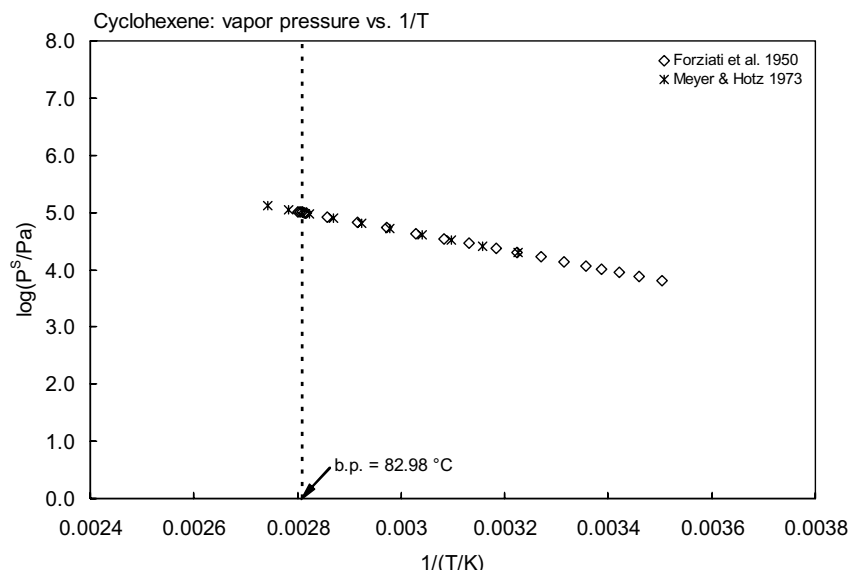


FIGURE 2.1.2.4.2.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexene.

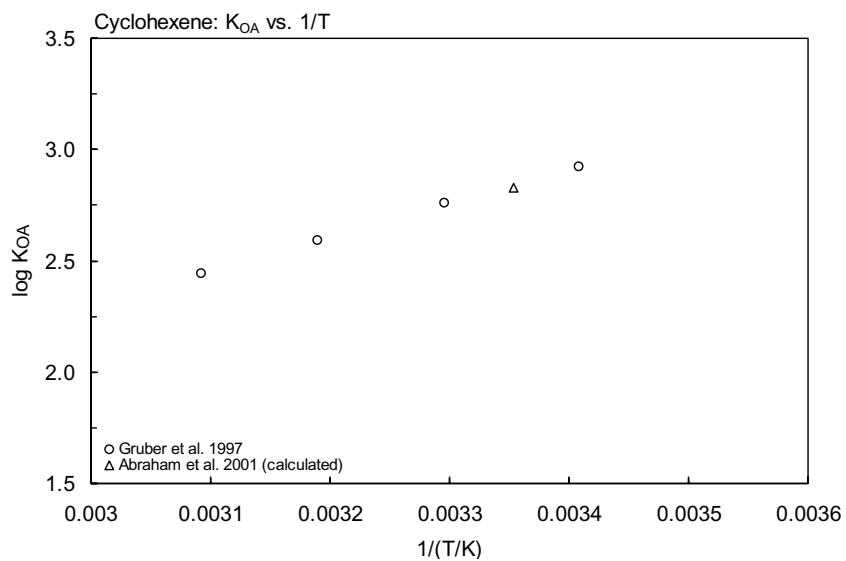
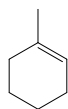


FIGURE 2.1.2.4.2.3 Logarithm of K_{OA} versus reciprocal temperature for cyclohexene.

2.1.2.4.3 1-Methylcyclohexene



Common Name: 1-Methylcyclohexene

Synonym:

Chemical Name: 1-methylcyclohexene

CAS Registry No: 591-49-1

Molecular Formula: C_7H_{12}

Molecular Weight: 96.170

Melting Point ($^{\circ}C$):

-120.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

110.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8102, 0.8058 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Weast 1982–83)

Molar Volume (cm^3/mol):

118.7 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

133.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

37.75, 32.70 (25° , bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.63 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

43.16, 44.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

52.0 (shake flask-GC, McAuliffe 1966)

64.1 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4080 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.86861 - 1308.0/(218.0 + t/^{\circ}C)$; temp range 25 – $165^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1955)

3933 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_l/kPa) = 6.0101 - 1311.087/(-56.045 + T/K)$; temp range 333 – $384\ K$ (Antoine eq., Stephenson & Malanowski 1987)

4858 ($25.25^{\circ}C$, transpiration method, Verevkin et al. 2000)

$\ln(P/Pa) = 23.65 - 4531/(T/K)$; temp range 275.4 – $313.4\ K$ (transpiration method, Verevkin et al. 2000)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

7660 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

7485, 14260 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

11070 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.05 (calculated-regression of Lyman et al. 1982, Wang et al. 1992)

2.20 (calculated-molar volume V_M , Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 9.44 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 305 K (Darnall et al. 1976, Atkinson 1989)

$k_{NO_3} = (2.87 \pm 0.34) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson et al. 1984a)

$k_{NO_2} < 0.20 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{O_3} = 1.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH} = 6.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{NO_3} = 2.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{O(3P)} = 2.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $O(3P)$ atom at room temp. (relative rate method, Atkinson et al. 1984b)

$k_{OH} = 9.45 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (Atkinson 1985)

$k_{OH} = 9.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1990)

$k_{OH} = 9.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}^* = 1.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = 1.65 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O(3P)} = 9.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(3P)$ atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals in aquatic system, and $t_{1/2} = 40 \text{ d}$, based on rate constant $k = 2 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for the oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.4.4 Cycloheptene



Common Name: Cycloheptene

Synonym: suberene

Chemical Name: cycloheptene

CAS Registry No: 628-92-2

Molecular Formula: C_7H_{12}

Molecular Weight: 96.170

Melting Point ($^{\circ}C$):

−56 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

115 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8228 (Weast 1982–83)

Molar Volume (cm^3/mol):

116.9 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)

129.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

36.73 ($27^{\circ}C$, Lister 1941)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.28, 0.71, 0.97; 6.96 (-119.15 , -63.15 , $-56.15^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

42.14, 45.0 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

66.0 (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

188, 821, 2636, 6547 (-21.44 , 0 , 19.82 , $39.06^{\circ}C$, static method-quartz spiral gauge, Lister 1941)

2670 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.27243 - 2011.9/(T/K)$; temp range 251 – 313 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.57 (calculated- π substituent constants, Hansch et al. 1968)

2.75 (calculated-MCI χ , Murray et al. 1975)

3.073 (calculated-UNIFAC group contribution, Chen et al. 1993)

2.58 (calculated-molar volume V_M , Wang et al. 1992)

3.37 (calculated-fragment const., Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = (3.19 \pm 0.36) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 1 \text{ K}$ (Atkinson et al. 1983a; quoted, Atkinson & Carter 1984)

$k_{OH} = (7.08 \pm 0.11) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Atkinson et al. 1983b)

$k_{OH} = 7.44 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1983b, Atkinson 1989)

$k_{O_3} = (28.3 \pm 1.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ in a smog chamber (Nolting et al. 1988)

$k_{NO_3} = 2.80 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = 7.13 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{NO_3} = 4.84 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1991)

$k_{OH} = 7.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 4.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O_3}^* = 2.45 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals in aquatic system, and $t_{1/2} = 40 \text{ d}$, based on rate constant $k = 2 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill & Mabey 1985).

2.1.2.4.5 Cyclooctene



Common Name: Cyclooctene

Synonym:

Chemical Name: cyclooctene

CAS Registry No: 931-87-3 (*cis*-octene), 931-89-5 (*trans*-octene)

Molecular Formula: C₈H₁₄

Molecular Weight: 110.197

Melting Point (°C):

–12, –59 (*cis*-, *trans*-cyclooctene, Weast 1982–83; Lide 2003)

–14.5 to –15.5 (*cis*-cyclooctene, Stephenson & Malanowski 1987)

Boiling Point (°C):

138, 143 (*cis*-, *trans*-cyclooctene, Weast 1982–83; Lide 2003)

Density (g/cm³):

0.8472, 0.8483 (20°C, *cis*-, *trans*-cyclooctene, Weast 1982–83)

Molar Volume (cm³/mol):

130.1 (*cis*-, 20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)

129.9 (*trans*-, 20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)

146.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.57 (27°C, Lister 1941)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

22.9* (generator column-GC/FID, measured range 273.15–313.15 K, Dohányosová et al. 2004)

$\ln x = -33.3561 + 20.8640/\tau + 43.2804 \cdot \ln \tau$, $\tau = [(T/K)/298.15]$, temp range 273.15–313.15 K (generator column-GC/FID, Dohányosová et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

209.3, 774.6, 2333, 5948 (0, 19.83, 40.36, 60.22°C, static method-quartz spiral manometer, Lister 1941)

$\log (P_L/\text{kPa}) = 7.3641 - 2194.3/(T/K)$, temp range 273–441 K (*cis*-cyclooctene, Antoine eq., Stephenson & Malanowski 1987)

1010 (interpolated from data of Lister 1941, temp range 273.15–313.15 K, Dohányosová et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C. Additional data at other temperatures designated * are compiled at the end of this section.):

4842* (derived from measured mole fraction solubility and solute fugacity, temp range 273.15–313.15 K, Dohányosová et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3}^* = 3.75 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (*cis*-cyclooctene, recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 2.1.2.4.5.1

Reorted aqueous solubilities and Henry's law constants of cyclooctene at various temperatures

Aqueous solubility				Henry's law constant	
Dohányosová et al. 2004				Dohányosová et al. 2004	
generator column-GC/FID		smoothed raw exptl data		from solute fugacity <i>f</i> and <i>x</i>	
T/K	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	H/(Pa m ³ /mol)
	raw data				
274.15	20.39	273.15	19.9	273.15	1184.4
274.15	20.14	278.15	20.2	278.15	1625.4
278.15	20.39	283.15	20.7	283.15	2196
278.15	19.59	288.15	21.3	288.15	2898
283.15	21.24	293.15	22.0	293.15	3780
283.15	20.45	298.15	22.9	298.15	4842
288.15	20.94	303.15	23.9	303.15	6120
288.15	20.63	308.15	25.1	308.15	7614
293.15	21.92	313.15	26.5	313.15	9378
298.15	23.63				
298.15	24.61	ln <i>x</i> = A + B/τ + C ln τ			
303.15	22.84	τ = T/298.15			
303.15	23.14	A	−33.3561		
308.15	27.24	B	20.8640		
308.15	24.73	C	23.4396		
308.15	26.88				
313.15	27.31				
313.15	24.80				

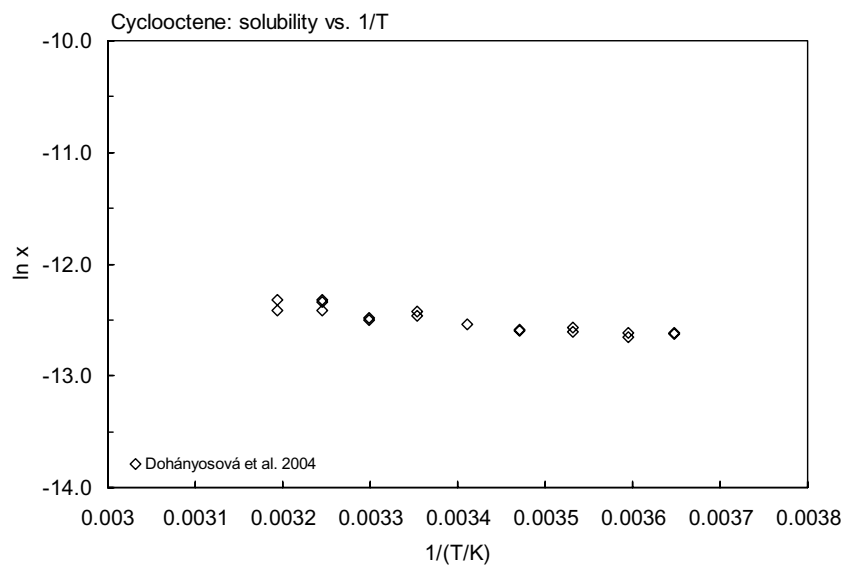


FIGURE 2.1.2.4.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cyclooctene.

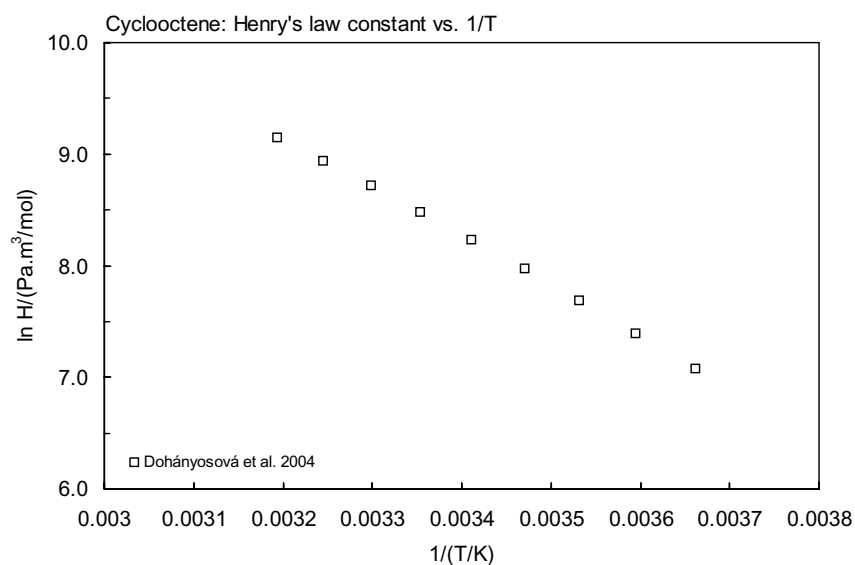


FIGURE 2.1.2.4.5.2 Logarithm of Henry's law constant versus reciprocal temperature for cyclooctene.

2.1.2.4.6 1,4-Cyclohexadiene



Common Name: 1,4-Cyclohexadiene

Synonym: 1,4-dihydrobenzene

Chemical Name: 1,4-cyclohexadiene

CAS Registry No: 628-41-1

Molecular Formula: C_6H_8

Molecular Weight: 80.128

Melting Point ($^{\circ}C$):

−49.2 (Weast 1983–83; Lide 2003)

Boiling Point ($^{\circ}C$):

85.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8471 (Weast 1982–83)

Molar Volume (cm^3/mol):

93.60 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

103.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

0.82, 5.72; 6.53 (-81.15 , $-49.15^{\circ}C$, total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

29.16, 38.0 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

700 (shake flask-GC, McAuliffe 1966)

930* (shake flask-GC, measured range 5.11 – $45.21^{\circ}C$, Pierotti & Liabstre 1972)

800* (recommended, temp range 5 – $45^{\circ}C$, IUPAC Solubility Data Series, Shaw 1989a)

979* (calculated-liquid-liquid equilibrium LLE data, temp range 278.3 – $318.4 K$, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

11892* ($31.1^{\circ}C$, static method-Hg manometer, measured range 304.25 – $322.23 K$, Letcher & Marsicano 1974)

$\log (P/mmHg) = [1 - 368.566/(T/K)] \times 10^4 \{0.916704 - 6.81678 \times 10^{-4} \cdot (T/K) - 7.02362 \times 10^{-7} \cdot (T/K)^2\}$; temp range 304.25 – $322.23 K$ (Cox eq., Chao et al. 1983)

8973 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.86553 - 1176.707/(214.528 + t/^{\circ}C)$; temp range 31.1 – $49.08^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

9009 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.41736 - 1475.149/(-26.108 + T/K)$; temp range: 304 – $360 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$

2.30 (shake flask, Log P Database, Hansch & Leo 1987)

2.48 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)

2.30 (recommended, Sangster 1989, 1993)

2.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = (0.639 \pm 0.074) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 1 \text{ K}$ (Atkinson et al. 1983a)

$k_{OH} = (9.48 \pm 0.39) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1983b)

$k_{NO_3} = (2.89 \pm 0.035) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson et al. 1984a)

$k_{O_3} = 63.9 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = 9.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 0.29 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{NO_2} < 0.4 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with NO_2 (Atkinson et al. 1984b)

$k_{OH}(\text{exptl}) = 9.90 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.03 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1985)

$k_{NO_3} = 7.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (fast flow system, Benter & Schindler 1988)

$k_{OH} = (99.2 - 99.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Atkinson 1989)

$k_{OH} = 9.91 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{NO_3} = 5.30 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with NO_3 radical at nights (Sabljic & Güsten 1990)

$k_{NO_3} = 6.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{OH} = 9.95 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 6.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O_3}^* = 4.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO_2 radicals for olefins in aquatic system, and $t_{1/2} = 19 \text{ h}$, based on rate constant $k = 1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill & Mabey 1985).

TABLE 2.1.2.4.6.1

Reported aqueous solubilities of 1,4-cyclohexadiene at various temperatures

Aqueous solubility						Vapor pressure	
Pierotti & Liabastre 1972		Shaw 1989a		Góral et al. 2004		Letcher & Marsicano 1974	
shake flask-GC/FID		IUPAC "tentative" values		calc-recommended LLE data		static method-Hg manometer	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
5.11	851.9	5	900	5.1	1068	304.25	11892
15.21	958.5	15	900	15.2	979	307.67	13826
25.11	936.2	25	800	25.0	979	310.76	15812
35.21	963.4	35	1000	25.1	979	312.92	42655
45.21	1010	45	1000	35.2	979	316.67	20238
				45.2	1068	319.94	22998
						322.23	25251
						Antoine eq.,	P/mmHg
						log P = A - B/(C + T/K)	
						A	7.2687
						B	1461.75
						C	-29.4

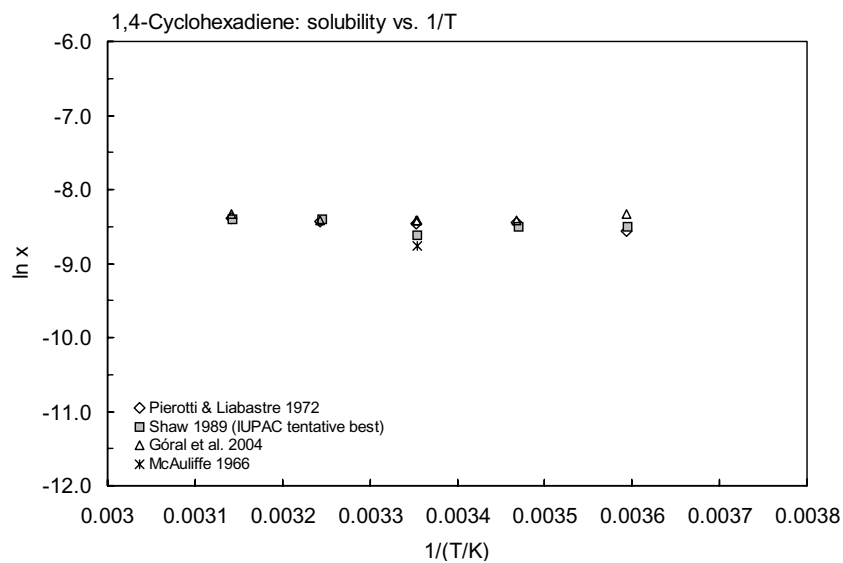


FIGURE 2.1.2.4.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,4-cyclohexadiene.

2.1.2.4.7 Cycloheptatriene



Common Name: Cycloheptatriene

Synonym: tropilidene

Chemical Name: 1,3,5-cycloheptatriene

CAS Registry No: 544-25-2

Molecular Formula: C_7H_8

Molecular Weight: 92.139

Melting Point ($^{\circ}C$):

−79.5 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

117 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8875 (Weast 1982–83)

Molar Volume (cm^3/mol):

103.0 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)

114.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

2.35, 1.16; 3.51 (−93.15, −75.15 $^{\circ}C$, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

21.11, 38.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

620 (shake flask-GC, McAuliffe 1966)

669* ($25.11^{\circ}C$, shake flask-GC, measured range 5.11 – $40.21^{\circ}C$, Pierotti & Liabastre 1972)

640* (recommended best value, temp range 5 – $45^{\circ}C$, IUPAC Solubility Data Series, Shaw 1989)

563* (calculated-liquid-liquid equilibrium LLE data, temp range 278.3 – $318.4\ K$, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

3136* (ebulliometry, measured range 0 – $65^{\circ}C$, Finke et al. 1956)

$\log(P/mmHg) = 6.97032 - 1374.065/(t/^{\circ}C + 220.538)$; temp range 0 – $65^{\circ}C$ (Antoine eq., ebulliometry, Finke et al. 1956)

2825, 3138 (interpolated-Antoine eq-I, II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.09522 - 1374.656/(-52.612 + T/K)$; temp range 273 – $390\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.12574 - 1390.771/(-53.069 + T/K)$; temp range 273 – $390\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

432 (calculated-P/C from selected data)

466 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.63 (shake flask, Eadsforth & Moser 1983)

3.03 (HPLC-RT correlation, Eadsforth & Moser 1983)

2.63 (recommended, Sangster 1989)

2.63 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = (5.39 \pm 0.078) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH} = (9.12 \pm 0.23) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for at 294 ± 2 K (Atkinson et al. 1984b)

$k_{O_3} = 5.39 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for at 294 K (Atkinson & Carter 1984)

$k_{OH} = 9.74 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (Atkinson 1985)

$k_{NO_3} = 1.18 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{OH} = 9.44 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljić & Güsten 1990)

$k_{OH} = 96.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (Atkinson 1989)

$k_{NO_3} = 1.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (quoted, Atkinson 1991)

$k_{OH} = 9.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O_3} = 5.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 2.1.2.4.7.1

Reported aqueous solubilities and vapor pressures of cycloheptatriene at various temperatures

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

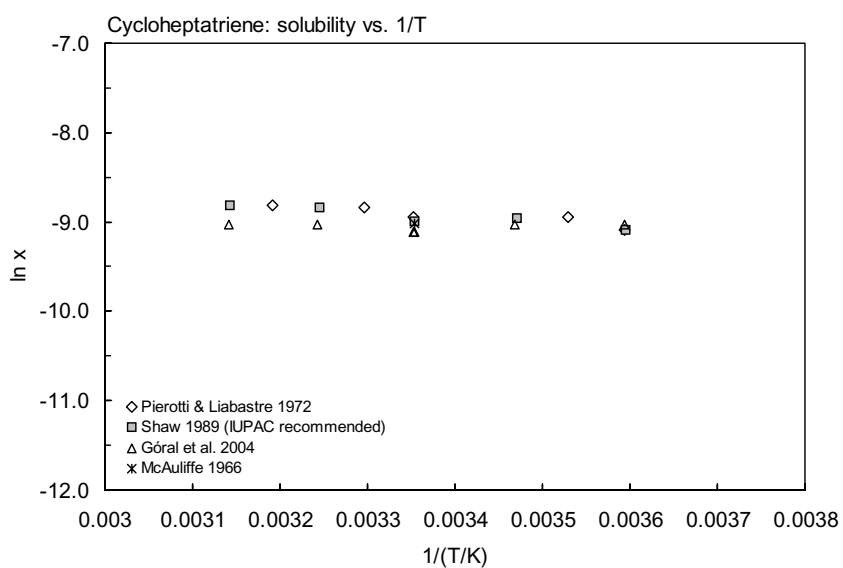
$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Aqueous solubility						Vapor pressure	
Pierotti & Liabastre 1972		Shaw 1989a		Góral et al. 2004		Finke et al. 1956	
shake flask-GC		IUPAC recommended		calc-recommended LLE data		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa
5.11	580.9	5	580	5.1	614	0	733.3
10.21	664.5	15	660	15.2	614	15	1815
25.11	669.4	25	640	25.0	563	20	2400
30.21	741.8	35	740	25.1	563	25	3136
40.21	764.8	45	760	35.2	614	30	4058
				45.2	614	35	5198
						40	6591
						45	8286
						50	10327
						55	12774
						60	15672
						65	19094

TABLE 2.1.2.4.7.1 (Continued)

Aqueous solubility						Vapor pressure	
Pierotti & Liabastre 1972		Shaw 1989a		Góral et al. 2004		Finke et al. 1956	
shake flask-GC		IUPAC recommended		calc-recommended LLE data		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa
						bp/°C	115.60
						$\Delta H_v/(\text{kJ mol}^{-1}) = 38.70$ at 25°C	
						eq. 2	P/mmHg
						A	6.97032
						B	1374.656
						C	220.538

FIGURE 2.1.2.4.7.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cyclohepta-triene.

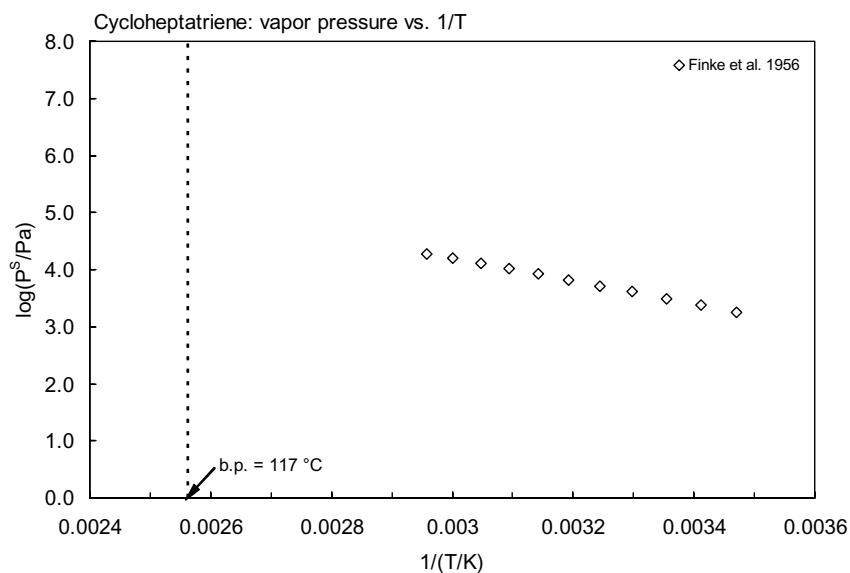
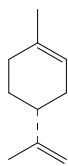


FIGURE 2.1.2.4.7.2 Logarithm of vapor pressure versus reciprocal temperature for cycloheptatriene.

2.1.2.4.8 dextro-Limonene [(R)-(+)-Limonene]



Common Name: *d*-Limonene

Synonym: *d*-*p*-mentha-1,8,-diene, (R)-(+)-*p*-mentha-1,8-diene, (+)-1-methyl-4-(1-methylethenyl)cyclohexene, *p*-mentha-1,8-diene, carvene, cinene, citrene, cajeputene, kautschin

Chemical Name: *dextro*-limonene, (R)-(+)-limonene

CAS Registry No: 5989-27-5

Molecular Formula: C₁₀H₁₆

Molecular Weight: 136.234

Melting Point (°C):

−74 (Lide 2003)

Boiling Point (°C):

178 (Weast 1982–83; Lide 2003)

Density (g/cm³ at 25°C):

0.8403, 0.8383 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

162.1 (20°C, calculated-density, Stephenson & Malanowski 1987)

192.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.1 (25°C, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

13.49 (shake flask-GC, Massaldi & King 1973)

13.8 (selected lit., Riddick et al. 1986)

20.44 (shake flask-GC/FID, Fichan et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

275.64 (calculated-Antoine eq. regression, Stull 1947)

275.5 (interpolated-Antoine eq., Weast 1972–73)

log (P/mmHg) = [−0.2185 × 10508.4/(T/K)] + 8.016262; temp range 14.0–175°C (Antoine eq., Weast 1972–73)

2670 (68.2°C, Riddick et al. 1986)

278, 202 (calculated-Antoine eq.-I, II, Stephenson & Malanowski 1987)

log (P_l/kPa) = 6.81591 − 2075.62/(−16.65 + T/K); temp range 287–448 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_l/kPa) = 7.67098 − 2494.342/(T/K); temp range 288–323 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 9.3771 − 2.8246 × 10³/(T/K) + 1.0584·log (T/K) − 8.9107 × 10^{−3}·(T/K) + 4.8462 × 10^{−6}·(T/K)²; temp range 199–660 K (vapor pressure eq., Yaws 1994)

213 (activity coefficient-GC, Fichan et al. 1999)

Henry's Law Constant (Pa m³/mol at 25°C):

2725 (calculated-P/C from selected data)

Octanol/Water Partition Coefficient, log K_{ow}:

4.38 (RP-HPLC-RT correlation, Griffin et al. 1999)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = 9 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, with $t_{1/2} < 0.24 \text{ h}$ (Darnall et al. 1976)

$k_{OH} = (9.0 \pm 1.35) \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ at 1 atm and $305 \pm 2 \text{ K}$ (relative rate method, Winer et al. 1976)

$k_{OH} = 9.0 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$, $k_{O_3} = 3.9 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$, and $k_{O(^3P)} = (6.50 \pm 0.52) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with $O(^3P)$ atom at room temp. (Winer et al. 1976)

$k_{OH}(\text{calc}) = 13.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = (14.0, 14.2) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1983b)

$k_{NO_3} = (7.7 \pm 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate technique, Atkinson et al. 1984a)

$k_{O_3} = 6.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetimes $\tau = 6 \text{ min}$ and 11 min in 24-h in clean and moderately polluted atmosphere, respectively; $k_{OH} = 1.42 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated $\tau = 2.0 \text{ h}$ and 1.0 h during daytime in clean and moderately polluted atmosphere respectively, $k_{NO_3} = 7.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated $\tau = 9 \text{ min}$ and 0.9 min during nighttime in clean and moderately polluted atmosphere, respectively, at room temp. (Atkinson et al. 1984a)

$k_{NO_2} < 3.5 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas phase reaction with NO_2 at 295 K (Atkinson et al. 1984b)

$k_{O_3} = 6.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH} = 1.42 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 7.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{O(^3P)} = 1.29 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $O(^3P)$ atom at room temp. (Atkinson et al. 1984b)

$k_{O_3} = 6.0 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 36 d^{-1} ; $k_{OH} = 1.4 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 12 d^{-1} , and $k_{NO_3} = 1.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 290 d^{-1} (Atkinson & Carter 1984)

$k_{O_3} = 6.0 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 36 d^{-1} ; $k_{OH} = 1.7 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 7.3 d^{-1} , and $k_{NO_3} = 1.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 290 d^{-1} at room temp. (Atkinson 1985)

$k_{OH} = (16.9 \pm 0.5) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 1 \text{ K}$ (relative rate method, Atkinson et al. 1986)

$k_{O_3} = 6.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated $\tau = 36 \text{ min}$; $k_{OH} = 1.7 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 1.6 \text{ h}$, $k_{NO_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 5.0 \text{ min}$ for clean tropospheric conditions at room temp. (Atkinson et al. 1986)

$k_{OH} = (146-171) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294–305 K (review, Atkinson 1989)

$k_{OH} = 1.71 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 1.22 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = 2.03 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O(^3P)} = 7.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(^3P)$ atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

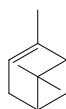
Half-Lives in the Environment:

Air: $t_{1/2} < 24 \text{ h}$ in air based on its photooxidation rate constant of $9 \times 10^{13} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the gas phase reaction with hydroxyl radical (Darnall et al. 1976; Lloyd et al. 1976);

calculated lifetimes: $\tau = 36 \text{ min}$ due to reaction with O_3 in 24-h period, $\tau = 2.0 \text{ h}$ with OH radical during daytime, and $\tau = 9 \text{ min}$ for NO_3 radical during nighttime for "clean" atmosphere; $\tau = 11 \text{ min}$ for reaction with O_3 in 24-h period, $\tau = 1.0 \text{ h}$ with OH radical during daytime, and $\tau = 0.9 \text{ min}$ for NO_3 radical during nighttime in moderately polluted atmosphere (Atkinson et al. 1984a);

calculated atmospheric lifetimes, $\tau = 36 \text{ min}$, 1.6 h and 5.0 min for reaction with O_3 , OH and NO_3 radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);

calculated tropospheric lifetimes $\tau = 1.1 \text{ h}$, 1.9 h and 53 min due to reactions with OH radical, O_3 and NO_3 radical, respectively, at room temp. (Corchnoy & Atkinson 1990).

2.1.2.4.9 α -PineneCommon Name: α -PineneSynonym: *dl*-pinene, 2-pinene

Chemical Name: 2,6,6-trimethylbicyclo[3,1,1]hept-2-ene

CAS Registry No: 7785-70-8

 α -pinene *d*-Form 80-56-8Molecular Formula: C₁₀H₁₆

Molecular Weight: 136.234

Melting Point (°C):

- 55 (*dl*-Form, Weast 1982–83)
- 64 (*d*-Form, Riddick et al. 1986; Lide 2003)
- 50 (*d*-Form, Stephenson & Malanowski 1987)

Boiling Point (°C):

- 156.2 (*dl*-Form, Weast 1982–83; Lide 2003)
- 156 (*d*-Form, Stephenson & Malanowski 1987)
- 155–156 (*d*-, *l*-Form, Budavari 1989)

Density (g/cm³):

- 0.8582 (20°C, *dl*-Form, Weast 1982–83)
- 0.8582, 0.8539 (*d*-Form, Riddick et al. 1986)
- 0.8592, 0.8591, 0.8590 (20°C, *dl*-, *d*-, *l*-Form, Budavari 1989)

Molar Volume (cm³/mol):

- 157.4 (*d*-Form, Stephenson & Malanowski 1987)
- 183.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

- 46.61, 39.673 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

- 21.8, 3.42; 5.04 (quoted lit. values; shake flask-GC/FID, Fichan et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 640*, 800 (22.2, 22.5°C, measured range 21.1–148°C, Pickett & Peterson 1929)
- 237.3* (13.25°C, Hg manometer, measured range –6.0 to 13.25°C, Linder 1931)
- 666.6* (24.6°C, summary of literature data, temp range –1.0 to 155.0°C, Stull 1947)
- 457*, 655 (21.2, 27.2°C, measured range 19.4–155.75°C, Hawkins & Armstrong 1954)
- 678 (interpolated-Antoine eq., Weast 1972–73)
- log (P/mmHg) = $[-0.2185 \times 9813.6/(T/K)] + 7.898207$; temp range –1.0 to 155°C (Antoine eq., Weast 1972–73)
- 667 (Verschuereen 1983)
- 605, 587 (interpolated-Antoine equations, Boublik et al. 1984)
- log (P/kPa) = $6.37971 - 1692.803/(231.558 + t/°C)$; temp range 21.1–148°C (Antoine eq. from reported exptl. data of Pickett & Peterson 1929, Boublik et al. 1984)
- log (P/kPa) = $6.95174 - 1430.936/(206.42 + t/°C)$; temp range 19.44–155.75°C (Antoine eq. from reported exptl. data of Hawkins & Armstrong 1954, Boublik et al. 1984)
- 655 (selected, Riddick et al. 1986)
- log (P/kPa) = $25.52644 - 3134.525/(T/K) - 6.16045 \cdot \log (T/K)$ (Riddick et al. 1986)

- 582 (α -pinene *d*-Form, interpolated-Antoine eq., temp range 292–433 K, Stephenson & Malanowski 1987)
 $\log(P/\text{kPa}) = 5.92666 - 1414.16/(T/\text{K})$ (Antoine eq., liquid, temp range 292–433 K (α -pinene *d*-Form, Stephenson & Malanowski 1987))
 588 (interpolated-Antoine eq., temp range 19–156°C, Dean 1992)
 $\log(P/\text{mmHg}) = 6.8525 - 1446.4/(t/^\circ\text{C} + 208.0)$; temp range 19–156°C (Antoine eq., Dean 1992)
 $\log(P/\text{mbar}) = 7.076588 - 1511.961/[(T/\text{K}) - 57.730]$; temp range 365–430 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)
 $\log(P/\text{mmHg}) = 21.4735 - 2.7156 \times 10^3/(T/\text{K}) - 5.0076 \cdot \log(T/\text{K}) + 2.8146 \times 10^{-3} \cdot (T/\text{K}) - 1.5389 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 209–632 K (vapor pressure eq., Yaws 1994)
 613, 581, 465; 529 (quoted lit. values; deduced from exptl. determined activity coeff. at infinite dilution, Fichan et al. 1999)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

- 0.194* (20°C, calculated from measured liquid-phase diffusion coefficients, measured range –10 to 20°C, Zhang et al. 2003)
 $\ln[H^*/(M/\text{atm})] = -6.590 + 3800/(T/\text{K})$; temp range 263–293 K (Zhang et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 4.44 ((+)- α -pinene, RP-HPLC-RT correlation, Griffin et al. 1999)
 4.48 ((-)- α -pinene, RP-HPLC-RT correlation, Griffin et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants k_{O_3} for reaction with O_3 , k_{OH} with OH radical and k_{NO_3} with NO_3 radical at 25°C or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

- $k_{\text{OH}} = (3.48 \pm 0.52) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Winer et al. 1976)
 $k_{\text{OH}} = 3.5 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3} = 2.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$, and $k_{\text{O(3P)}} = (1.60 \pm 0.06) \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with O(³P) atom at room temp. (Winer et al. 1976)
 $k_{\text{OH}} = 32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{O}_3} = 67 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Gaffney & Levine 1979)
 $k_{\text{O}_3}^* = (8.4 \pm 1.9) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 276–324 K, atmospheric lifetime $\tau = 3\text{--}4 \text{ h}$ due to reaction with O_3 , and $\tau \sim 4 \text{ h}$ due to reaction with OH radical (Atkinson et al. 1982)
 $k_{\text{OH}}^* = (6.01 \pm 0.82) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–422 K (flash photolysis-resonance fluorescence, Kleindienst et al. 1982)
 $k_{\text{OH}}(\text{calc}) = 8.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs}) = (7.6, 5.5, 6.01) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1983b)
 $k_{\text{OH}}^* = 60.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–422 K (Flash photolysis-resonance fluorescence, Kleindienst et al. 1982; Atkinson 1985)
 $k_{\text{NO}_3} = (3.4 \pm 0.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate method, Atkinson et al. 1984a)
 $k_{\text{O}_3} = 8.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetimes of 4.6 h and 1.4 h in 24-h in clean and moderately polluted atmosphere, respectively; $k_{\text{OH}} = 6.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetimes of 4.6 h and 2.3 h during daytime in clean and moderately polluted atmosphere, respectively, $k_{\text{NO}_3} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetimes of 20 min and 2 min during nighttime in clean and moderately polluted atmosphere respectively at room temp. (Atkinson et al. 1984a)
 $k_{\text{NO}_2} < 2.1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas phase reaction with NO_2 at 295 K (Atkinson et al. 1984b)

$k_{O_3} = 8.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH} = 6.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{O(^3P)} = 640 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $O(^3P)$ at room temp. (Atkinson et al. 1984b)
 $k_{O_3} = 8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 5 d^{-1} ; $k_{OH} = 6.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 5 d^{-1} , and $k_{NO_3} = 6.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 130 d^{-1} (Atkinson & Carter 1984)
 $k_{OH} = (5.45 \pm 0.32) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 1 \text{ K}$ (relative rate method, Atkinson et al. 1986)
 $k_{O_3} = 8.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated $\tau = 5.6 \text{ h}$; $k_{OH} = 5.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 5.1 \text{ h}$, $k_{NO_3} = 6.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 11 \text{ min}$ for clean tropospheric conditions at room temp. (Atkinson et al. 1986)
 $k_{O_3} = (8.6 \pm 1.3) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ in a smog chamber (Nolting et al. 1988)
 $k_{OH}^* = 5.37 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)
 $k_{OH}^* = 5.37 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 5.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} = (8.4, 8.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1990)
 $k_{OH} = 9.12 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{NO_3} = 5.75 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Müller & Klein 1991)
 $k_{OH} = 5.32 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 5.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljic & Güsten 1990)
 $k_{NO_3}^* = 6.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)
 $k_{OH}^* = 5.37 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3}^* = 6.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3}^* = 86.6 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O(^3P)} = 3.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(^3P)$ atom, at 298 K (recommended, Atkinson 1997)
 $k_{OH}(\text{lit.}) = 5.45 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH}(\text{calc}) = 8.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (quoted; calculated-QSAR, Peeters et al. 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated lifetimes: $\tau = 4.6 \text{ h}$ due to reaction with O_3 in 24-h period, $\tau = 4.6 \text{ h}$ with OH radical during daytime, and $\tau = 20 \text{ min}$ for NO_3 radical during nighttime for clean atmosphere; $\tau = 1.4 \text{ h}$ for reaction with O_3 in 24-h period, $\tau = 2.3 \text{ h}$ with OH radical during daytime, and $\tau = 2 \text{ min}$ with NO_3 radical during nighttime in moderately polluted atmosphere (Atkinson et al. 1984a, Winer et al. 1984);
 calculated atmospheric lifetimes of 5.6 h , 5.1 h and 11 min for reaction with O_3 , OH and NO_3 radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);
 calculated tropospheric lifetimes of 3.4 h , 4.6 h and 2.0 h due to reactions with OH radical, O_3 and NO_3 radical respectively at room temp. (Corchnoy & Atkinson 1990).

TABLE 2.1.2.4.9.1

Reported vapor pressures of α -pinene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Pickett & Peterson 1929				Linder 1931		Stull 1947	
Ramsay & Young method				Hg manometer		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
21.2	533	134.9	57128	-6.0	54.66	-1.0	133
22.0	573	135.4	57608	1.0	96.0	24.6	666.6
22.2	640	138.5	63728	13.25	237.3	37.3	1333
22.5	800	138.8	64261			51.4	2666

(Continued)

TABLE 2.1.2.4.9.1 (Continued)

Pickett & Peterson 1929				Linder 1931		Stull 1947	
Ramsay & Young method				Hg manometer		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
54.7	3040	139.8	65861			66.8	5333
55.3	3200	140.1	66794			76.8	7999
55.5	3306	140.5	67461			90.1	13332
77.4	7839	141.2	68794			110.2	26664
77.5	7906	141.3	69327			132.3	53329
77.7	7959	141.9	70394			155.0	101325
77.9	8026	147.0	80526				
78.6	8253	148.0	83060			mp/°C	−55
79.3	8519						
79.6	8639	bp/°C	155–158				
101.1	19625						
102.8	20758						
103.2	21025						
103.5	21238						
103.7	21371						
103.8	21451						
131.2	52196						
132.3	53462						
132.4	53862						
132.5	53902						
132.7	54089						
132.9	54275						
133.0	54755						
133.1	54862						
133.2	54995						

2.

Hawkins & Armstrong 1954

Hg manometer							
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
19.45	408.0	65.63	4858	95.27	16164	155.77	100601
21.3	457.3	66.54	5121	102.25	20717	155.76	100793
27.25	654.6	68.27	5554	105.9	23430		
29.72	790.6	70.45	6073	106.76	24217	bp/°C	155.9
37.07	1201	75.1	7430	110.53	27438		
46.92	2015	76.04	7698	113.5	30135	eq. 4	P/mmHg
53.69	2832	77.12	8033	115.07	31795	A	26.40174
54.18	2877	79.75	8905	122.11	39478	B	3134.525
56.57	3234	84.71	10859	125.02	42963	C	6.16045
57.09	3309	86.23	11536	129.87	49509	155.77	100601
57.3	3393	88.42	12512	135.72	58678		
62.28	4221	92.01	14299	147.48	80731		

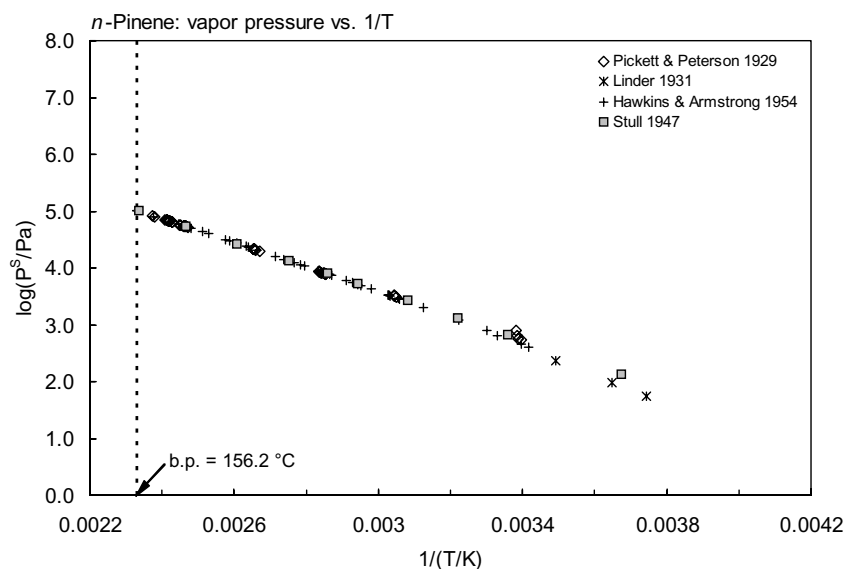


FIGURE 2.1.2.4.9.1 Logarithm of vapor pressure versus reciprocal temperature for α -pinene.

TABLE 2.1.2.4.9.2

Reported Henry's law constants of α -pinene at various temperatures

Zhang et al. 2003

liquid-phase diffusion coefficient

$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
-10	0.0397
0	0.0618
10	0.113
20	0.194
$\ln(kH/\text{atm}) = A - B/(T/K)$	
eq. 3	$H'/(M \text{ atm}^{-1})$
A	-6.59
B	3800

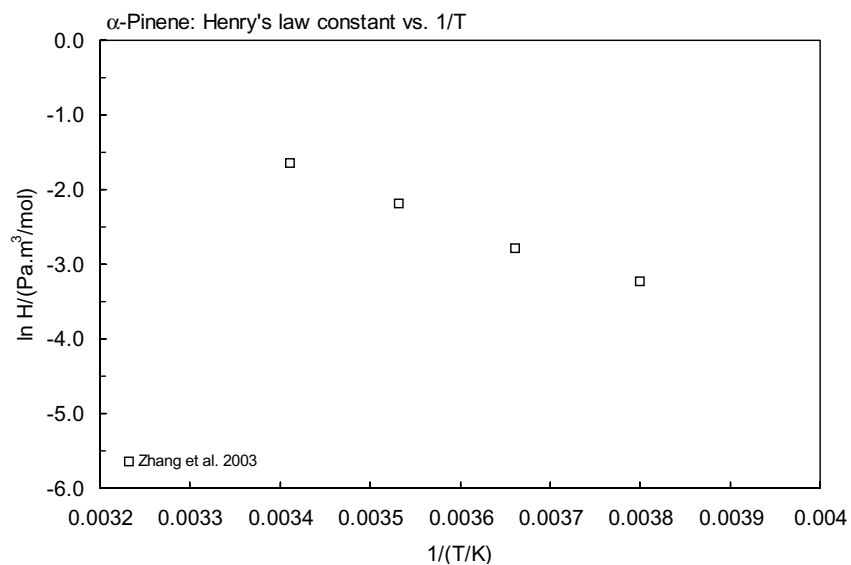
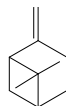


FIGURE 2.1.2.4.9.2 Logarithm of Henry's law constant versus reciprocal temperature for α -pinene.

2.1.2.4.10 β -Pinene

Common Name: β -Pinene

Synonym: β -Pinene *d*, or nopinene; β -Pinene *l*, or 2(10)-pinene

Chemical Name: 6,6-dimethyl-2-methylene bicyclo[3,1,1]heptane

CAS Registry No: 19172-67-3

β -pinene *l*-Form 127-91-3

Molecular Formula: $C_{10}H_{16}$

Molecular Weight: 136.234

Melting Point ($^{\circ}C$):

−61.54 (*l*-Form, Riddick et al. 1986)

−50 (*l*-Form, Stephenson & Malanowski 1987)

−61.5 (*l*-Form, Lide 2003)

Boiling Point ($^{\circ}C$):

164–166, 162.4 (*d*-Form, *l*-Form, Weast 1982–83)

166 (*l*-Form, Riddick et al. 1986; Lide 2003)

163 (*l*-Form, Stephenson & Malanowski 1987)

165–166, 164–166, 162–163 (*dl*-, *d*-, *l*-Form, Budavari 1989)

Density (g/cm^3):

0.8654, 0.8694 (20 $^{\circ}C$, *d*-, *l*-Form, Weast 1982–83)

0.8667 (25 $^{\circ}C$, *l*-Form, Riddick et al. 1986)

Molar Volume (cm^3/mol):

157.4 (*l*-Form, Stephenson & Malanowski 1987)

183.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

43.471, 40.208 (25 $^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

32.7, 6.27; 11.04 (quoted lit. values; shake flask-GC, Fichan et al. 1999)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

613* (Ramsay & Young method, measured range 24.3–158.1 $^{\circ}C$, Pickett & Peterson 1929)

666.6* (30.0 $^{\circ}C$, summary of literature data, temp range 4.2–158.3 $^{\circ}C$, Stull 1947)

345*, 447 (23.06, 26.8 $^{\circ}C$, measured range 18.71–165.91 $^{\circ}C$, Hawkins & Armstrong 1954)

501 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 10235.8/(T/K)] + 8.633424$; temp range 4.2–158.3 $^{\circ}C$ (Antoine eq., Weast 1972–73)

667 (Verschuereen 1983)

395 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.02052 - 1509.944/(210.05 + t/^{\circ}C)$; temp range 18.71–165.9 $^{\circ}C$ (Antoine eq. from reported exptl. data of Hawkins & Armstrong 1954, Boublik et al. 1984)

610 (selected, Riddick et al. 1986)

$\log(P/kPa) = 27.90258 - 3318.845/(T/K) - 6.94263 \cdot \log(T/K)$ (Riddick et al. 1986)

391 (*l*-Form, interpolated-Antoine eq., temp range 291–441K, Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.04993 - 1520.15/(T/K + 62.75)$; temp range 291–441 K (*l*-Form, Antoine eq., liquid, Stephenson & Malanowski 1987)

394 (interpolated-Antoine eq., Dean 1992)

$\log(P/\text{mmHg}) = 6.8984 - 1511.7/(t/^\circ\text{C} + 210.2)$; temp range 19–156°C (Antoine eq., Dean 1992)

$\log(P/\text{mbar}) = 7.067997 - 1539.348/[(T/\text{K}) - 59.937]$; temp range 364–439 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)

$\log(P/\text{mmHg}) = 46.3728 - 3.9789 \times 10^3/(T/\text{K}) - 13.284 \cdot \log(T/\text{K}) - 1.3113 \times 10^{-10} \cdot (T/\text{K}) + 3.4783 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 120–651 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.16 (RP-HPLC-RT correlation, Griffin et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for second order gas-phase rate constants k_{OH} , k_{O_3} and k_{NO_3} for reactions with OH radicals, O_3 and NO_3 radicals or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = 42 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$, with $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ (Darnall et al. 1976)

$k_{\text{OH}} = (4.06 \pm 0.61) \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ at 1 atm and $305 \pm 2 \text{ K}$ (relative rate method, Winer et al. 1976)

$k_{\text{OH}} = 4.1 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$; $k_{\text{O}_3} = 2.2 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$; and $k_{\text{O(}^3\text{P)}} = (1.51 \pm 0.06) \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with $\text{O(}^3\text{P)}$ atom (Winer et al. 1976)

$k_{\text{O}_3} = 30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{OH}} = 65 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Gaffney & Levine 1979)

$k_{\text{O}_3} = (2.1 \pm 0.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ with atmospheric lifetime $\tau \sim 13 \text{ h}$ due to reaction with O_3 and $\tau \sim 4 \text{ h}$ due to reaction with OH radical (Atkinson et al. 1982)

$k_{\text{OH}}^* = (7.76 \pm 1.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 297–423 K (flash photolysis-resonance fluorescence, Kleindienst et al. 1982; Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 5.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs}) = (6.4, 7.76) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1983b)

$k_{\text{NO}_3} = (1.4 \pm 0.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate method, Atkinson et al. 1984a)

$k_{\text{O}_3} = 2.1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetimes $\tau = 18 \text{ h}$ and 5.5 h in clean and moderately polluted atmosphere respectively; $k_{\text{OH}} = 7.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated $\tau = 3.6 \text{ h}$ and 1.8 h during daytime in clean and moderately polluted atmosphere, respectively; $k_{\text{NO}_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated $\tau = 50 \text{ min}$ and 5 min during nighttime in clean and moderately polluted atmosphere, respectively, at room temp. (Atkinson et al. 1984a)

$k_{\text{NO}_2} = < 2.4 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas phase reaction with NO_2 at 295 K (Atkinson et al. 1984b)

$k_{\text{O}_3} = 2.1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{OH}} = 7.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{\text{O(}^3\text{P)}} = 640 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O(}^3\text{P)}$ atom, at room temp. (Atkinson et al. 1984b)

$k_{\text{OH}} = (7.95 \pm 0.52) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 1 \text{ K}$ (relative rate method, Atkinson et al. 1986)

$k_{\text{O}_3} = 2.1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated $\tau = 18 \text{ h}$; $k_{\text{OH}} = 8.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 3.5 \text{ h}$, $k_{\text{NO}_3} = 2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 28 \text{ min}$ for clean tropospheric conditions at room temp. (Atkinson et al. 1986)

$k_{\text{NO}_3} = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1988)

$k_{\text{O}_3} = (1.4 \pm 0.2) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ in a smog chamber (Nolting et al. 1988)

$k_{\text{OH}}^* = 7.89 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}^* = 7.89 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}_3} = (2.1; 1.4) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1990)

$k_{\text{OH}} = 5.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{NO}_3} = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Müller & Klein 1991)
 $k_{\text{OH}} = 7.82 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at 298K (Sabljić & Güsten 1990)
 $k_{\text{NO}_3} = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)
 $k_{\text{O}_3} = 12.2 \pm 1.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $22 \pm 1^\circ\text{C}$ (Grosjean et al. 1993)
 $k_{\text{OH}}^* = 7.89 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}_3}^* = 1.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}(^3\text{P})} = 2.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom, at 298 K (recommended, Atkinson 1997)
 $k_{\text{OH, lit}} = 7.95 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{OH}}(\text{calc}) = 6.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (quoted; calculated-QSAR, Peters et al. 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated lifetimes: $\tau = 18 \text{ h}$ due to reaction with O_3 in 24-h period, $\tau = 3.6 \text{ h}$ with OH radical during daytime, and $\tau = 50 \text{ min}$ for NO_3 radical during nighttime for “clean” atmosphere; $\tau = 5.5 \text{ h}$ for reaction with O_3 in 24-h period, $\tau = 1.8 \text{ h}$ with OH radical during daytime, and $\tau = 5 \text{ min}$ with NO_3 radical during nighttime hours in “moderately polluted” atmosphere (Atkinson et al. 1984a, Winer et al. 1984);
 calculated atmospheric lifetimes of 18 h, 3.5 h and 28 min for reaction with O_3 , OH and NO_3 radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);
 calculated tropospheric lifetimes of 2.3 h, 1.1 d and 4.9 h due to reactions with OH radical, O_3 and NO_3 radical respectively at room temp. (Corchnoy & Atkinson 1990).

TABLE 2.1.2.4.10.1

Reported vapor pressures of β -pinene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Pickett & Peterson 1929						Stull 1947	
Ramsay & Young method						summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.3	453.3	94.7	13839	131.9	47809	4.2	133.3
24.5	480	95.1	14225	132.1	48329	30.0	666.6
24.7	520	95.7	14585	132.6	48889	42.3	1333
24.8	400	96.0	14705	132.9	49583	58.1	2666
25.0	613	96.2	14905	133.6	50623	71.5	5333
25.4	653	96.5	14905	133.9	50796	81.2	7999
53.5	2486	105.8	20825	154.7	91792	94.0	13332
54.0	2440	106.0	20998	154.9	92126	114.1	26664
54.4	2466	106.4	21305	155.2	92459	136.1	53329
54.6	2520	106.9	21665	156.2	94859	158.3	101325
55.0	2586	107.1	21812	158.0	100258		
68.7	4680	108.2	21932	158.1	100926	mp/°C	—
68.9	4720	131.2	47529				
69.1	4866	131.6	47929	bp/°C	160.2–163.8		
70.9	5240	131.7	47929				

(Continued)

TABLE 2.1.2.4.10.1 (Continued)

2.

Hawkins & Armstrong 1954							
Hg manometer							
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
18.72	252.0	50.11	1644	81.23	6949	161.22	89634
20.05	284.0	52.32	1812	85.96	8266	165.8	100788
23.09	345.3	56.57	2268	85.86	9983	157.82	101194
26.82	446.6	56.94	2341	90.80	11346		
29.45	517.3	58.86	2550	94.12	12828	bp/°C	166.0
31.68	592.0	59.48	3056	97.33	15948		
32.03	592.0	62.62	3084	103.41	19288	eq. 4	P/mmHg
36.78	793.3	66.52	3534	108.81	24117	A	28.77768
37.09	803.9	68.75	4014	115.50	27972	B	3318.845
39.41	929.3	72.23	4677	125.33	33079	C	6.94243
41.34	1037	75.43	5384	131.39	39762		
45.52	1289	78.59	6141	136.02	45106		
49.41	1580	80.88	6810	149.55	65069		

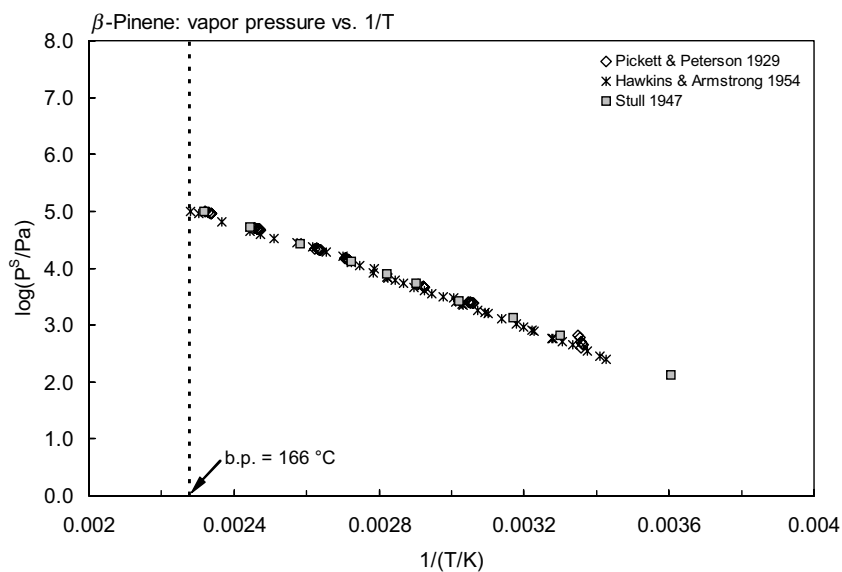


FIGURE 2.1.2.4.10.1 Logarithm of vapor pressure versus reciprocal temperature for β -pinene.

2.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 2.2.1
Summary of physical properties of aliphatic and cyclic hydrocarbons

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p.°C	b.p.°C	Fugacity ratio, F at 25°C*	Density, ρ g/cm³ at 20°C	Molar volume, V _M cm³/mol	
								MW/ρ at 20°C	Le Bas
Alkanes:									
Isobutane (2-Methylpropane)	75-28-5	C ₄ H ₁₀	58.122	−159.4	−11.73	1	0.5571	104.33	96.2
2,2-Dimethylpropane (Neopentane)	463-82-1	C ₅ H ₁₂	72.149	−16.4	9.48	1	0.5910	122.08	118.4
<i>n</i> -Butane	106-97-8	C ₄ H ₁₀	58.122	−138.3	−0.5	1	0.5786	100.45	96.2
2-Methylbutane (Isopentane)	78-78-4	C ₅ H ₁₂	72.149	−159.77	27.88	1	0.6193	116.50	118.4
2,2-Dimethylbutane	75-83-2	C ₆ H ₁₄	86.175	−98.8	49.73	1	0.6492	132.74	140.6
2,3-Dimethylbutane	79-29-8	C ₆ H ₁₄	86.175	−128.10	57.93	1	0.6616	130.25	140.6
2,2,3-Trimethylbutane	464-06-2	C ₇ H ₁₆	100.202	−24.6	80.86	1	0.6901	145.20	162.8
<i>n</i> -Pentane	109-66-0	C ₅ H ₁₂	72.149	−129.67	36.06	1	0.6262	115.22	118.4
2-Methylpentane (Isohexane)	107-83-5	C ₆ H ₁₄	86.175	−153.6	60.26	1	0.6322	136.31	140.6
3-Methylpentane	96-14-0	C ₆ H ₁₄	86.175	−162.90	63.27	1	0.66431	129.72	140.6
2,2-Dimethylpentane	590-35-2	C ₇ H ₁₆	100.202	−123.7	79.2	1	0.6739	148.69	162.8
2,4-Dimethylpentane	108-08-7	C ₇ H ₁₆	100.202	−119.5	80.49	1	0.6727	148.95	162.8
3,3-Dimethylpentane	562-49-2	C ₇ H ₁₆	100.202	−134.4	86.06	1	0.6933	144.53	162.8
2,2,4-Trimethylpentane (Isooctane)	540-84-1	C ₈ H ₁₈	114.229	−107.3	99.22	1	0.6919	165.09	185.0
2,3,4-Trimethylpentane	565-75-3	C ₈ H ₁₈	114.229	−109.2	113.5	1	0.7191	158.85	185.0
<i>n</i> -Hexane	110-54-3	C ₆ H ₁₄	86.175	−95.35	68.73	1	0.6593	130.71	140.6
2-Methylhexane (Isoheptane)	591-76-4	C ₇ H ₁₆	100.202	−118.2	90.04	1	0.6786	147.66	162.8
3-Methylhexane	589-34-4	C ₇ H ₁₆	100.202	−119.4	92	1	0.6871	145.83	162.8
2,2,5-Trimethylhexane	3522-94-9	C ₉ H ₂₀	128.255	−105.7	124.09	1	0.7072	181.36	207.2
<i>n</i> -Heptane	142-82-5	C ₇ H ₁₆	100.202	−90.55	98.4	1	0.6837	146.56	162.8
2-Methylheptane	592-27-8	C ₈ H ₁₈	114.229	−109.02	117.66	1	0.698	163.65	185.0
3-Methylheptane	589-81-1	C ₈ H ₁₈	114.229	−120.48	118.9	1	0.7075	161.45	185.0
<i>n</i> -Octane	111-65-9	C ₈ H ₁₈	114.229	−56.82	125.67	1	0.70256	162.59	185.0
4-Methyloctane	2216-34-4	C ₉ H ₂₀	128.255	−113.3	142.4	1	0.7199	178.16	207.2
<i>n</i> -Nonane	111-84-2	C ₉ H ₂₀	128.255	−53.46	150.82	1	0.7177	178.70	207.2
<i>n</i> -Decane	124-18-5	C ₁₀ H ₂₂	142.282	−29.6	174.15	1	0.7301	194.88	229.4
<i>n</i> -Undecane	1120-21-4	C ₁₁ H ₂₄	156.309	−25.5	195.9	1	0.7402	211.17	251.6
<i>n</i> -Dodecane	112-40-3	C ₁₂ H ₂₆	170.334	−9.57	216.32	1	0.7487	227.51	273.8
<i>n</i> -Tridecane	629-50-5	C ₁₃ H ₂₈	184.361	−5.4	235.47	1	0.7564	243.73	296.0

(Continued)

TABLE 2.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MWg/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρg/cm ³ at 20°C	Molar volume, V _M cm ³ /mol	
								MW/ρ at 20°C	Le Bas
<i>n</i> -Tetradecane	629-59-4	C ₁₄ H ₃₀	198.388	5.82	253.58	1	0.7628	260.08	318.2
<i>n</i> -Pentadecane	629-62-9	C ₁₅ H ₃₂	212.415	9.95	270.6	1	0.7685	276.40	340.4
<i>n</i> -Hexadecane	544-76-3	C ₁₆ H ₃₄	226.441	18.12	286.86	1	0.77344	292.77	362.6
<i>n</i> -Heptadecane	629-78-7	C ₁₇ H ₃₆	240.468	22.0	302.0	1	0.7780	309.08	384.8
<i>n</i> -Octadecane	593-45-3	C ₁₈ H ₃₈	254.495	28.2	316.3	0.930	0.7819	325.48	407.0
<i>n</i> -Eicosane	112-95-8	C ₂₀ H ₄₂	282.547	36.6	343	0.769	0.7887	358.24	451.4
<i>n</i> -Tetracosane	646-31-1	C ₂₄ H ₅₀	338.654	50.4	391.3	0.563	0.7991	423.79	540.2
<i>n</i> -Hexacosane	630-01-3	C ₂₆ H ₅₄	366.707	56.1	412.2	0.495	0.8032	456.56	584.6
Cycloalkanes:									
Cyclopentane	287-92-3	C ₅ H ₁₀	70.133	-93.4	49.3	1	0.7454	94.09	99.5
Methylcyclopentane	96-37-7	C ₆ H ₁₂	84.159	-142.42	71.8	1	0.7487	112.41	121.7
1,1,3-Trimethylcyclopentane	4516-69-2	C ₈ H ₁₆	112.213	-142.4	104.9	1	0.7483	149.96	166.1
Propylcyclopentane	2040-96-2	C ₈ H ₁₆	112.213	-117.3	131	1	0.7763	144.55	166.1
Pentylcyclopentane	3741-00-2	C ₁₀ H ₂₀	140.266	-83	180	1	0.7912	177.28	210.5
Cyclohexane	110-82-7	C ₆ H ₁₂	84.159	6.59	80.73	1	0.7786	108.09	118.2
Methylcyclohexane	108-87-2	C ₇ H ₁₄	98.186	-126.6	100.93	1	0.7694	127.61	140.4
1,2- <i>cis</i> -Dimethylcyclohexane	2207-01-4	C ₈ H ₁₆	112.213	-49.8	129.8	1	0.7963	140.92	162.6
1,4- <i>trans</i> -Dimethylcyclohexane	2207-04-7	C ₈ H ₁₆	112.213	-36.93	119.4	1	0.7626	147.15	162.6
1,1,3-Trimethylcyclohexane	3073-66-3	C ₉ H ₁₈	126.239	-65.7	136.6	1	0.7664	165.72	184.8
Ethylcyclohexane	1678-91-7	C ₈ H ₁₆	112.213	-111.3	131.9	1	0.7880	142.40	162.6
Cycloheptane	291-64-5	C ₇ H ₁₄	98.186	-8.46	118.4	1	0.8098	121.25	136.4
Cyclooctane	292-64-8	C ₈ H ₁₆	112.213	14.59	149	1	0.8340	134.55	154.1
<i>cis</i> -Decalin	493-01-6	C ₁₀ H ₁₈	138.250	-42.9	195.8	1	0.8931	154.80	184.6
<i>trans</i> -Decalin	493-02-7	C ₁₀ H ₁₈	138.250	-30.4	187.3	1	0.8662	159.60	184.6
Alkenes:									
2-Methylpropene	115-11-7	C ₄ H ₈	56.107	-140.7	-6.9	1	0.5942	94.42	88.8
1-Butene	106-98-9	C ₄ H ₈	56.107	-185.34	-6.26	1	0.5951	94.28	88.8
2-Methyl-1-butene	563-46-2	C ₅ H ₁₀	70.133	-137.53	31.2	1	0.6504	107.83	111.0
3-Methyl-1-butene	563-45-1	C ₅ H ₁₀	70.133	-168.43	20.1	1	0.6272	111.82	111.0
2-Methyl-2-butene	513-35-9	C ₅ H ₁₀	70.133	-133.72	38.56	1	0.6623	105.89	111.0
1-Pentene	109-67-1	C ₅ H ₁₀	70.133	-165.12	29.96	1	0.6405	109.50	111.0
<i>cis</i> -2-Pentene	627-20-3	C ₅ H ₁₀	70.133	-151.36	36.93	1	0.6556	106.98	111.0
2-Methyl-1-pentene	763-29-1	C ₆ H ₁₂	84.159	-135.7	62.1	1	0.6799	123.78	133.2
4-Methyl-1-pentene	691-37-2	C ₆ H ₁₂	84.159	-153.6	53.9	1	0.6642	126.71	133.2

1-Hexene	592-41-6	C ₆ H ₁₂	84.159	-139.76	63.48	1	0.6732	125.01	133.2
1-Heptene	592-76-7	C ₇ H ₁₄	98.186	-118.9	93.64	1	0.6970	140.87	155.4
1-Octene	111-66-0	C ₈ H ₁₆	112.213	-101.7	121.29	1	0.7149	156.96	177.6
1-Nonene	124-11-8	C ₉ H ₁₈	126.239	-81.3	146.9	1	0.7292	173.12	199.8
1-Decene	872-05-9	C ₁₀ H ₂₀	140.266	-66.3	170.5	1	0.7408	189.34	222.0
Dienes:									
1,3-Butadiene	106-99-0	C ₄ H ₆	54.091	-108.91	-4.41	1	0.6211	87.09	81.4
2-Methyl-1,3-butadiene (Isoprene)	78-79-5	C ₅ H ₈	68.118	-145.9	34.0	1	0.6809	100.04	103.6
2,3-Dimethyl-1,3-butadiene	513-81-5	C ₆ H ₁₀	82.143	-76	68.8	1	0.7267	113.04	125.8
1,4-Pentadiene	591-93-5	C ₅ H ₈	68.118	-148.2	26	1	0.6608	103.08	103.6
1,5-Hexadiene	592-42-7	C ₆ H ₁₀	82.143	-140.7	59.4	1	0.6923	118.65	125.8
1,6-Heptadiene	3070-53-9	C ₇ H ₁₂	96.170	-129	90	1	0.714	134.69	148.0
Alkynes:									
1-Butyne	107-00-6	C ₄ H ₆	54.091	-125.7	8.08	1	0.650	83.22	81.4
1-Pentyne	627-19-0	C ₅ H ₈	68.118	-90	40.1	1	0.6901	98.71	103.6
1-Hexyne	693-02-7	C ₆ H ₁₀	82.143	-131.9	71.3	1	0.7155	114.81	125.8
1-Heptyne	628-71-7	C ₇ H ₁₂	96.170	-81	99.7	1	0.7328	131.24	148.0
1-Octyne	629-05-0	C ₈ H ₁₄	110.197	-79.3	126.3	1	0.7461	147.70	170.2
1-Nonyne	3452-09-3	C ₉ H ₁₆	124.223	-50	150.8	1	0.7568	164.14	192.4
Cycloalkenes:									
Cyclopentene	142-29-0	C ₅ H ₈	68.118	-135.0	44.2	1	0.772	88.24	92.1
Cyclohexene	110-83-8	C ₆ H ₁₀	82.143	-103.5	82.98	1	0.8110	101.29	110.8
1-Methylcyclohexene	591-49-1	C ₇ H ₁₂	96.170	-120.4	110.3	1	0.8102	118.70	133.0
Cycloheptene	628-92-2	C ₇ H ₁₂	96.170	-56	115	1	0.8228	116.88	129.0
<i>cis</i> -Cyclooctene	931-87-3	C ₈ H ₁₄	110.197	-12	138	1	0.8472	130.07	146.7
<i>trans</i> -Cyclooctene	931-89-5	C ₈ H ₁₄	110.197	-59	143	1	0.8483	129.90	146.7
1,4-Cyclohexadiene	628-41-1	C ₆ H ₈	80.128	-49.2	85.5	1	0.8471	94.59	103.4
1,3,5-Cycloheptatriene	544-25-2	C ₇ H ₈	92.139	-79.5	117	1	0.8875	103.82	114.2
<i>d</i> -Limonene	5989-27-5	C ₁₀ H ₁₆	136.234	-74.0	178	1	0.8403	162.13	192.2
α -Pinene	80-56-8	C ₁₀ H ₁₆	136.234	-64	156.2	1	0.8582	158.74	183.7
β -Pinene	127-91-3	C ₁₀ H ₁₆	136.234	-61.5	166	1	0.8694	156.70	183.7

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

TABLE 2.2.2

Summary of selected physical-chemical properties of aliphatic and cyclic hydrocarbons at 25°C

Compound	Selected properties					log K _{ow}	Henry's law constant H/(Pa·m ³ /mol) calculated P/C
	Vapor pressure		Solubility				
	P ^s /Pa	P _L /Pa	S/(g/m ³)	C ^s /(mol/m ³)	C _L /(mol/m ³)		
Alkanes:							
Isobutane (2-Methylpropane)	357000	357000	48.9	0.8413	0.8413	2.76	120435*
2,2-Dimethylpropane	172000	172000	33.2	0.4602	0.4602	3.11	220195*
<i>n</i> -Butane	243000	243000	61.4	1.0564	1.0564	2.90	95915*
2-Methylbutane (Isopentane)	91640	91640	47.8	0.6625	0.6625	2.30	138320
2,2-Dimethylbutane	42600	42600v	18.4	0.2135	0.2135	3.82	199515
2,3-Dimethylbutane	32010	32010	19.1	0.2216	0.2216	3.85	144422
2,2,3-Trimethylbutane	13652	13652	4.38	0.0437	0.0437		312320
<i>n</i> -Pentane	68400	68400	38.5	0.5336	0.5336	3.45	128180
2-Methylpentane (Isohexane)	28200	28200	13.8	0.1601	0.1601	2.80	176097
3-Methylpentane	25300	25300	12.8	0.1485	0.1485	3.60	170330
2,2-Dimethylpentane	14000	14000	4.4	0.0439	0.0439	3.10	318825
2,4-Dimethylpentane	13100	13100	4.06	0.0405	0.0405	3.10	323312
3,3-Dimethylpentane	10940	10940	5.94	0.0593	0.0593		184550
2,2,4-Trimethylpentane (Isooctane)	6560	6560	2.44	0.0214	0.0214		307110
2,3,4-Trimethylpentane	3600	3600	2.0	0.0119	0.0119		205614
<i>n</i> -Hexane	20200	20200	9.5	0.1102	0.1102	4.11	183235
2-Methylhexane (Isoheptane)	8780	8780	2.54	0.0253	0.0253		346370
3-Methylhexane	8210	8210	3.3	0.0329	0.0329		249290
2,2,5-Trimethylhexane	2210	2210	1.15	0.0090	0.0090	4.50	246472
<i>n</i> -Heptane	6110	6110	2.93	0.0292	0.0292	5.00	208955
2-Methylheptane	2600	2600	0.85	0.00744	0.0074		349410
<i>n</i> -Octane	1800	1800	0.66	0.005778	0.0058	5.15	311536
<i>n</i> -Nonane	571	571	0.22	0.001715	0.0017	5.65	332880
<i>n</i> -Decane	175	175	0.052	0.000365	0.00037	6.25	478840
<i>n</i> -Undecane	52.2	52.2	0.004	0.000026	0.000026		2039835
<i>n</i> -Dodecane	18.02	18.02	0.0037	0.000022	0.000022	6.80	829570
<i>n</i> -Tridecane	6.682	6.682					
<i>n</i> -Tetradecane	1.804	1.804				8.00	
<i>n</i> -Hexadecane	0.191	0.191					
<i>n</i> -Heptadecane	0.0615	0.0615					
<i>n</i> -Octadecane	0.02	0.019					

<i>n</i> -Eicosane	0.00209	0.00161					
Cycloalkanes:							
Cyclopentane	42400	42400	166	2.3669	2.3669	3.00	17915
Methylcyclopentane	18300	18300	43	0.5109	0.5109	3.37	35815
1,1,3-Trimethylcyclopentane	5300	5300	3.73	0.0332	0.0332		159440
Propylcyclopentane	1640	1640	2.04	0.0182	0.0182		90210
Pentylcyclopentane	152	152	0.115	0.0008	0.0008		185395
Cyclohexane	13014	13014	58	0.6892	0.6892	3.44	18885
Methylcyclohexane	6180	6180	15.1	0.1538	0.1538	3.88	40185
1,2- <i>cis</i> -Dimethylcyclohexane	1930	1930	6	0.0535	0.0535		36095
1,4- <i>trans</i> -Dimethylcyclohexane	3020	3020	3.84	0.0342	0.0342		88250
1,1,3-Trimethylcyclohexane	1480	1480	1.77	0.0140	0.0140		105560
Cycloheptane	2924	2924	23.5	0.2393	0.2393		12220
Cyclooctane	748	748	5.80	0.0517	0.0517	4.45	14470
Alkenes:							
2-Methylpropene	304000	304000	263	4.6875	4.6875		21620*
1-Butene	297000	297000	222	3.9567	3.9567		25610*
2-Methyl-1-butene	81330	81330					
3-Methyl-1-butene	120000	120000	130	1.8536	1.8536		54670*
2-Methyl-2-butene	62410	62410	325	4.634	4.634		13470
1-Pentene	85000	85000	148	2.1103	2.1103	2.20	40280
<i>cis</i> -2-Pentene	66000	66000				2.20	
2-Methyl-1-pentene	26000	26000	78	0.9268	0.9268		28050
4-Methyl-1-pentene	36100	36100	48	0.5703	0.5703	2.50	63295
1-Hexene	24800	24800	50	0.5941	0.5941	3.39	41743
1-Heptene	7510	7510	18.3	0.1864	0.1864	3.99	40295
1-Octene	2320	2320	2.7	0.0241	0.0241	4.57	96420
1-Nonene	712	712	1.12	0.0089	0.0089	5.15	80250
1-Decene	218	218					
Dienes:							
1,3-Butadiene	281000	281000	735	13.588	13.588	1.99	7458*
2-Methyl-1,3-butadiene (Isoprene)	73300	73300	642	9.4248	9.4248		7780
2,3-Dimethyl-1,3-butadiene	20160	20160	327	3.9809	3.9809		5065
1,4-Pentadiene	98000	98000	558	8.1917	8.1917	2.48	11965
1,5-Hexadiene	29690	29690	169	2.0574	2.0574	2.75	14430
1,6-Heptadiene			44	0.4575	0.4575		

(Continued)

TABLE 2.2.2 (Continued)

Compound	Selected properties					log K _{ow}	Henry's law constant H/(Pa·m ³ /mol) calculated P/C
	Vapor pressure		Solubility				
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		
Alkynes:							
1-Butyne	188000	188000	2870	53.059	53.059		1910*
1-Pentyne	57600	57600	1570	23.048	23.048	1.98	2500
1-Hexyne	18140	18140	360	4.3830	4.3830	2.73	4140
1-Heptyne	7500	7000	94	0.9774	0.9774	2.98	7675
1-Octyne	1715	1715	24	0.2178	0.2178		7875
1-Nonyne			7.2	0.0580	0.0580		
Cycloalkenes:							
Cyclopentene	50710	50706	535	7.8540	7.8540	2.48	6455
Cyclohexene	11850	11850	213	2.5928	2.5928	2.86	4570
1-Methylcyclohexene	4689	4689	52	0.5407	0.5407		8670
Cycloheptene	2670	2670	66	0.6863	0.6863		3890
Cyclooctene	1010	1010	22.9	0.2078	0.2078	2.47	4860
1,4-Cyclohexadiene	9009	9009	800	9.9840	9.9840		902
1,3,5-Cycloheptatriene	3140	3140	620	7.7376	7.7376	2.63	467
<i>d</i> -Limonene	270	270	13.8	0.1013	0.1013		2665
α-Pinene	582	582					
β-Pinene	395	395					

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H/(Pa·m³/mol) = 101325 Pa/C^s mol/m³.

TABLE 2.2.3

Suggested half-life classes of hydrocarbons in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Alkanes:				
<i>n</i> -Pentane	2	5	6	7
<i>n</i> -Hexane	2	5	6	7
<i>n</i> -Octane	2	5	6	7
<i>n</i> -Decane	2	5	6	7
<i>n</i> -Dodecane	2	5	6	7
Cycloalkanes:				
Cyclopentane	2	5	5	6
Methylcyclopentane	2	5	5	6
Cyclohexane	2	5	5	6
Methylcyclohexane	2	5	5	6
Cyclooctane	2	5	5	6
Alkenes:				
1-Pentene	1	4	5	6
1-Octene	1	4	5	6
1,3-Butadiene	1	4	5	6
1,4-Pentadiene	1	4	5	6
Alkynes:				
1-Hexyne	1	4	5	6
Cycloalkenes:				
Cyclopentene	1	4	5	6
Cyclohexene	1	4	5	6

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

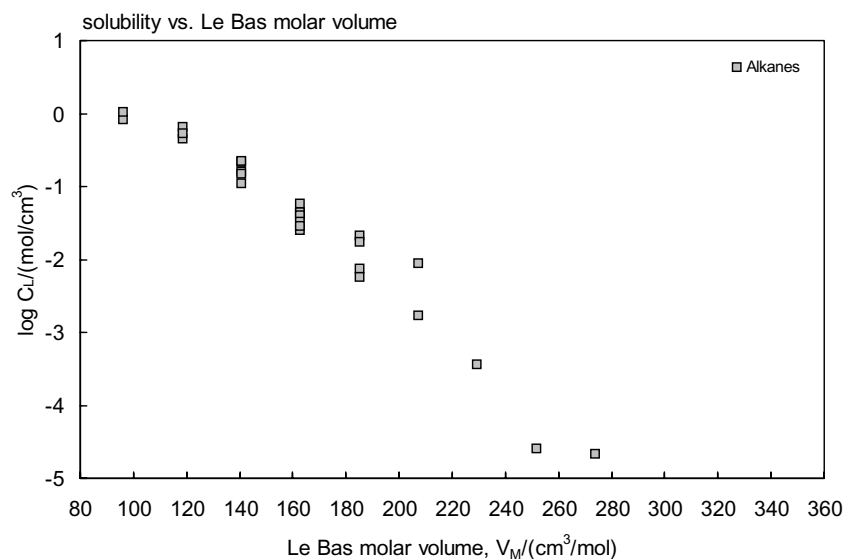


FIGURE 2.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alkanes.

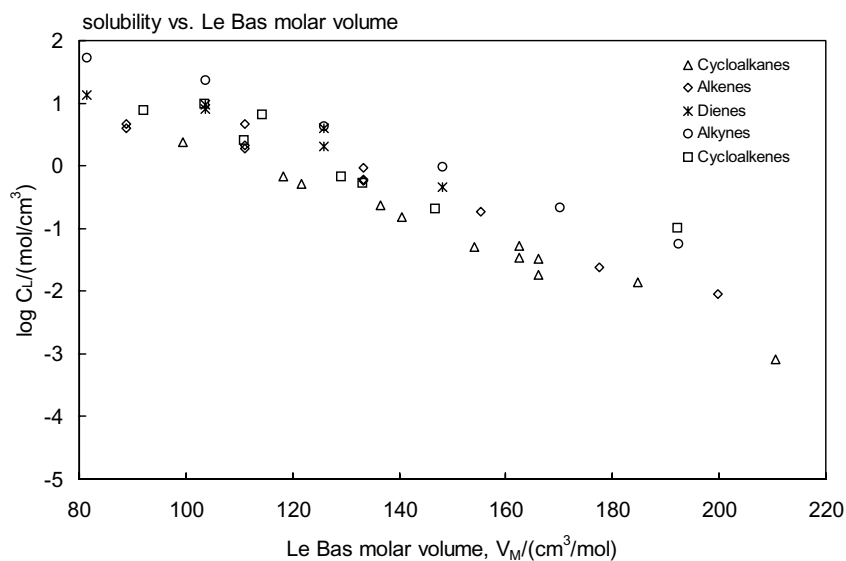


FIGURE 2.2.2 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.

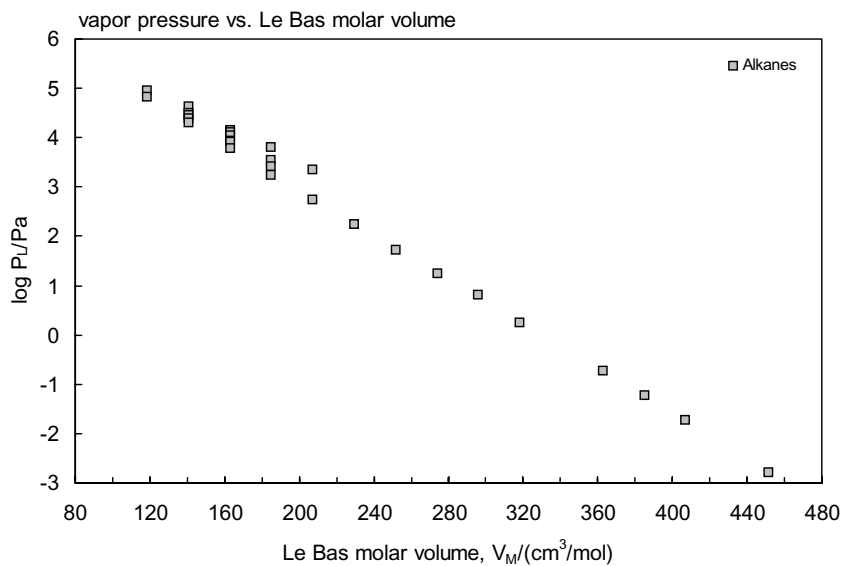


FIGURE 2.2.3 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alkanes.

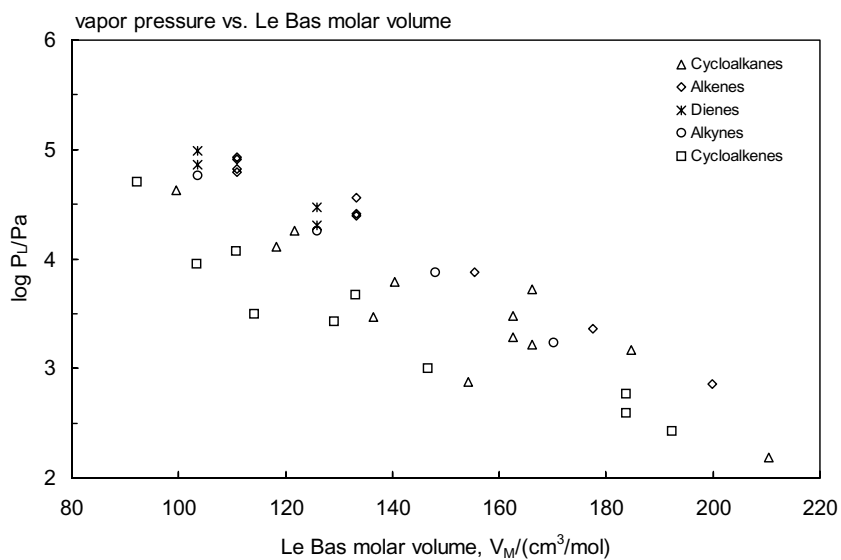


FIGURE 2.2.4 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.

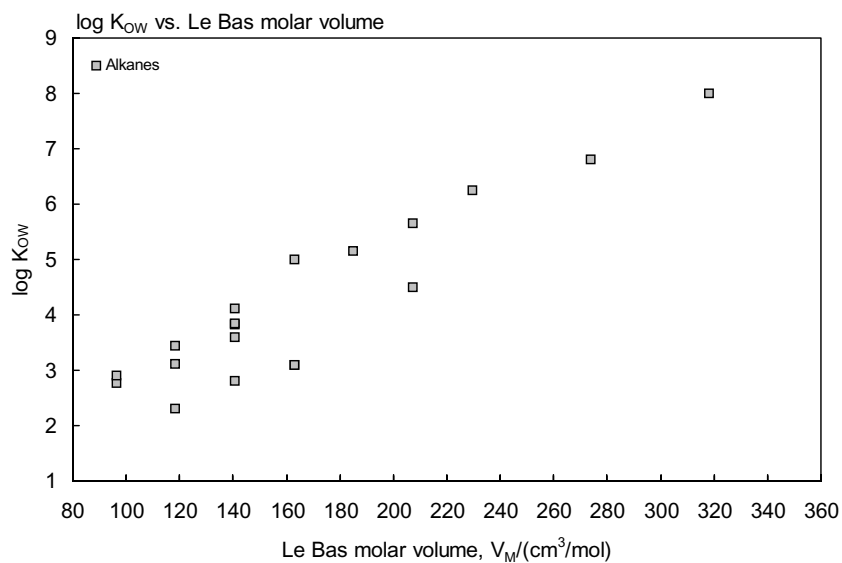


FIGURE 2.2.5 Octanol-water partition coefficient versus Le Bas molar volume for alkanes.

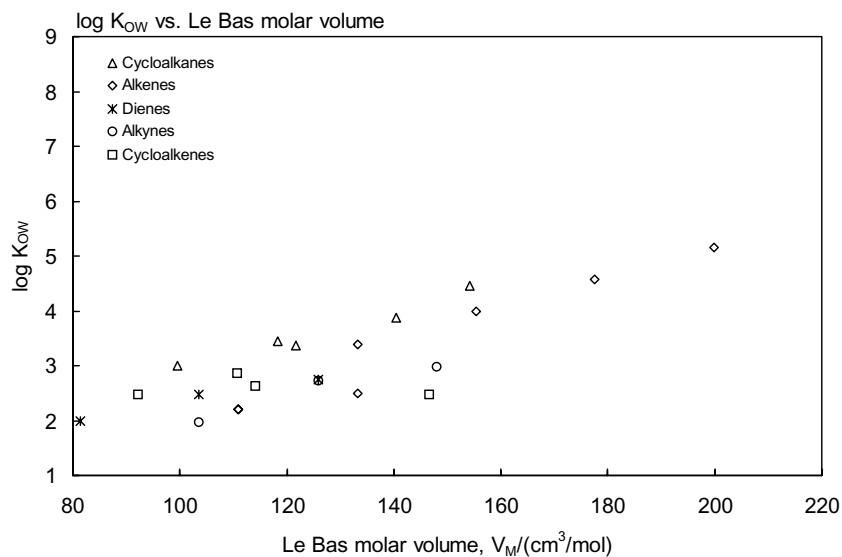


FIGURE 2.2.6 Octanol-water partition coefficient versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.

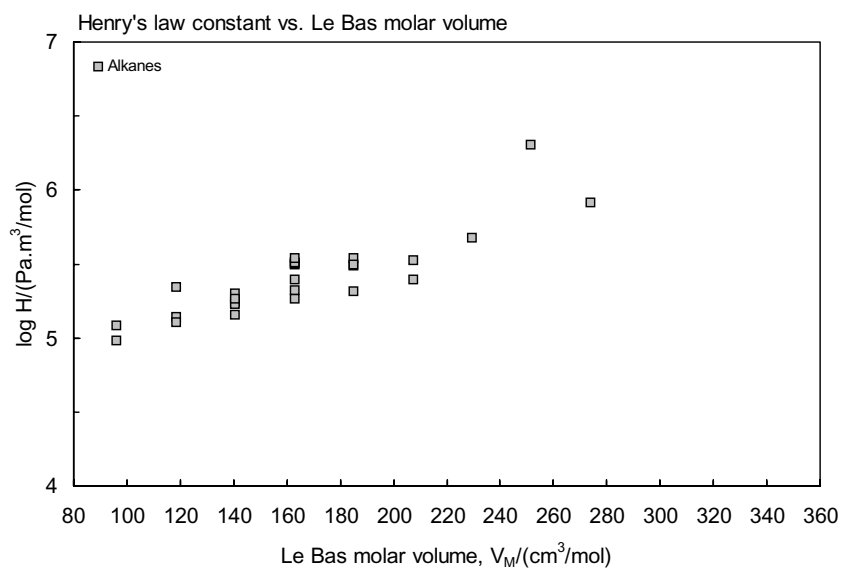


FIGURE 2.2.7 Henry's law constant versus Le Bas molar volume for alkanes.

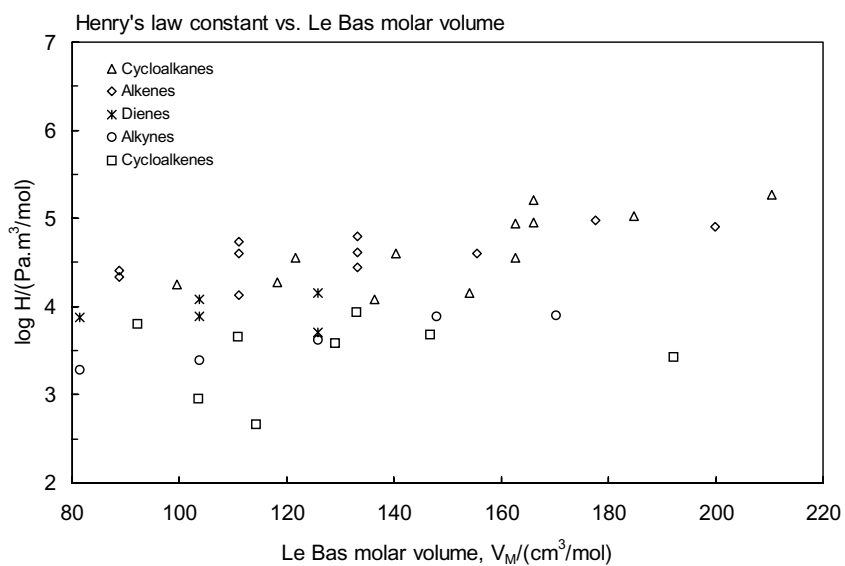


FIGURE 2.2.8 Henry's law constant versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.

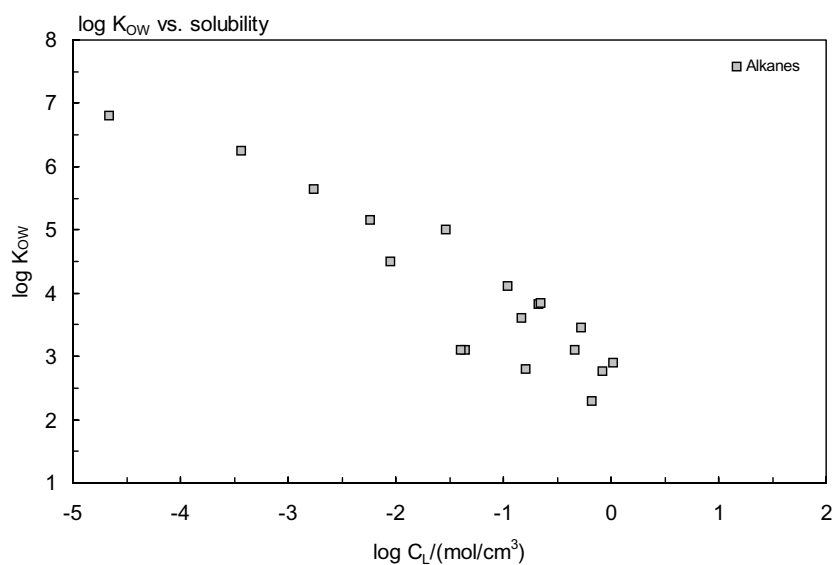


FIGURE 2.2.9 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alkanes.

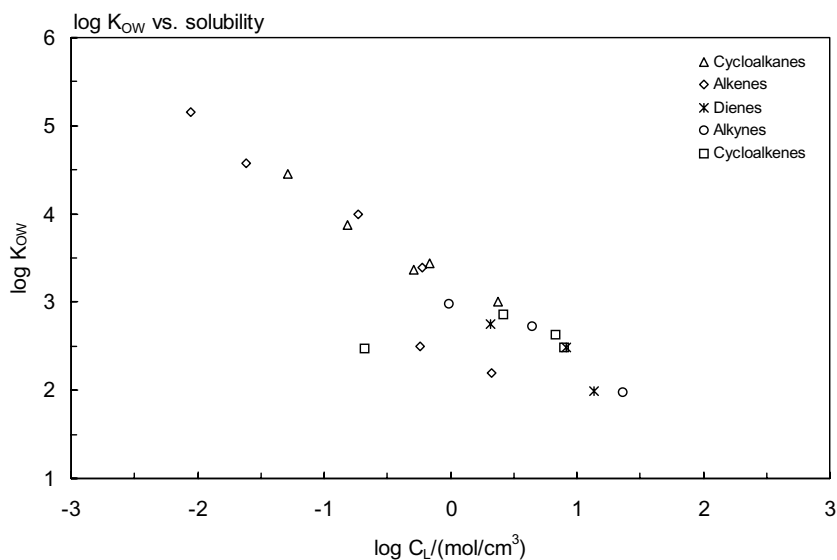


FIGURE 2.2.10 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for aliphatic and cyclic hydrocarbons.

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3 Mononuclear Aromatic Hydrocarbons

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3.1 LIST OF CHEMICALS AND DATA COMPILATIONS

3.1.1 MONONUCLEAR AROMATIC HYDROCARBONS

3.1.1.1 Benzene



Common Name: Benzene

Synonym: benzol, cyclohexatriene

Chemical Name: benzene

CAS Registry No: 71-43-2

Molecular Formula: C_6H_6

Molecular Weight: 78.112

Melting Point ($^{\circ}C$):

5.49 (Lide 2003)

Boiling Point ($^{\circ}C$):

80.09 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8765 (Weast 1982–1983)

Molar Volume (cm^3/mol):

89.1 ($20^{\circ}C$, calculated from density)

96.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

33.843, 30.726 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

9.916 (Tsonopoulos & Prausnitz 1971)

9.866 (Riddick et al. 1986)

9.87 (exptl., Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

35.564 (Tsonopoulos & Prausnitz 1971)

35.4, 44.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1850 ($30^{\circ}C$, shake flask-interferometer, Gross & Saylor 1931)

1786 (shake flask-turbidimetric method, Stearns et al. 1947)

1402 (residue-volume method, Booth & Everson 1948)

1740 (shake flask-UV spec., Andrews & Keefer 1949)

1860 (shake flask-UV, Klevens 1950)

1790* (shake flask-UV, Bohon & Claussen 1951)

1755 (shake flask-UV, McDevit & Long 1952)

1718 (shake flask-UV, Morrison & Billett 1952)

1796 (Hayashi & Sasaki 1956; quoted, Keeley et al. 1988)

1780, 1823 (selected, calculated-molar volume, Lindenburg 1956; quoted, Horvath 1982)

1760 (Brady & Huff 1958)

1740* (shake flask-UV, measured range $0.4\text{--}45^{\circ}C$, Arnold et al. 1958)

$S/(wt.\%) = 0.1806 - 0.001095 \cdot (t/^{\circ}C) + 3.170 \times 10^{-5} \cdot (t/^{\circ}C)^2$; temp range $5\text{--}45^{\circ}C$ (shake flask-UV, Arnold et al. 1958); or

$S/(wt.\%) = 0.1784 - 0.0007436 \cdot (t/^{\circ}C) + 1.1906 \times 10^{-5} \cdot (t/^{\circ}C)^2 + 1.217 \times 10^{-7} \cdot (t/^{\circ}C)^3$; temp range $5\text{--}45^{\circ}C$ (shake flask-UV, Arnold et al. 1958)

1800* ($24^{\circ}C$, shake flask-UV, measured range $0.8\text{--}64.5^{\circ}C$, Alexander 1959)

1890 ($35^{\circ}C$, shake flask-UV spectrophotometry, Hine et al. 1962)

1742* (shake flask-UV, measured range $17\text{--}63^{\circ}C$, Franks et al. 1963)

- 1780 (shake flask-GC, McAuliffe 1963, 1966)
- 2100* (20°C, polythermic method, measured range 20–79.5°C, Udovenko & Aleksandrova 1963)
- 1778 (calculated-group contribution, Irmann 1965; quoted, Horvath 1982)
- 2167 (vapor saturation-UV, Worley 1967)
- 1740 (21°C, extraction by nonpolar resins/elution, Chey & Calder 1972)
- 1765* (shake flask-GC, measured range 4–25°C, Leinonen 1972)
- 1830* (shake flask-UV spectroscopy, measured range 25–55°C, Bradley et al. 1973)
- 1755 (shake flask-GC, Polak & Lu 1973)
- 1755* (shake flask-GC, measured range 25–84.7°C, Price 1973)
- 1765 (shake flask-GC, Leinonen & Mackay 1973)
- 1760* (shake flask-UV, measured range 4.5–20.1°C, Brown & Wasik 1974)
- 1906 (shake flask-UV, Vesala 1974)
- 1769 (shake flask-GC, Mackay et al. 1975)
- 1780 (shake flask-GC, Mackay & Shiu 1975)
- 1740 (shake flask-GC, Price 1976)
- 1791* (generator column-HPLC/UV, May et al. 1978; May 1980)
- $S/(\mu\text{g/kg}) = [1833 + 0.3166 \cdot (t/^\circ\text{C})^2 - 0.6838 \cdot (t/^\circ\text{C})^3] \times 10^3$; temp range 0.2–25.8°C (generator column-HPLC/UV, May et al. 1978, 1980)
- $\log x = 424.544/(T/K)^2 - 2955.82/(T/K) + 1.6606$; temp range 0–55°C (Ueda et al. 1978)
- 1769 (shake flask-fluorescence spectrophotometry, Aqun-Yuen et al. 1979)
- 1734* (20°C, shake flask-UV, Ben-Naim & Wilf 1979)
- 1790* (20°C, shake flask-GC, Bittrich et al. 1979)
- 1820–1930 (elution chromatography-UV, Schwarz 1980)
- 1750 (shake flask-LSC, Banerjee et al. 1980)
- 1610* (vapor saturation-UV spec., measured range 5–45°C, Sanemasa et al. 1981)
- 1787 (shake flask-GC, Chiou et al. 1982; 1983)
- 1620* (vapor saturation-UV spec., measured range 5–45°C, Sanemasa et al. 1982)
- 1792* (generator column-HPLC/UV, May et al. 1983)
- 1789 (generator column-HPLC, Wasik et al. 1983)
- 1809 (HPLC- k' correlation, converted from reported γ_w , Hafkenschied & Tomlinson 1983a)
- 1617 (vapor saturation-UV spec., Sanemasa et al. 1984)
- 1810 (shake flask-radiometric method, Lo et al. 1986)
- 1695 (shake flask-GC, Keeley et al. 1988)
- 1650 (shake flask-GC, Coutant & Keigley 1988)
- 1770* (IUPAC recommended, temp range 0–70°C, Shaw 1989a)
- $S/(\text{g}/100 \text{ g soln}) = 5.5773 - 4.6067 \times 10^{-2} \cdot (T/K) + 1.2504 \times 10^{-4} \cdot (T/K)^2 - 1.0489 \times 10^{-7} \cdot (T/K)^3$; temp range 0–70°C (summary of literature data, Shaw 1989a)
- 1732* (20°C, activity coefficient-GC, Cooling et al. 1992)
- 1840* (30°C, equilibrium flow cell-GC, measured range 30–100°C, Chen & Wagner 1994a)
- $\ln(1/x) = -6.191 + 14.03 \cdot [(T/K)/562.2]^{-1} - 3.511 \cdot [(T/K)/562.2]^{-2}$; temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994a)
- $\ln x = 6.191 - 14.03 \cdot (T_r/K)^{-1} + 3.511 \cdot (T_r/K)^{-2}$, $T_r = T/T_c$, the reduced temp, system temp T divided by critical temp T_c (Chen & Wagner 1994c)
- 1760 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
- $\ln x = -15.544647 - 1442.4276/(T/K) - 3.283 \times 10^{-5} \cdot (T/K)^2$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
- $\ln x = -180.368 + 7524.83/(T/K) + 25.8585 \cdot \ln(T/K)$; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 12654 (Hg manometer, Hovorka & Dreisbach 1934)
- 9960* (20°C, manometer, measured range 0–50°C, Stuckey & Saylor 1940)
- $\log(P/\text{mmHg}) = 7.12491 - 1323.06/(T/K - 41.23)$; temp range 0–75°C (manometer, Stuckey & Saylor 1940)

- 11700* (23.7°C, ebulliometry-manometer, measured range 14.5–80.9°C, Willingham et al. 1945)
 $\log (P/\text{mmHg}) = 6.89324 - 1203.835/(219.924 + t/^\circ\text{C})$; temp range 14.5–80.9°C (ebulliometry-manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
- 13332* (26.1°C, summary of literature data, Stull 1947)
- 11720* (23.27°C, ebulliometry, measured range 10.9–80.9°C, Forziati et al. 1949)
 $\log (P/\text{mmHg}) = 6.91210 - 1214.645/(221.205 + t/^\circ\text{C})$; temp range 10.9–80.9°C (ebulliometry-manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
- 12690 (interpolated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 6.90565 - 1211.033/(220.79 + t/^\circ\text{C})$; temp range 0–160°C (Antoine eq. for liquid state, Dreisbach 1955)
- 23450* (39.093°C, summary of literature data, temp range 7.565–260°C, Bond & Thodos 1960)
- 545800* (146.85°C, ebulliometry, measured range 146.85–286.85°C, Ambrose et al. 1967)
- 32045* (46.85°C, summary of literature data, temp range 46.85–286.85°C, Ambrose et al. 1970)
- 12700* (extrapolated-Antoine eq., Zwolinski & Wilhoit, 1971)
 $\log (P/\text{mmHg}) = 6.90565 - 1211.033/(220.790 + t/^\circ\text{C})$; temp range –11.6 to 103.92°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 12680 (extrapolated, Antoine eq., Boublik et al. 1973; 1984)
 $\log (P/\text{mmHg}) = [-0.2185 \times 10254.2/(T/\text{K})] + 9.5560$; temp range –58 to –30°C (Antoine eq., Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 8146.5/(T/\text{K})] + 7.833714$; temp range –36.7 to 290.3°C (Antoine eq., Weast 1972–73)
- 12339* (24.396°C, ebulliometry, measured range 19.071–32.467°C, Osborn & Scott 1978)
- 19933* (32.182°C, ebulliometry, measured range 32.182–115.697°C, Scott & Osborn 1979)
- 12640* (average, ebulliometry-bubble cap boilers, measured range 290–378 K, Ambrose 1981)
- 12100 (gas saturation-GC, Politzki et al. 1982)
 $\log (P/\text{atm}) = (1 - 353.214/T) \times 10^{(0.832632 - 6.72598 \times 10^4 \cdot T + 6.38324 \times 10^7 \cdot T^2)}$; T in K, temp range 280.0–562.6 K (Cox vapor pressure eq., Chao et al. 1983)
- 12690, 12680 (interpolated-Antoine equations, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.01905 - 1204.637/(220.069 + t/^\circ\text{C})$; temp range 21.2–105°C (Antoine eq. from reported exptl. data of Ambrose 1981, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.01788 - 1203.677/(219.904 + t/^\circ\text{C})$; temp range 14.5–80.9°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
- 12690 (extrapolated, Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 9.1064 - 1885.9/(244.2 + t/^\circ\text{C})$; temp range –12 to 3°C (Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 6.90565 - 1211.033/(220.79 + t/^\circ\text{C})$; temp range 8–103°C (Antoine eq., Dean 1985, 1992)
- 12716 (headspace-GC, Hussam & Carr 1985)
 $\log (P/\text{kPa}) = 6.02232 - 1206.33/(220.91 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
- 12700 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 10.0091 - 2836/(25.31 + T/\text{K})$; temp range 223–279 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 8.45261 - 1986.69/(-23.089\text{C} + T/\text{K})$; temp range 218–279 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.01907 - 1204.682/(-53.072 + T/\text{K})$; temp range 279–377 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.06832 - 1236.034/(-48.99 + T/\text{K})$; temp range 353–422 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.3607 - 1466.083/(-15.44 + T/\text{K})$; temp range 420–502 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.51922 - 2809.514/(171.489 + T/\text{K})$; temp range 501–562 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
- 13100* (gas saturation, measured range –15.4 to 40°C, Liu & Dickhut 1994)
 $\log (P/\text{mmHg}) = 31.7718 - 2.7254 \times 10^3/(T/\text{K}) - 8.4442 \cdot \log (T/\text{K}) - 5.3534 \times 10^{-9} \cdot (T/\text{K}) + 2.7187 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 279–562 K (vapor pressure eq., Yaws 1994)
 $\log (P/\text{kPa}) = 6.02994 - 1211.033/[(T/\text{K}) - 52.36]$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 653 (30°C, concn ratio-UV, Saylor et al. 1938)
 576 (Taha et al. 1966)
 442* (20.06°C, headspace-GC, Brown & Wasik 1974)
 $\ln [H/(\text{Pa m}^3/\text{mol})] = 21.26071 - 4445.58/(T/K)$; temp range 4.5–20°C (regression eq. of exptl. data of Brown & Wasik 1974, Shiu & Ma 2000)
 555, 530 (calculated as $1/K_{AW}$, calculated-bond contribution, Hine & Mookerjee 1975)
 551 (headspace-GC, Vitenberg et al. 1975)
 562, 556 (batch air stripping-GC, calculated-P/C, Mackay et al. 1979)
 552* (shake flask-concn. ratio-UV, measured range 10–30°C, Green & Frank 1979)
 $\log (H/\text{atm}) = 8.58 - 1852.308/(T/K)$; temp range 10–30°C (shake flask-concn-UV, Green & Frank 1979)
 $\ln (H/\text{atm}) = 8.58 - 1852.038/(T/K)$ (Kavanaugh & Trussell 1980)
 554* (equilibrium cell-concentration ratio-GC/FID, Leighton & Calo 1981)
 $\ln (k_H/\text{atm}) = 19.02 - 3964/(T/K)$; temp range 1.0–27.2°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
 610* (vapor-liquid equilibrium-GC, measured range 15–45°C, Sanemasa et al. 1981)
 608* (vapor-liquid equilibrium-GC, measured range 5–45°C, Sanemasa et al. 1982)
 562 (gas stripping-GC, Warner et al. 1987)
 740; 441 (20°C, EPICS-GC, calculated-P/C, Yurteri et al. 1987)
 535; 588; 557; 554; 555 (EPICS-GC/FID; batch air stripping-GC; calculated P/C; direct concentration ratio; calculated-UNIFAC, Ashworth et al. 1988)
 535* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 5.534 - 3194/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 586 (concentration ratio, Keeley et al. 1988)
 555 (infinite activity coeff. γ^∞ from solubility measurement, Abraham et al. 1990)
 564 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 570* (extrapolated from equilibrium headspace-GC data, measured range 40–80°C, Ettre et al. 1993)
 $\log (1/K_{AW}) = -2.1678537 + 836.2228/(T/K)$; temp range: 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)
 569 (infinite activity coeff. γ^∞ in water determined by inert gas stripping-GC, Li et al. 1993)
 604* (equilibrium headspace-GC, measured range 10–30°C, Perlinger et al. 1993)
 535* (static headspace-GC, measured range 25–50°C, Robbins et al. 1993)
 644 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
 488 (23°C, gas stripping-IR, Nielsen et al. 1994)
 481* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)
 267, 612 (6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35‰, Dewulf et al. 1995)
 $\ln K_{AW} = -3640/(T/K) + 0.00786 \cdot Z + 10.577$; with Z salinity 0–35.5‰, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)
 552* (25.4°C, gas stripping-HPLC/UV/fluorescence, Alaei et al. 1996)
 $\ln [H/(\text{Pa m}^3/\text{mol})] = 21.87689 - 4672.28/(T/K)$; temp range: 4–34.9°C and enthalpy of volatilization $\Delta H_{vol} = 32.2 \text{ kJ/mol}$ at 20°C; (gas stripping-HPLC/UV measurements, Alaei et al. 1996)
 485 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 640* (vapor-liquid equilibrium-GC, measured range 10–35°C, Turner et al. 1996)
 $K_{AW} = 0.0763 + 0.00211 \cdot (T/K) + 0.000162 \cdot (T/K)^2$; temp range 0–50°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)
 538* (headspace equilibrium-GC, Peng & Wan 1997)
 $\ln K_{AW} = 7.15 - 1397/(T/K)$; temp range 15–45°C (headspace equilibrium-GC, Peng & Wan 1997)
 272 (gas stripping-GC, Altschuh et al. 1999)
 439 (20°C, headspace equilibrium-GC, Peng & Wan 1998)
 $\ln K_{AW} = 7.44 - 1448/(T/K)$; temp range 0–45°C (seawater with salinity of 36‰, headspace-GC, Peng & Wan 1998)
 466 (21°C, headspace equilibrium-GC, de Wolf & Lieder 1998)
 558 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 580.6 (modified EPICS method-GC, Ryu & Park 1999)
 556 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)
 466 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

- $\log K_{AW} = 5.053 - 1693/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
 538* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)
 $\ln K_{AW} = 8.1648 - 2889.4/(T/K)$; temp range 15–40°C (SPME-GC, Bierwagen & Keller 2001)
 573.4* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
 $\ln K_{AW} = 10.01 - 3430.4/(T/K)$; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)
 514–606 (27°C, headspace equilibrium-GC, at different solute concn: 0.48–19.1 mg/L, measured temp range 300–315 K, Cheng et al. 2003)
 558* (headspace-GC, measured range 10–25°C, Bakierowska & Trzeszczyński 2003)
 $\ln (1/K_{AW}) = 11.663 - 3920/(T/K)$; temp range 10–25°C, headspace-GC, Bakierowska & Trzeszczyński 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 2.13 (shake flask-UV, Fujita et al. 1964)
 1.56, 1.65 (shake flask-UV, calculated-M.O. indices, Rogers & Cammarata 1969)
 2.13 (calculated-fragment const., Rekker 1977)
 2.13, 1.56, 2.15, 2.03, 2.04 (Hansch & Leo 1979)
 2.39 (HPLC-RT correlation, Veith et al. 1979a)
 2.12 (shake flask-LSC, Banerjee et al. 1980)
 2.28 (HPLC- k' correlation, Hanai et al. 1981)
 2.11 (HPLC-RT correlation, McDuffie 1981)
 2.43 (HPLC- k' correlation, McDuffie 1981)
 2.16 (HPLC- k' correlation, D'Amboise & Hanai 1982)
 2.13 (shake flask-GC, Watarai et al. 1982)
 2.20 (shake flask-HPLC, Hammers et al. 1982)
 2.18 (HPLC- k' correlation, Miyake & Terada 1982)
 2.02 (shake flask method, Eadsforth & Moser 1983)
 2.38 (HPLC method, Eadsforth & Moser 1983)
 2.10 (shake flask-GC, Platford 1983)
 2.48 (HPLC-RT correlation, Swann et al. 1983)
 2.10 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983b)
 2.04 (HPLC-RV correlation, Garst 1984)
 2.25 (RP-HPLC- k' correlation, Rapaport & Eisenreich 1984)
 2.13 (generator column-GC/ECD, Miller et al. 1984)
 2.26 (HPLC- k' correlation, De Kock & Lord 1987)
 2.01 (generator column-reversed phase-LC, Schantz & Martire 1987)
 2.16 (RP-HPLC-capacity factor correlation, Sherblom & Eganhouse 1988)
 1.91 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
 2.13 (recommended, Sangster 1989, 1993)
 2.186 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 2.21 (normal phase-HPLC- k' correlation, Govers & Evers 1992)
 2.13 (recommended, Hansch et al. 1995)
 1.97* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 2.90* (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.290–50.28°C, Gruber et al. 1997)
 2.80 (head-space GC-FID both phases, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 0.64 (pacific herring, Korn et al. 1977)
 0.54 (eels, Ogata & Miyake 1978; Ogata et al. 1984)
 1.10 (fathead minnow, Veith et al. 1980)
 1.48, 1.0 (algae, fish, Freitag et al. 1984)
 1.48 (algae, Geyer et al. 1984)
 0.63 (gold fish, Ogata et al. 1984)

- < 1.0, 3.23 (fish, activated sludge, Freitag et al. 1985)
 0.54, 0.64, 0.63; 1.38 (selected: eels, pacific herring, gold fish; calculated, Howard 1990)
 1.63 (*S. capricornutum*, Herman et al. 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 1.92 (sediment, sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
 1.63; 1.82 (Hastings soil pH 5.6; Overton soil pH 7.8, batch equilibrium, Rogers et al. 1980)
 1.78 (average of 17 sediments and soils, sorption isotherms by batch equilibrium, Karickhoff 1981)
 1.58; 1.73; 1.64 (forest soil pH 5.6; forest soil pH 4.2; agricultural soil pH 7.4, Seip et al. 1986)
 1.42 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
 1.34 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.08, 2.04 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.65, 2.59, 2.25 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.69, 2.66 (organic cations HDTMA treated soils: St. Clair soil B_t horizon OC 3.25%; Oshtemo soil B_t horizon OC 0.83%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 1.89 (aquifer material with f_{OC} of 0.006 and measured partition coeff. $K_p = 0.47$ mL/g., Abdul et al. 1990)
 1.58, 1.49 (Riddles soil top layer, pH 5.0; below top layer pH 5.3, batch equilibrium, Boyd et al. 1990)
 1.82, 1.87 (RP-HPLC- k' correlation, humic acid-silica column, Szabo et al. 1990a,b)
 1.74; 1.81 (Captina silt loam pH 4.97; McLaurin sandy loam pH 4.43, batch equilibrium, Walton et al. 1992)
 1.75 (average of 5 soils, sorption isotherms by batch equilibrium method-GC, Xing et al. 1994)
 1.96 (soil, calculated-molecular connectivity indices, Sabljic et al. 1995)
 1.57, 1.62, 1.74 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
 1.82, 1.84 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 1.84, 1.86, 1.87, 1.88, 1.90, 1.87, 1.90 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)
 2.76, 2.41 (natural zeolite modified with a cation surfactant HDTMA with surface coverage of 100, 200 mmol/kg at pH 7, batch equilibrium-sorption isotherm, Li et al. 2000)
 1.64, 1.58, 1.78 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM} :

- 1.26 (Woodburn silt loam soil, 1.9% organic matter, equilibrium isotherm-GC, Chiou et al. 1983)
 1.04 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 1.89, 1.81 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.53, 2.46, 2.08 (organic cations treated Marlette soil B_t horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil B_t horizon OM 4.38%; Oshtemo soil B_t horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 1.34; 1.14 (high-organic-content soils: Florida peat - 57.1% C; Michigan muck - 53.7% C, equilibrium isotherm-GC, Rutherford & Chiou 1992)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2} = 4.81$ h from water depth of 1 m (calculated, Mackay & Leinonen 1975; Haque et al. 1980);
 $k = 0.03$ d⁻¹ with $t_{1/2} = 23$ d in spring at 8–16°C, $k = 0.22$ d⁻¹ with $t_{1/2} = 31$ d in summer at 20–22°C, $k = 0.054$ d⁻¹ with $t_{1/2} = 13$ d in winter at 3–7°C during the periods when volatilization appears to dominate, and $k = 0.101$ d⁻¹ with $t_{1/2} = 6.9$ d with HgCl₂ in September 9–15, 1980 in marine mesocosm experiments (Wakeham et al. 1983);
 $t_{1/2} \sim 27$ h from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s is 2.7 h at 20°C (Lyman et al. 1982).

Photolysis: atmospheric photolysis $t_{1/2} = 2808\text{--}16152$ h, based on measured photolysis half-lives in deionized water (Hustert et al. 1981; Howard et al. 1991);

aqueous photolysis $t_{1/2} = 2808\text{--}16152$ h, based on measured photolysis half-lives in deionized water (Hustert et al. 1981; Howard et al. 1991);

reaction rate constants, $k = 8.64 \times 10^{-4} \text{ h}^{-1}$ in air, and $k = 1.8 \times 10^{-4} \text{ h}^{-1}$ in water (Mackay et al. 1985).

Oxidation: rate constant k ; and gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

$k_{\text{OH}} = 1.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{O}(3\text{P})} = 0.24 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction of $\text{O}(3\text{P})$ atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{\text{OH}} \leq 2.3 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} \geq 5.1$ h; $k_{\text{O}(3\text{P})} = (0.144 \pm 0.2) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ with $\text{O}(3\text{P})$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{\text{OH}} = 0.85 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$, with $t_{1/2} = 2.4\text{--}24$ h (Darnall et al. 1976)

$k_{\text{OH}}^* = (1.20 \pm 0.15) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

photooxidation $t_{1/2} = 8.021 \times 10^3\text{--}3.21 \times 10^5$ h in water, based on measured rate constant for reaction with OH radical in water (Güsten et al. 1981)

$k_{\text{OH}} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and residence time of 8.3 d, loss of 11.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}} = 28 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k_{\text{OH}} = 0.82 \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 6.8$ d in the atmosphere (Mill 1982)

$k = (2.0 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 50–1000 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}} = (8.8 \pm 0.4) 1.45 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{\text{NO}_3} < 2.3 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 1.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1985)

$k_{\text{OH}}^* = 1.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}} = 1.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K. (relative rate method, Ohta & Ohya 1985)

$k_{\text{OH}} = 1.26 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 23.8°C, with an atmospheric lifetime of 9.1 d (Edney et al. 1986)

$k_{\text{OH}}^* = 1.14 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 239–354 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{\text{OH}}(\text{calc}) = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}}^* = (1.29 \pm 1.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{OH}} = 1.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{NO}_3} < 3.2 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson & Aschmann 1988)

$k_{\text{OH}}^* = 1.40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 1.23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}}(\text{calc}) = 1.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

$t_{1/2} = 6$ d in estuarine water (estimated, Lee & Ryan 1976)

$t_{1/2}(\text{aq. aerobic}) = 120\text{--}384$ h, based on seawater dieaway test data (Van der Linden 1978) and river dieaway data (Vaishnav & Babeu, 1987; Howard et al. 1991)

$k = 4.58 \times 10^{-3} \text{ h}^{-1}$ in water (Lee & Ryan 1979; Mackay et al. 1985)

$k = 0.2 \text{ yr}^{-1}$ with $t_{1/2} = 110$ d (Zoeteman et al 1981; Olsen & Davis 1990)

$k = 0.5 \text{ d}^{-1}$ significant degradation in favourable aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2}(\text{aq. anaerobic}) = 2688\text{--}17280$ h, based on unacclimated aqueous anaerobic biodegradation screening test data (Horowitz et al. 1982; Howard et al. 1991)

$k = 0.12 \text{ d}^{-1}$ in river water (estimated, Bartholomew & Pfaender 1983; quoted, Battersby 1990)

$t_{1/2} = 8.6$ d in activated sludge (estimated, Freitag et al. 1985, quoted, Anderson et al. 1991)

$k = 0.025 \text{ d}^{-1}$ with $t_{1/2} = 28 \text{ d}$ in groundwater, $k = 0.044 \text{ d}^{-1}$ with $t_{1/2} = 16 \text{ d}$ in Lester River with nutrient and microbial addition, and $k = 0.082 \text{ d}^{-1}$ with $t_{1/2} = 8 \text{ d}$ in Superior harbor waters (Vaishnav & Babeu 1987)
 $t_{1/2}(\text{aerobic}) = 5 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 110 \text{ d}$ in natural waters (Capel & Larson 1995)
 $k = 0.58 \text{ d}^{-1}$ associated with microbial population growth initially followed by a slower second phase with $k = 0.12 \text{ d}^{-1}$ degradation by *P. aeruginosa* is a two-stage process (Kim et al. 2003).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Constants or Half-Lives:

$t_{1/2} = 0.5 \text{ d}$ for elimination from eels, 0.5 d (Ogata & Miyake 1978).

Half-Lives in the Environment:

Air: $t_{1/2} \geq 5.1 \text{ h}$, based on a determined rate of disappearance in ambient LA basin air for reaction with OH radical at 300 K (Doyle et al. 1975);

$t_{1/2} = 2.4\text{--}24 \text{ h}$, based on rate of disappearance for the reaction with OH radical (Darnall et al. 1976);
 residence time of 8.3 d, loss of 11.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981);

$t_{1/2} = 50.1\text{--}501 \text{ h}$, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);
 calculated lifetime of 9.1 d due to reaction with OH radical (Edney et al. 1986);
 summer daylight lifetime of 115 h due to reaction with OH radical (Altshuller 1991);
 calculated lifetimes of 9.4 d, $> 4 \text{ yr}$ and $> 4.5 \text{ yr}$ for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

Surface Water:

$t_{1/2} = 4.81 \text{ h}$, based on evaporation loss at 25°C and 1 m depth of water (Mackay & Leinonen 1975)
 biodegradation $t_{1/2} \sim 6 \text{ d}$ in estuarine water (Lee & Ryan 1976)

$t_{1/2} = 120\text{--}384 \text{ h}$, based on unacclimated aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991);

$t_{1/2} = 23 \text{ d}$ at $8\text{--}16^\circ\text{C}$ in the spring, $t_{1/2} = 3.1 \text{ d}$ at $20\text{--}22^\circ\text{C}$ in the summer and $t_{1/2} = 13 \text{ d}$ at $3\text{--}7^\circ\text{C}$ in the winter, and $t_{1/2} = 6.9 \text{ d}$ with HgCl_2 in September 9–15 from mesocosm experiments (Wakeham et al. 1983).

Ground water: $t_{1/2} \sim 1 \text{ yr}$ from persistence observed in the groundwater of Netherlands (Zoeteman et al. 1981),
 $t_{1/2} = 240\text{--}17280 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991).

Soil: $t_{1/2} = 120\text{--}384 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991);

$t_{1/2} < 10 \text{ d}$ (Ryan et al. 1988);

$t_{1/2} = 365 \text{ d}$, assumed first-order biological/chemical degradation in the soil (Jury et al. 1990);
 disappearance $t_{1/2} < 2 \text{ d}$ for test soils (Anderson et al. 1991).

Biota:

TABLE 3.1.1.1.1

Reported aqueous solubilities of benzene at various temperatures and reported temperature dependence equations

$$R \cdot \ln x = -[\Delta H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K) \quad (1)$$

$$S(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t_{1/2} + c \cdot t + d \quad (2)$$

$$\ln x = A - B/T(K) \quad (3)$$

$$\ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_0, T_0 = 298.15 \text{ K} \quad (4)$$

1.

Bohon & Claussen 1951		Arnold et al. 1958		Alexander 1959		Franks 1963	
shake flask-UV		shake flask-UV		shake flask-UV		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0.4	1741	4.5	1720	0.8	1840	17	1714
5.2	1810	4.9	1770	9.4	1790	22	1723
10	1800	5.0	1740	16.8	1770	25	1742
14.9	1770	6.7	1740	24	1800	29	1745
21	1790	9.0	1730	31	1830	32	1788
25.6	1790	12.5	1720	38	1920	35	1823
30.2	1843	15	1730	44.7	2030	40.5	1905
34.9	1877	20	1710	51.5	2140	42	1910
42.8	1998	20.6	1720	65.4	2340	44	1931
		24.8	1710			46	1983
		24.9	1740			51	2075
		27.3	1745			56	2183
ΔH _{sol} /(kJ mol ⁻¹) =							
25	2.42	30	1775			61	2305
12	-2.30	30.9	1884			63	2352
17	-0.25	45	1975				
18	0	49.8	2044				
22	1.34	54.5	2152				
27	3.01	59.8	2265				
32	4.435	64.8	2313				
37	5.86						
		ΔH _{sol} /(kJ mol ⁻¹) = 2.27					
		at 25°C					

2.

Leinonen 1972		Udovenko & Aleksandrova 1963		Price 1973		Bradley et al. 1973	
shake flask-GC		polythermic method		shake flask-GC		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4	1710	20	2100	25	1755	25	1830
5	1737	40	2270	55.3	3980	45	2160
5.4	1746	40.5	2480	84.7	6468	55	2380
6.1	1735	44.5	2590				
7.0	1781	56.5	2880				
10.3	1748	60	3000				
13	1741	65	3190				
16	1730	79.5	3730				
19.1	1721						
22.1	1739						

(Continued)

TABLE 3.1.1.1.1 (Continued)

3.

Brown & Wasik 1974		May et al. 1980, 1983		Ben-Naim & Wiff 1979		Bittrich et al. 1979	
shake flask-UV		generator column-HPLC/UV		shake flask-UV		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4.5	1840	0.2	1836	10	1625	20	1790
6.3	1850	6.2	1804	20	1734	40	2025
7.1	1810	11	1799			69	2442
9.0	1810	13	1770				
11.8	1770	16.9	1762				
12.1	1770	18.6	1767				
15.1	1790	25.0	1790				
17.9	1790	25.8	1819				
20.1	1760						

temp dependence eq. 2
given in May et al. 1978b and
May 1980

S	mg/kg
a	0.0247
b	-0.6838
c	0.3166
d	1833

4.

Sanemasa et al. 1981		Shaw 1989a (IUPAC)		Cooling et al. 1992		Chen & Wagner 1994a	
vapor saturation-UV		recommended values		activity coefficient-GC		equilibrium flow cell-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	1540	0	1690	20	1732	30	1840
25	1610	5	1800	30	1688	40	2014
35	1770	10	1780	40	1712	50	2213
45	1870	15	1760	50	1760	60	2452
		20	1760			70	2713
		25	1770			80	3033
		30	1810			90	3472
		35	1860			100	4123
		40	1930				
		45	1990				
		50	2080				
		55	2190				
		60	2310				
		65	2410				
		70	2670				

Sanemasa et al. 1982
vapor saturation-UV

t/°C	S/g·m ⁻³
5	1620
15	1580
25	1620
35	1710
45	1800

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.07$
at 25°C

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.69$
25°C

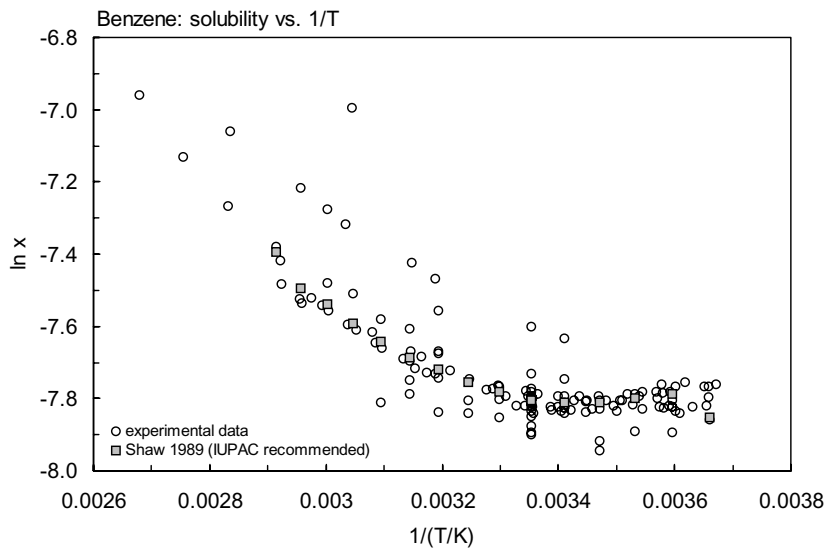


FIGURE 3.1.1.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzene.

TABLE 3.1.1.1.2
Reported vapor pressures of benzene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)

log P = A – B/(C + t/°C)

log P = A – B/(C + T/K)

log P = A – B/(T/K) – C·log (T/K)

log P = A – B/(T/K) – C·log (T/K) + D·P/(T/K)²

(1)

(2)

(3)

(4)

(5)

ln P = A – B/(T/K)

ln P = A – B/(C + t/°C)

(1a)

(2a)

1.

Stuckey & Saylor 1940		Willingham et al. 1945		Stull 1947		Forziati et al. 1949	
mercury manometer		ebulliometry		summary of lit. data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	3509	14.548	7654	–36.7	133.3*	10.983	6397
12.5	6040	17.720	8962	–19.6	266.6*	14.575	7690
25	9960	20.504	10303	–11.5	1333*	17.697	8989
37.5	15800	23.270	11699	–2.60	2666*	20.028	11700
40	24240	26.886	13818	7.60	5333	23.271	11720
50	36050	31.004	16621	15.4	7999	26.908	13840
		35.191	19922	26.1	13332	31.013	16631
eq. 4	P/mmHg	30.078	23450	42.2	26664	35.207	19942
A	7.12491	44.284	28952	60.5	53323	39.095	23465
B	1323.06	49.066	34897	80.1	101325	44.294	28976
C	41.23	54.832	43320			49.084	34924
		60.784	53652		*solid	54.852	43358
bp/°C	80.06	67.135	66753	mp/°C	5.5	60.803	53697
		74.028	83717			67.148	66795
		78.891	97601			74.035	83746
		79.413	99197			78.903	97643
		79.898	100689			79.424	99230

(Continued)

TABLE 3.1.1.1.2 (Continued)

1.

Stuckey & Saylor 1940		Willingham et al. 1945		Stull 1947		Forziati et al. 1949	
mercury manometer		ebulliometry		summary of lit. data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		80.442	102384			79.090	100722
		80.922	106570			80.461	102460
						80.948	104000
		eq. 2	P/mmHg			eq. 2	P/mmHg
		A	6.89324			A	6.9210
		B	1203.835			B	1214.645
		C	219.924			B	221.205
		bp/°C	80.103			bp/°C	80.099

2.

Bond & Thodos 1960		Ambrose et al. 1967		Ambrose et al. 1970		Zwolinski & Wilhoit 1971	
compiled data		ebulliometry		compiled data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
7.565	5333	146.85	545800	46.85	32045	-11.6	1333*
39.093	23450	166.85	809200	66.85	66116	-2.60	2666*
67.15	66753	186.85	1156700	86.85	124180	3.0	4000*
95.713	159987	206.85	1603700	106.85	215960	7.55	5333
110.015	231848	226.85	2166700	126.85	352460	11.80	6666
150.015	577419	246.85	2864400	146.85	545760	15.39	7999
180.015	1017250	266.85	3719300	166.85	809050	21.293	10666
240.015	2589787	286.85	4771700	186.85	1156600	26.075	13332
260.015	3376922			206.85	1603800	35.266	19998
		eq. 5	P/mmHg	226.85	2166900	42.214	26664
eq. 5	P/mmHg	A	20.87440	246.85	2864000	47.868	33331
A	23.36128	B	2472.77	266.85	3718800	52.672	39997
B	2457.12	C	5.44671	286.85	4772600	60.611	53329
C	5.28840	D	1238			67.093	66661
D	1.56738					72.616	79993
bp/°C	80.115					77.454	93326
						78.354	95991
						79.236	98659
						80.100	101325
						25.0	12690
							*solid
						eq. 2	P/mmHg
						A	9.1064
						B	1885.9
						C	244.2
							for liquid
						eq. 2	P/mmHg
						A	6.90565
						B	1211.033
						C	220.790

TABLE 3.1.1.1.2 (Continued)

Bond & Thodos 1960		Ambrose et al. 1967		Ambrose et al. 1970		Zwolinski & Wilhoit 1971	
compiled data		ebulliometry		compiled data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						bp/°C	80.100
						$\Delta H_v/(\text{kJ mol}^{-1})$	
						at 25°C	33.85
						at bp	30.76

3.

Osborn & Scott 1978		Scott & Osborn 1979		Ambrose 1981			
ebulliometry		ebulliometry		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
				set 1		set 2	
19.071	9585	32.182	19933	290.076	8634	294.165	10527
21.728	10887	40.637	25023	302.392	15388	297.699	12431
24.396	12339	46.139	31177	311.186	22484	303.293	16017
27.0755	13955	51.684	38565	318.694	30464	306.060	18080
29.765	15748	57.276	47375	325.097	38953	314.942	26227
32.467	17735	62.991	57817	330.437	47571	318.971	30791
		68.591	70120	334.886	55511	323.246	36326
		74.319	84532	338.935	63815	328.325	43899
		80.092	101325	342.946	72985	334.125	54050
		85.911	120791	346.244	81275	338.779	63474
		91.777	143240	349.910	91346	348.400	87089
		97.689	169030	353.469	102043	352.356	98297
		103.645	198490	356.187	110854	353.212	101226
		109.648	232020	358.873	120137	353.802	103094
		115.697	270030	362.286	132779	357.611	115693
				365.234	144528	363.086	135887
				367.897	155797	367.789	155309
				370.527	167605	372.897	178812
				373.151	180059	378.152	205747
				375.844	193529		
				378.523	207939		
				381.325	223436		

4.

Ambrose 1981 (continued)				Liu & Dickhut 1994	
ebulliometry		ebulliometry		gas saturation-GC	
T/K	P/Pa	T/K	P/Pa	t/°C	P/Pa
set 3		set 4			
285.957	7014	297.769	12471	-15.4	880
292.893	9903	302.633	15553	-5.0	1750
298.684	13007	307.159	18957	10	6540
302.619	15545	308.384	19979	25	13100
304.302	16745	314.503	25716	40	26400
310.167	21539	319.907	31940		
314.406	25665	324.512	38019		
319.512	31444	329.473	45774		

(Continued)

TABLE 3.1.1.1.2 (Continued)

4.

Ambrose 1981 (continued)				Liu & Dickhut 1994	
ebulliometry		ebulliometry		gas saturation-GC	
T/K	P/Pa	T/K	P/Pa	t/°C	P/Pa
323.921	37264	333.842	53510		
329.536	45876	338.144	62115		
334.406	54580	342.687	77356		
339.063	64081	347.828	85511		
343.751	74940	352.112	97852		
348.357	86959	352.617	99394		
352.594	99320	352.955	100439		
353.078	100816	358.109	117426		
353.660	102633	362.258	132666		
358.727	119597	367.239	152938		
363.062	135783	372.175	175319		
367.554	154281	377.584	202669		
372.630	177510				
377.875	204219				
383.175	234260				

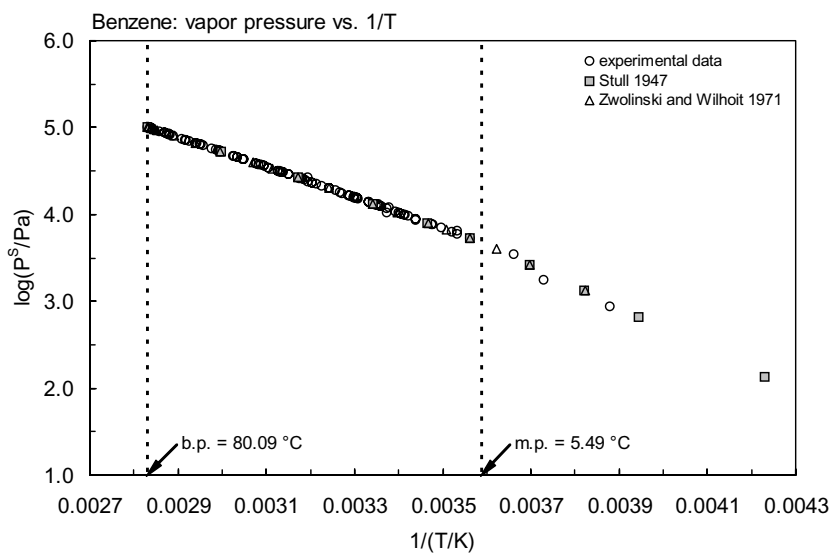


FIGURE 3.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for benzene.

TABLE 3.1.1.1.3

Reported Henry's law constants of benzene at various temperatures and reported temperature dependence equations

$$\begin{aligned} \ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) & (4) & \ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K) & (4a) \\ K_{AW} &= A - B/(T/K) + C\cdot(T/K)^2 & (5) & & \end{aligned}$$

1.

Brown & Wasik 1974		Green & Frank 1979		Leighton & Calo 1981		Sanemasa et al. 1981	
headspace-GC		concentration ratio-UV		equilibrium cell-GC		vapor-liquid equilibrium	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
4.5	187.2	10	262	1.0	178	15	396
6.33	209.3	15	332	1.3	174	25	610
7.06	222.9	20	430	11	280	35	877
8.96	246.4	25	552	13	330	45	1267
11.75	289.9	30	688	21	470		
12.1	295.3			33	482		
15.1	346.8	eq. 3	k _H /atm	27.2	597	Sanemasa et al. 1982	
17.93	391.6	A	8.58	25	554	vapor liquid-equilibrium	
20.06	442.4	B	1852.308			t/°C	H/(Pa m ³ /mol)
				eq. 3	k _H /atm	5	225
				A	19.02	15	387
				B	3964	25	608
						35	905
						45	1321

2.

Ashworth et al. 1988		Robbins et al. 1993		Perlinger et al. 1993		Ettre et al. 1993	
EPICS-GC		static headspace-GC		headspace-GC		equil. headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
10	334	25	535	10	290	25	570
15	391	30	679	15	380	45	912
20	458	40	890	20	460	60	1220
25	535	45	1236	25	604	70	1668
30	730	50	1450	30	741	80	1767
eq. 4	H/(atm·m ³ /mol)					eq.2	1/K _{AW}
A	5.534					A	-2.1678537
B	3194					B	836.2228

3.

Dewulf et al. 1995		Alaee et al. 1996		Turner et al. 1996		Peng & Wan 1997	
EPICS-GC		gas stripping-GC		vapor phase-equilibrium		headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
2.0	162	4	169	10	287	15	366
6.0	208	10	228	15	390	20	436
10	228	15	326	25	640	25	538

(Continued)

TABLE 3.1.1.1.3 (Continued)

3.

Dewulf et al. 1995		Alaee et al. 1996		Turner et al. 1996		Peng & Wan 1997	
EPICS-GC		gas stripping-GC		vapor phase-equilibrium		headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
18.2	366	20.6	441	35	986	30	675
25	481	25.4	552			35	766
		30.1	744			40	947
eq. 1	K _{AW}	34.9	874	eq. 5	K _{AW}	45	1053
A	10.577			A	0.0763		
B	3640			B	0.00211		
				C	0.000162		
		enthalpy of volatilization: $\Delta H_{vol}/(kJ \cdot mol^{-1}) = 32.2$ at 20°C				eq.1	K _{AW}
		eq. 1	K _{AW}			A	7.15
		A	11.5352			B	1397
		B	3873				

4.

Bierwagen & Keller 2001		Görgényi et al. 2002		Bakierowska & T. 2003	
SPME-GC		EPICS-SPME method		headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
15	376	2	172.2	10	294
25	538	6	235.6	15	353.5
30	675	10	279.2	20	440
40	893	18	441.3	25	558
		25	573.4		
eq. 1	K _{AW}	30	740.0	Eq. 2	1/K _{AW}
A	8.1648	40	1033	A	11.663
B	2889.4	50	1429	B	3920
		60	1844		
		eq. 1	K _{AW}		
		A	10.01		
		B	3430.4		

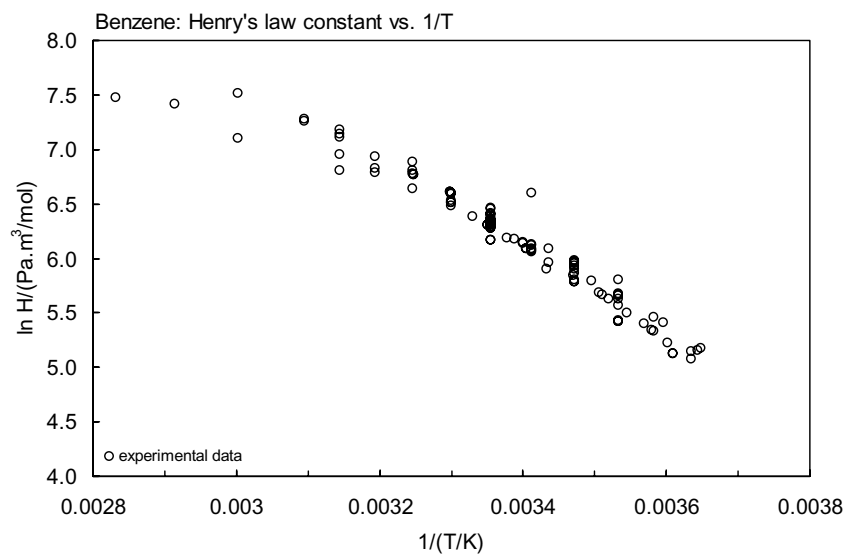


FIGURE 3.1.1.1.3 Logarithm of Henry’s law constant versus reciprocal temperature for benzene.

TABLE 3.1.1.1.4
Reported octanol-water partition coefficients and octanol-air partition coefficients of benzene at various temperatures

log K _{OW}		log K _{OA}	
Dewulf et al. 1999		Gruber et al. 1997	
EPICS-GC, both phases		activity coefficient-GC	
t/°C	log K _{OW}	t/°C	log K _{OA}
2.2	1.973	20.29	2.9
6	1.961	30.3	2.71
10	2.053	40.4	2.56
14.1	2.01	50.28	2.42
18.7	2.04		
24.8	1.974		
change in enthalpy:			
$\Delta H_{OW}/(\text{kJ mol}^{-1}) = 1.7$			
(-8.3 to 11.8)			
enthalpy of transfer			
$\Delta H_{oct}/(\text{kJ mol}^{-1}) = 8.1$			
(-1.9 to 18.2)			

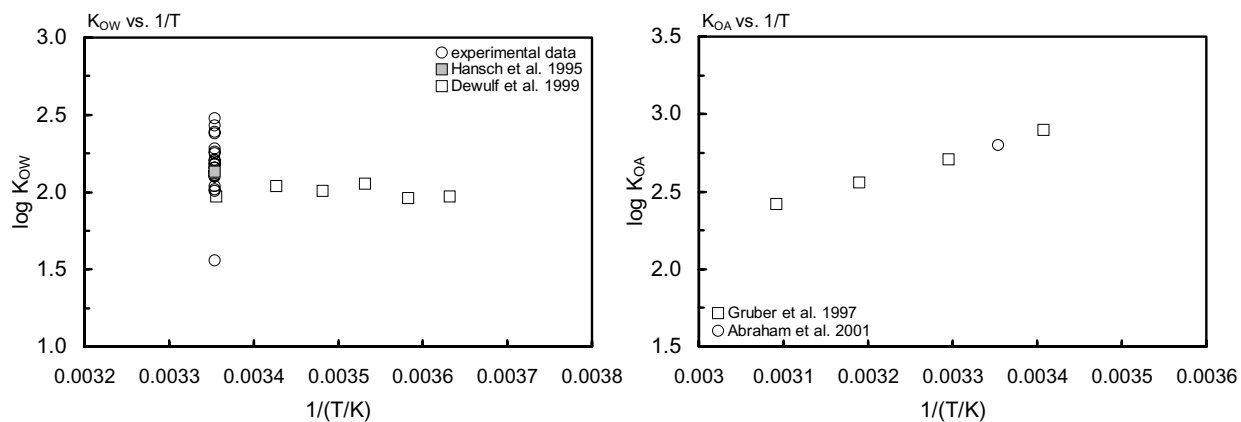
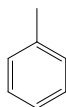


FIGURE 3.1.1.1.4 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for benzene.

3.1.1.2 Toluene



Common Name: Toluene

Synonym: methyl benzene, phenylmethane, toluol, methylbenzol, methacide

Chemical Name: toluene

CAS Registry No: 108-88-3

Molecular Formula: C_7H_8 , $C_6H_5CH_3$

Molecular Weight: 92.139

Melting Point ($^{\circ}C$):

-94.95 (Lide 2003)

Boiling Point ($^{\circ}C$):

110.63 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8669 (Weast 1982-83)

Molar Volume (cm^3/mol):

106.3 ($20^{\circ}C$, calculated from density)

118.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

37.99, 33.183 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

6.636 (Riddick et al. 1986)

6.62 (exptl., Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

37.15, 45.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or indicated. Additional data at other temperatures designated * are compiled at the end of this section):

470	($16^{\circ}C$, shake flask, Fühner, 1924)
570	($30^{\circ}C$, shake flask-interferometer, Gross & Saylor 1931)
347	(residue-volume method, Booth & Everson 1948)
530	(shake flask-UV, Andrews & Keffer 1949)
500	(flask flask-UV, Klevens 1950)
627*	(shake flask-UV, measured range $0.4-45.3^{\circ}C$, Bohon & Claussen 1951)
546	(shake flask-UV, Morrison & Billett 1952)
550	(Dreisbach 1955)
595	(quoted, Deno & Berkheimer 1960)
538	(shake flask-GC, McAuliffe 1963)
515	(shake flask-GC, McAuliffe 1966)
479	($21^{\circ}C$, shake flask-GC, Chey & Calder 1972)
530*	(shake flask-GC, measured range $5-45^{\circ}C$, Pierotti & Liabastre 1972)
547*	(shake flask-UV, measured $25-55^{\circ}C$, Bradley et al. 1973)
573*	(shake flask-GC, Polak & Lu 1973)
517	(shake flask-GC, Mackay & Wolkoff 1973)
573*	(headspace-GC, measured range $4.5-20.1^{\circ}C$, Brown & Wasik 1974)
627	(shake flask-UV, Vesala 1974)
520	(shake flask-GC, Mackay & Shiu 1975)
534.8	(shake flask-GC, Sutton & Calder 1975)
554	(shake flask-GC, Price 1976)
488; 563	(shake flask-titration, shake flask-cloud point, Sada et al. 1975)

- 534 (shake flask-fluorescence, Schwarz 1977)
 554 (shake flask-GC, Krzyzanowska & Szeliga 1978)
 $\log x = 626.526/(T/K)^2 - 4300.59/(T/K) + 3.3585$, temp range 0–50°C (Ueda et al. 1978)
 572, 587 (10, 20°C, shake flask-UV, Ben-Naim & Wiff 1979)
 660 (elution chromatography, Schwarz 1980)
 732*, 739* (20°C, exptl.-elution chromatography, shake flask-UV, Schwarz & Miller 1980)
 155 (shake flask-LSC, Banerjee et al. 1980)
 507 (shake flask-GC, Rossi & Thomas 1981)
 557* (vapor saturation-UV spec., measured range 15–45°C, Sanemasa et al. 1981)
 526* (vapor saturation-UV spec., measured range 15–45°C, Sanemasa et al. 1982)
 585 (generator column-HPLC/UV, Tewari et al. 1982b)
 578 (generator column-HPLC/UV, Tewari et al. 1982c)
 580 (generator column-HPLC/UV, Wasik et al. 1983)
 524 (shake flask-HPLC/UV, Banerjee 1984)
 521 (vapor saturation-UV spec., Sanemasa et al. 1984)
 $\ln x = -185.1695 + 7348.55/(T/K) + 26.34525 \cdot \ln (T/K)$; temp range 310–560 K (Heidman et al. 1985)
 520 (shake flask-radiometry, Lo et al. 1986)
 580 (shake flask-GC, Keeley et al. 1988)
 538 (shake flask-GC, Coutant & Keigley 1988)
 530* (IUPAC recommended value, temp range 5–55°C, Shaw 1989a)
 599* (30°C, equilibrium flow cell-GC; measured range 30–100°C Chen & Wagner 1994b)
 $\ln (1/x) = -12.21 + 21.39 \cdot [(T/K)/591.8]^{-1} - 3.572 \cdot [(T/K)/591.8]^{-2}$; temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994b)
 $\ln x = 12.21 - 21.39 \cdot (T_r/K)^{-1} + 5.372 \cdot (T_r/K)^{-2}$, $T_r = T/T_c$, the reduced temp, system temp T divided by critical temp T_c (Chen & Wagner 1994c)
 562.9 (shake flask-UV spectrophotometry, Poulson et al. 1999)
 $\ln x = -46.05 - 7268.85/(T/K) - 1.411 \times 10^{-4} \cdot (T/K)^2$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
 519* (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)
 556* (vapor absorption technique-HPLC/UV, measured range 0.5–55°C, Dohányosová et al. 2001)
 558* (shake flask-UV, measured range 0–50°C, Sawamura et al. 2001)
 $\ln x = -221.739 + 9274.79/(T/K) + 31.8721 \cdot \ln (T/K)$; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section):

- 920* (0°C, mercury manometer, measured range –9.70 to 0°C, Linder 1931)
 3786* (Hg manometer measurements, Pitzer & Scott 1943)
 $\log (P/\text{mmHg}) = -2866.53/(T/K) - 6.7 \log (T/K) + 27.6470$; temp range: 0–50°C (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)
 6357* (35.366°C, ebulliometry, measured range 35.366–111.509°C, Willingham et al. 1945)
 $\log (P/\text{mmHg}) = 6.95337 - 1343.943/(219.377 + t/^\circ\text{C})$; temp range 35.4–111.5°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
 2666* (18.4°C, summary of literature data, temp range –16.7 to 110.6°C, Stull 1947)
 6386* (35.504°C, ebulliometry, measured range 35.504–111.545°C, Forziati et al. 1949)
 $\log (P/\text{mmHg}) = 6.95508 - 1345.087/(219.516 + t/^\circ\text{C})$; temp range 35.5–111.5°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
 3792 (calculated from det. data, Dreisbach 1955)
 $\log (P/\text{mmHg}) = 6.95334 - 1343.943/(219.377 + t/^\circ\text{C})$; temp range 20–200°C (Antoine eq. for liquid state, Dreisbach 1955)
 1333* (6.375°C, compiled data, temp range 6.375–136.435°C, Bond & Thodos 1960)
 256200* (146.85°C, ebulliometry, measured range 146.85–306.85°C, Ambrose et al. 1967)
 48898* (86.85°C, compiled data, temp range 86.85–306.85°C, Ambrose et al. 1970)
 3792* (interpolated, Antoine eq., Zwolinski & Wilhoit 1971)

- log (P/mmHg) = $6.95464 - 1344.80/(219.482 + t/^{\circ}\text{C})$; temp range; 6.36–136.42°C (Antoine eq., Zwolinski & Wilhoit 1971)
- log (P/mmHg) = $[-0.2185 \times 9368.5/(T/K)] + 8.3300$; temp range –92 to –15°C (Antoine eq., Weast 1972–73)
- log (P/mmHg) = $[-0.2185 \times 8586.5/(T/K)] + 8.719392$; temp range –26.7 to 319°C (Antoine eq., Weast 1972–73)
- 2904* (19.99°C, differential capacitance gauge, measured range 0–49.26°C, Munday et al. 1980)
- log (P/mmHg) = $-5541.623/(T/K) + 25.08047 - 0.01055321(T/K)$; temp range 0–49.26°C (differential capacitance gauge, Munday et al. 1980)
- 3560 (gas saturation-GC, Politzki et al. 1982)
- log (P/atm) = $(1 - 383.737/T) \times 10^{(0.837122 - 6.48791 \times 10^4/T + 5.91293 \times 10^7/T^2)}$; T in K, temp range 245.0–590.0 K (Cox vapor pressure eq., Chao et al. 1983)
- log (P/kPa) = $6.08436 - 1347.62/(219.787 + t/^{\circ}\text{C})$; temp range 35.37–111.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- log (P/kPa) = $6.37988 - 1575.007/(249.372 + t/^{\circ}\text{C})$; temp range 86.85–306.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 3786 (Daubert & Danner 1985)
- 3790 (interpolated-Antoine eq., Dean 1985, 1992)
- log (P/mmHg) = $6.95464 - 1344.80/(219.48 + t/^{\circ}\text{C})$; temp range 6–137°C (Antoine eq., Dean 1985, 1992)
- 3790 (headspace-GC, Hussam & Carr 1985)
- log (P/kPa) = $6.08540 - 1348.77/(219.976 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
- 3800 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.08627 - 1349.122/(-53.154 + T/K)$; temp range 308–386 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.1258 - 1376.61/(-51.1 + T/K)$; temp range 210–219 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.12012 - 1374.901/(-49.657 + T/K)$; temp range 383–445 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.40815 - 1615.834/(-15.897 + T/K)$; temp range 440–531 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $7.65383 - 3153.235/(188.566 + T/K)$; temp range 530–592 K (liquid, Antoine eq.-V, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.16273 - 1391.005/(-48.974 + T/K)$; temp range 273–295 K (liquid, Antoine eq.-VI, Stephenson & Malanowski 1987, selected, Shiu & Ma 2000)
- 3090* (20.98°C, static method, measured range 199.22–402.21 K, Mokbel et al. 1998)

Henry's Law Constant (Pa m³/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 474* (headspace-GC, Brown & Wasik 1974)
- 527 (headspace-GC, Vitenberg et al. 1975)
- 673 (batch air stripping-GC, Mackay et al. 1979)
- 625* (23.0°C, equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
- ln (k_H/atm) = $18.46 - 3751/(T/K)$; temp range: 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
- 628* (vapor-liquid equilibrium-GC., Sanemasa et al. 1981)
- 664* (vapor-liquid equilibrium, Sanemasa et al. 1982)
- 647 (EPICS-GC, Garbarnini & Lion 1985)
- 634* (20°C, headspace-GC, measured range 20–46°C, Schoene & Steinhanses 1985)
- 601 (gas stripping-GC, Warner et al. 1987)
- 594 (20°C, EPICS, Yurteri et al. 1987)
- 651* (EPICS-GC, Ashworth et al. 1988)
- ln [H/(atm m³/mol)] = $5.133 - 3024/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
- 652 (infinite activity coeff. γ[∞] from solubility measurement, Abraham et al. 1990)
- 644 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 933* (40°C, static headspace-GC, measured range 40–80°C, Kolb et al. 1992)
- ln (1/K_{AW}) = $-6.03 + 2198/(T/K)$; temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
- 1116* (45°C, headspace-GC, measured range 45–80°C, Ettre et al. 1993)

$\log (1/K_{AW}) = -2.5323790 + 928.3536/(T/K)$; temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)

631 (infinite activity coeff. γ^∞ in water determined by inert gas stripping-GC, Li et al. 1993)

660* (equilibrium headspace-GC, Perlinger et al. 1993)

652* (static headspace-GC, Robbins et al. 1993)

644 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)

676 (23°C, gas stripping-IR, Nielsen et al. 1994)

555* (EPICS-GC/FID, Dewulf et al. 1995)

699 (EPICS-GC/FID, natural seawater with salinity of 35‰ Dewulf et al. 1995)

$\ln K_{AW} = -4064/(T/K) + 0.00834 \cdot Z + 12.150$; with Z salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)

541 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

684* (vapor-liquid equilibrium.-GC, Turner et al. 1996)

595 (gas stripping-GC, Altschuh et al. 1999)

605* (headspace equilibrium-GC, Peng & Wan 1997)

$\ln K_{AW} = 7.94 - 1621/(T/K)$; temp range 15–45°C (headspace equilibrium-GC, Peng & Wan 1997)

478 (headspace-GC, Peng & Wan 1998)

$\ln K_{AW} = 7.89 - 1565/(T/K)$; temp range 0–45°C (seawater with salinity of 36‰, headspace-GC, Peng & Wan 1998)

637.2 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

674.8 (modified EPICS method-GC, Ryu & Park 1999)

652 (EPICS-GC, David et al. 2000)

644 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

959 (EPICS-GC, Ayuttaya et al. 2001)

509 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 5.271 - 1745/(T/K)$ (van = t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

647.5* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)

$\ln K_{AW} = 11.25 - 3770.4/(T/K)$; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

556–574 (27°C, solid-phase microextraction-GC, solute concn 0.47–19.21 mg/L, measured range 15–40°C, Cheng et al. 2003)

612* (headspace-GC, measured range 10–25°C, Bakierowska & Trzeszczyński 2003)

$\ln (1/K_{AW}) = 11.926 - 3977/(T/K)$; temp range 10–25°C, headspace-GC, Bakierowska & Trzeszczyński 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:

2.69 (shake flask-UV, Fujita et al. 1964; quoted, Hansch et al. 1968; Hansch et al. 1972)

2.11 (shake flask-UV, Rogers & Cammarata 1969)

2.69, 2.73, 2.11, 2.80 (Leo et al. 1971; Hansch & Leo 1979)

2.21 (shake flask-LSC, Banerjee et al. 1980)

2.68 (shake flask-HPLC, Nahum & Horvath 1980)

2.59 (HPLC- k' correlation, Hanai et al. 1981)

2.97 (HPLC- k' correlation, McDuffie 1981)

2.78 (HPLC- k' correlation, Hammers et al. 1982)

2.59 (HPLC- k' correlation, D'Amboise & Hanai 1982)

2.65 (generator column-HPLC/UV, Tewari et al. 1982b,c)

2.62 (HPLC- k' correlation, Miyake & Terada 1982)

2.65 (generator column-HPLC/UV, Wasik et al. 1983)

2.74 (HPLC- k' correlation, Hafkanschheid & Tomlinson 1983b)

2.11–2.80, 2.65 (range, mean; shake flask method, Eadsforth & Moser 1983)

2.51–3.06, 2.88 (range, mean; HPLC method, Eadsforth & Moser 1983)

2.10 (shake flask, Platford 1979, 1983)

2.72 (HPLC-RV correlation, Garst & Wilson 1984)

2.89 (HPLC-RT correlation, Rapaport & Eisenreich 1984)

2.78 (HPLC/MS correlation, Burkhard et al. 1985)

3.00 (HPLC- k' correlation, De Kock & Lord 1987)

2.65 (generator column-RP-LC, Schantz & Martire 1987)

- 2.62 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
- 2.73 (recommended, Sangster 1989, 1993)
- 2.66, 2.69 (RP-HPLC capacity factor correlations, Sherblom & Eganhouse 1988)
- 2.786 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
- 2.63 ± 0.05, 2.786 ± 0.005 (shake flask/slow stirring, interlaboratory studies, Brooke et al. 1990)
- 2.76 (normal phase HPLC-*k'* correlation, Govers & Evers 1992)
- 2.73 (recommended, Hansch et al. 1995)
- 2.77 ± 0.02 (HPLC-*k'* correlation, Poulson et al. 1997)
- 2.32* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.42* (20.29°C, from GC-determined γ^∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
- 3.31 (head-space GC/FID both phases, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 1.12 (eels, Ogata & Miyake 1978)
- 0.22 (Manila clam, Nunes & Benville 1979)
- 0.62 (mussels, Geyer et al. 1982)
- 0.92 (goldfish, Ogata et al. 1984),
- 3.28, 2.58, 1.95 (activated sludge, algae, fish, Freitag et al. 1985)
- 1.99 (*S. capricornutum*, Herman et al. 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 2.39 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)
- 2.27, 1.89 (ICN humic acid, ICN HA coated Al_2O_3 , headspace equilibrium, Garbarnini & Lion 1985)
- 2.28, 1.89 (Offutt AFB soil, Whitean AFB soil, headspace equilibrium, Garbarnini & Lion 1985)
- 1.91, 1.13, 1.19, 2.18, 2.09, -1.30, 1.94 (Sapsucker Woods humic acid, Sapsucker Woods fulvic acid, tannic acid, lignin, zein, cellulose, Aldrich humic acid, headspace equilibrium, Garbarnini & Lion 1986)
- 2.18, 2.21, 2.43, 2.54 (Sapsucker Woods S.W. soil, S.W. ethyl ether extracted soil, humin, oxidized humin, headspace equilibrium, Garbarnini & Lion 1986)
- 1.74, 2.13, 1.98 (forest soil pH 5.6, forest soil pH 4.2, agricultural soil pH 7.4, Seip et al. 1986)
- 2.0 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
- 1.70 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.50, 2.39 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.86, 2.86, 2.43 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 1.59 (untreated St Clair soil B_t horizon, OC 0.44%, batch equilibrium, Lee et al. 1989)
- 3.03, 2.90 (organic cations HDTMA treated soils: St. Clair soil B_t horizon OC 3.25%; Oshtemo soil B_t horizon OC 0.83%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.01 (aquifer material with $f_{OC} = 0.006$ and measured partition coeff. $K_p = 0.61$ mL/g., Abdul et al. 1990)
- 2.10, 2.26 (HPLC-*k'* correlation, humic acid-silica column, Szabo et al. 1990a,b)
- 2.22, 2.16 (Captina silt loam, McLaurin sandy loam, batch equilibrium, Walton et al. 1992)
- 2.10 (average of 5 soils, sorption isotherms by batch equilibrium method-GC, Xing et al. 1994)
- 2.21, 2.31, 2.21 (RP-HPLC-*k'* correlation on 3 different stationary phases, Szabo et al. 1995)
- 2.17, 2.18 (RP-HPLC-*k'* correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 2.12 (HPLC-screening method, Müller & Kördel 1996)
- 2.23, 2.31, 2.33, 2.34, 2.40, 2.31, 2.34 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)
- 1.89, 2.00, 1.79 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, $\log K_{OM}$:

- 1.39 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.30, 2.16 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.74, 2.72, 2.28 (organic cations treated Marlette soil B₁ horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 1.29 (untreated St Clair soil B₁ horizon, OM 0.88%, batch equilibrium, Lee et al. 1989)
- 2.89; 2.74 (organic cations HDTMA treated soils: St. Clair soil B₁ horizon OM 4.38%; Oshtemo soil B₁ horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 5.18$ h from water depth of 1-m (Mackay & Leinonen 1975; Haque et al. 1980);

$k = 0.043$ d⁻¹ with $t_{1/2} = 16$ d in spring at 8–16°C, $k = 0.0463$ d⁻¹ with $t_{1/2} = 1.5$ d in summer at 20–22°C, $k = 0.053$ d⁻¹ with $t_{1/2} = 13$ d in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.088$ d⁻¹ with $t_{1/2} = 7.6$ d with HgCl₂, in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);

evaporation $t_{1/2} \sim 2.9$ d from a river of 1-m depth with wind speed of 3 m/s and water current of 1 m/s at 20°C (Lyman et al. 1982);

estimated $t_{1/2} = 1$ and 4 d for evaporation from a river and lake, respectively (Howard 1990).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982);

$k = 3.39 \times 10^{-3}$ h⁻¹ with H₂O₂ under photolysis at 25°C in F-113 solution and with HO· in the gas (Dilling et al. 1988); $t_{1/2} < 0.25$ h on silica gel under indoor artificial UV-light “continuous” condition (Söderström et al. 2004).

Oxidation: rate constant k ; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

$k_{OH} = (2.5 \pm 0.9) \times 10^9$ L mol⁻¹ s⁻¹ with $t_{1/2} = 4.6$ h; $k_{O(3P)} = (0.450 \pm 0.045) \times 10^8$ L mol⁻¹ s⁻¹ with O(3P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = 5.78 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹; $k_{O_3} = 0.75 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ for the reaction of O(3P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 3.6 \times 10^9$ L mol⁻¹ s⁻¹, with $t_{1/2} = 2.4$ –24 h at room temp. (Darnall et al. 1976)

$k_{OH}^* = (6.40 \pm 0.64) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH} = 6 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{NO_3} \leq 3 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹ at 300 ± 1 K (Carter et al. 1981)

$k_{OH} = 6.0 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ and residence time of 1.9 d, loss of 40.9% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360$ M⁻¹ h⁻¹ for singlet oxygen and $k = 144$ M⁻¹ h⁻¹ for RO₂ radical (Mabey et al. 1982)

$k_{O_3} = 160$ cm³ mol⁻¹ s⁻¹ at 300 K (Lyman et al. 1982)

$k_{OH} = 3.5 \times 10^9$ M⁻¹ s⁻¹ with $t_{1/2} = 1.6$ d in the atmosphere (Mill 1982)

$k = (14 \pm 3)$ M⁻¹ s⁻¹ for the reaction with ozone in water at pH 1.7 and 20–23°C (Hoigné & Bader 1983)

$k_{O_3} < 1.0 \times 10^{-20}$ cm³ molecule⁻¹ s⁻¹ with a loss rate of < 0.0006 d⁻¹; $k_{OH} = 6.4 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with a loss rate of 0.6 d⁻¹ and $k_{NO_3} = 3.7 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ with a loss rate of 0.0007 d⁻¹ at room temp. (review, Atkinson & Carter 1984)

$k_{NO_3} = 1.8 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 296 K (Atkinson et al. 1984)

$k_{OH}^* = 6.19 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1985)

$k_{OH}(\text{calc}) = 5.9 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(\text{obs.}) = 5.7 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH} = 5.7 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with $t_{1/2} = 10$ –104 h (Atkinson 1985; Howard 1991)

$k_{O_3} < 1.0 \times 10^{-20}$ cm³ molecule⁻¹ s⁻¹ with a loss rate of < 0.0006 d⁻¹; $k_{OH} = 6.2 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with a loss rate of 0.27 d⁻¹ and $k_{NO_3} = 3.6 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ with a loss rate of 0.0007 d⁻¹ at room temp. (review, Atkinson 1985)

$k_{OH} = 6.03 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (relative rate method, Ohta & Ohya 1985)

$k_{OH} = 5.35 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 24.2°C, with a calculated atmospheric lifetime $\tau = 2.2$ d (Edney et al. 1986)

$k_{\text{OH}}(\text{calc}) = 5.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{NO}_3} = 6.46 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{OH}} = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{NO}_3} = (7.8 \pm 1.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate method, Atkinson & Aschmann 1988)

$k_{\text{OH}}^* = 5.96 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

photooxidation $t_{1/2} = 10\text{--}104 \text{ h}$, based on measured rate data for the vapor phase reaction with OH radicals in air; $t_{1/2}(\text{aq.}) = 321\text{--}1284 \text{ h}$, based on measured rate data for hydroxyl radicals in aqueous solution (Howard et al. 1991)

$k_{\text{OH}}(\text{calc}) = 5.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 4.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (based on molecular orbital calculations, Klamt 1993)

Hydrolysis: not aquatically significant (Callahan et al. 1979);

no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of $2.22 \times 10^{-6} \text{ L/L}$ (Jamison et al. 1976)

$t_{1/2} \approx 90 \text{ d}$ in uncontaminated estuarine water; and $t_{1/2} \approx 30 \text{ d}$ in oil polluted water (Lee 1977)

$k = 0.5 \text{ d}^{-1}$, significant degradation in aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$k = 0.07 \text{ yr}^{-1}$ with $t_{1/2} = 39 \text{ d}$ (Zoeteman et al. 1981; Olsen & Davis 1990)

$t_{1/2}(\text{aq. anaerobic}) = 1344\text{--}5040 \text{ h}$, based on anaerobic screening test data and anaerobic sediment grab sample data (Horowitz et al. 1982; Howard et al. 1991)

$t_{1/2} = 9.5 \text{ d}$ in activated sludge (estimated, Freitag et al. 1985; quoted, Anderson et al. 1991)

$t_{1/2}(\text{aq. aerobic}) = 96\text{--}528 \text{ h}$, based on an acclimated seawater dieaway test (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 4 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 56 \text{ d}$ in natural waters (Capel & Larson 1995)

$t_{1/2} = 31\text{--}220 \text{ h}$ for toluene concn range from 0.5–200 $\mu\text{g/g}$ in sandy loam soil and degradation rate $k = 1.76 \times 10^{-2}$ and $0.42 \mu\text{g g}^{-1} \text{ h}^{-1}$ of soil for 0.5 and 5.0 $\mu\text{g/g}$, respectively; $t_{1/2} = 172$ and 165 h in sand and degradation rate $k = 1.05 \times 10^{-2}$ and $0.22 \mu\text{g g}^{-1} \text{ h}^{-1}$ of soil for toluene concn 0.5 and 5 $\mu\text{g/g}$ respectively in sand (Davis & Madsen 1996)

Biotransformation: $1.0 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$t_{1/2} \sim 1.4 \text{ d}$ elimination from eels in seawater (Ogata & Miyake 1978).

Half-Lives in the Environment:

Air: $t_{1/2} = 4.6 \text{ h}$ in ambient air based on reaction with OH radical at $\sim 300\text{K}$ (Doyle et al. 1975);

$t_{1/2} = 2.4\text{--}24 \text{ h}$ based on rate of disappearance for the reaction with hydroxyl radicals (Darnall et al. 1976)

photodecomposition $t_{1/2} = 6.8 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976)

residence time of 1.9 d, loss of 40.9% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

calculated lifetime $\tau = 2.2 \text{ d}$ due to reaction with OH radical (Edney et al. 1986)

summer daylight lifetime of 23 h due to reaction with OH radical (Altshuller 1991)

$t_{1/2} = 10\text{--}104 \text{ h}$, based on photooxidation in air (Howard et al. 1991)

calculated lifetimes, $\tau = 1.9 \text{ d}$, 1.9 yr and $> 4.5 \text{ yr}$ for reactions with OH radical, NO_3 radical and O_3 respectively (Atkinson 2000).

Surface Water: $t_{1/2} = 5.55 \text{ h}$, based on evaporative loss at 25°C and 1-m depth of water (calculated, Mackay & Leinonen 1975; Haque et al. 1980)

photooxidation $t_{1/2} = 321\text{--}1284 \text{ h}$ in water, based on measured rate data for hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)

$t_{1/2} = 16 \text{ d}$ in spring at 6–16°C, $t_{1/2} = 1.5 \text{ d}$ in summer at 20–22°C, $t_{1/2} = 13 \text{ d}$ in winter at 3–7°C when volatilization dominates and $t_{1/2} = 7.9 \text{ d}$ with HgCl_2 in marine mesocosm experiments (Wakeham et al. 1983)

$t_{1/2} = 96\text{--}528 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} \approx 0.3 \text{ yr}$ from observed persistence in groundwater of Netherlands (Zoeteman et al. 1981);

$t_{1/2} = 168\text{--}672 \text{ h}$, based on unacclimated grab sample data of aerobic soil from groundwater aquifers (Wilson et al. 1983; Swindoll et al. 1987; Howard et al. 1991).

Soil: $t_{1/2} < 10 \text{ d}$ (Ryan et al. 1988)

$t_{1/2} = 5 \text{ d}$ assumed first-order biological/chemical degradation in soil (Jury et al. 1990);

reported lit. $t_{1/2} = 0.1 - 1.7$ d and 7 d in soil, measured disappearance $t_{1/2} < 2.0$ d from test soils (Anderson et al. 1991)

$t_{1/2} = 96-528$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} = 31, 57, 96$ and 220 h with toluene concn range from 0.5, 5, 50 and 200 $\mu\text{g/g}$ in sandy loam soil, $t_{1/2} = 172$ and 165 h with toluene concn 0.5 and 5 $\mu\text{g/g}$, respectively, in sand (Davis & Madsen 1996).

Biota: $t_{1/2} = 10$ h clearance from fish (Neely 1980).

TABLE 3.1.1.2.1

Reported aqueous solubilities of toluene at various temperatures and reported enthalpy of solution

1.

Bohon & Claussen 1951		Pierotti & Liabastre 1972		Bradley et al. 1973		Brown & Wasik 1974	
shake flask-UV		shake flask-GC		shake flask-UV		headspace-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0.4	658	5	634	25	547	25	573
3.6	646	10	632	45	722	4.5	612
10	628	20	661	55	860	6.3	601
11.2	624	25	630			7.1	586
14.9	623	35	672			9	587
15.9	621	45	672			11.8	573
25	627			Polak & Lu 1973		12.1	575
25.6	625			shake flask-GC		15.1	569
30	640	$\Delta_{\text{sol}}H/(\text{kJ mol}^{-1}) = 1.50$ at 25°C		t/°C	S/g·m ⁻³	17.9	577
30.2	642			0	724	20.1	566
35.2	657			25	573		
42.8	701					$\Delta_{\text{sol}}H/(\text{kJ mol}^{-1}) = 4.70$ at 25°C	
45.3	717						
$\Delta_{\text{sol}}H/(\text{kJ mol}^{-1})$							
25°C	2.3						
2°C	-3.93						
7°C	-3.01						
12°C	-1.38						
17°C	0						
22°C	0.962						
27°C	3.22						
32°C	4.435						
37°C	5.73						
42°C	7.15						

2.

Ben-Naim & Wiff 1979		Schwarz & Miller 1980		Sanemasa et al. 1981		Shaw 1989a (IUPAC)	
shake flask-UV		shake flask-UV		vapor saturation-UV		recommended values	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	572	10	777	15	533	0	690
20	587	20	739	25	557	5	630
		30	754	35	587	10	590
				45	635	20	570
						25	530
						30	590
		Elution chromatography		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.70$ at 25°C		40	640
		t/°C	S/g·m ⁻³			45	660
		10	758				

TABLE 3.1.1.2.1 (Continued)

Ben-Naim & Wiff 1979		Schwarz & Miller 1980		Sanemasa et al. 1981		Shaw 1989 (IUPAC)	
shake flask-UV		shake flask-UV		vapor saturation-UV		recommended values	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
		20	732	Sanemasa et al. 1982		55	860
		30	920	vapor saturation-UV		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.70$ at 25°C	
				15	514		
				25	526		
				35	545		
				45	584		
				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.10$ at 25°C			
3.							
Chen & Wagner 1994b		Ma et al. 2001		Dohányosová et al.2001		Sawamura et al. 2001	
equilibrium flow cell-GC		shake flask-GC/FID		vapor absorption-HPLC/UV		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
30	599	5	540	0.5	563	0	583.5
40	609	15	516	5	552	5	670
50	650	25	519	15	542	10	558
60	737	35	555	25	556	15	553
70	875	45	632	35	590	20	553
80	1013			45	632	25	558
90	1187			55	704	30	573.8
100	1371					35	589.1
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 0.37$ at 25°C				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.0$ at 25°C		40	614.7
						45	640.3
						50	676.6

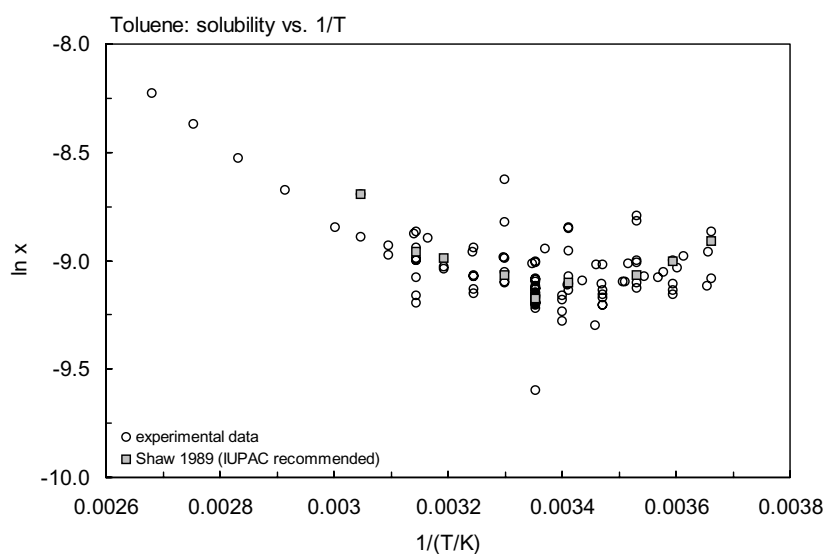
FIGURE 3.1.1.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for toluene.

TABLE 3.1.1.2.3

Reported Henry's law constants of toluene at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1) \qquad \log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \qquad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4) \qquad \ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

1.

Brown & Wasik 1974		Leighton & Calo 1981		Sanemasa et al. 1981		Schoene & S. 1985	
head space-GC		equilibrium cell-GC		vapor liquid-equilibrium		headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
4.5	179	1.0	222	15	382	20	634
6.33	204	1.3	236	25	628	36.9	670
7.06	218	12.4	373	35	979	41.5	680
8.96	244	12.5	361	45	1404	46	690
11.75	294	17.9	459				
12.1	299	19.1	525			eq. 1	K _{AW}
15.1	259	22.7	565	Sanemasa et al. 1982		A	6.90
17.93	414	23	625	vapor-liquid equilibrium		B	2194
20.06	474			t/°C	H/Pa m ³ /mol		
		eq. 3	k _H /atm				
		A	18.46	15	396		
		B	3751	25	664		
				35	1060		
				45	1571		

2.

Ashworth et al. 1988		Kolb et al. 1992		Ettre et al. 1993		Perlinger et al. 1993	
EPICS-GC		static headspace-GC		headspace-GC		equil. headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
10	386	40	933	45	1116	10	293
15	499	60	1565	60	1489	15	390
20	562	70	1915	70	1877	20	499
25	651	80	2312	80	2427	25	660
30	819					30	838
eq 4a	H/(atm m ³ /mol)	eq. 2	1/K _{AW}	eq. 2	1/K _{AW}		
A	5.133	A	7.61	A	-2.532379		
B	3024	B	2647	B	928.3536		

3.

Robbins et al. 1993		Dewulf et al. 1995		Turner et al. 1996		Peng & Wan 1997	
static headspace-GC		EPICS-GC		vapor phase-equilibrium		headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
25	652	2.0	175	11	376	15	391
30	835	6.0	203	15	460	20	475
40	1086	10	250	25	684	25	605

TABLE 3.1.1.2.3 (Continued)

Robbins et al. 1993		Dewulf et al. 1995		Turner et al. 1996		Peng & Wan 1997	
static headspace-GC		EPICS-GC		vapor phase-equilibrium		headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
45	1351	18.2	424	35	1202	30	774
50	1450	25	555			35	984
eq. 4a	H/(atm m ³ /mol)	eq. 1	K _{AW}	eq. 5	K _{AW}	40	1104
A	7.14	A	12.40	A	0.115	45	1309
B	3689	B	4064	B	0.00474		
				C	0.000466	eq. 1	K _{AW}
						A	7.94
						B	1621

4.

Görgényi et al. 2002		Bakierowska & T. 2003	
EPICS-SPME method		headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
2.0	169.3	10	288
6.0	238.2	15	358
10	304.9	20	467
18	476.9	25	612
25	647.5		
30	822.4	eq. 2	1/K _{AW}
40	1214	A	11.926
50	1758	B	3977
60	2286		
eq. 1	K _{AW}		
A	11.25		
B	3770.4		

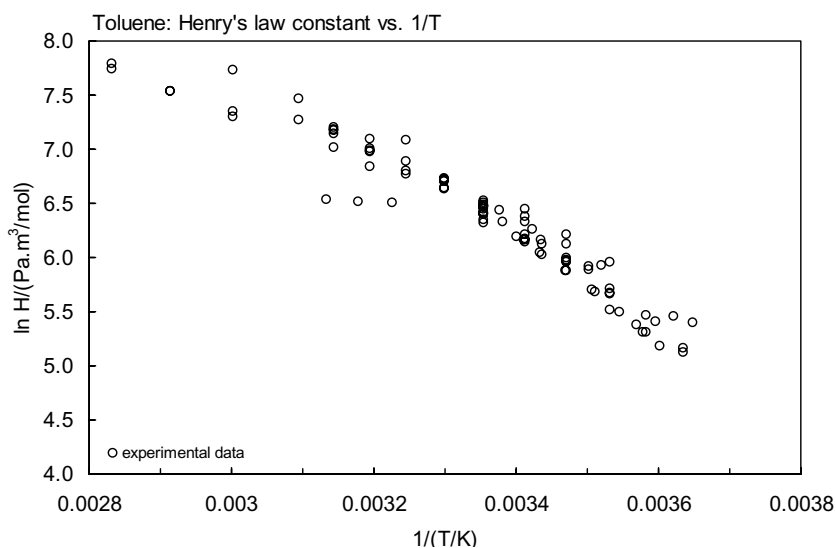


FIGURE 3.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for toluene.

TABLE 3.1.1.2.4

Reported octanol/water partition coefficients and octanol-air partition coefficients of toluene at various temperatures

log K _{OW}		log K _{OA}	
Dewulf et al. 1999		Gruber et al. 1997	
EPICS-GC, both phases		GC det'd activity coeff.	
t/°C	log K _{OW}	t/°C	log K _{OA}
2.2	2.316	20.29	3.42
6	2.405	30.3	3.2
10	2.464	40.4	3.03
14.1	2.38	50.28	2.86
18.7	2.41		
24.8	2.32		
enthalpy change $\Delta H/(\text{kJ mol}^{-1}) = -1.0$ (-16 to 13.9)			

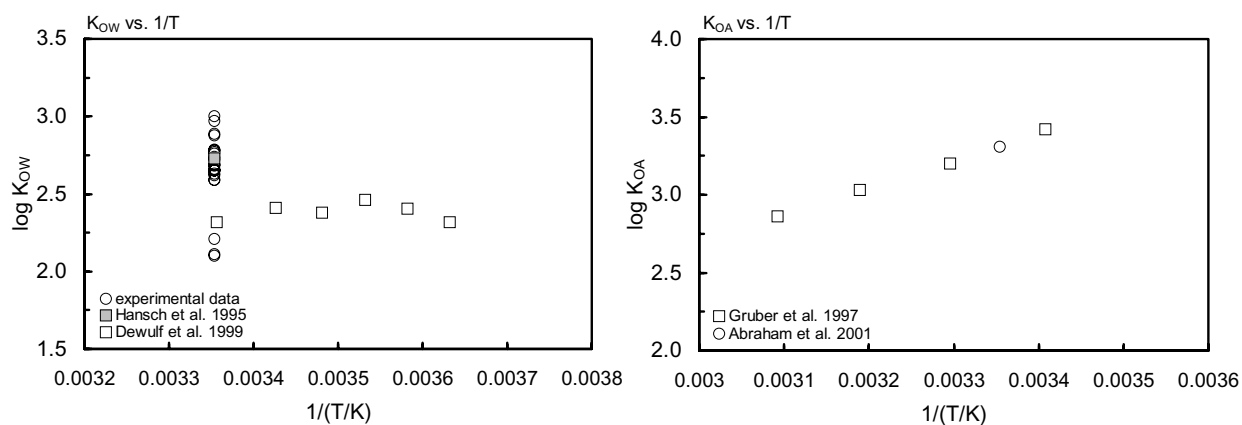
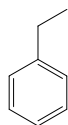


FIGURE 3.1.1.2.4 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for toluene.

3.1.1.3 Ethylbenzene



Common Name: Ethylbenzene

Synonym: phenylethane, ethylbenzol

Chemical Name: ethylbenzene

CAS Registry No: 100-41-4

Molecular Formula: C_8H_{10} , $C_2H_5C_6H_5$

Molecular Weight: 106.165

Melting Point ($^{\circ}C$):

−94.96 (Lide 2003)

Boiling Point ($^{\circ}C$):

136.2 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.867 (Weast 1982–83)

Molar Volume (cm^3/mol):

122.4 ($20^{\circ}C$, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)

140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

42.25, 35.2 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

9.184 (Riddick et al. 1986)

9.16 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

51.43, 52.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

140 ($15^{\circ}C$, shake flask, Fühner 1924)

168 (shake flask-UV, Andrews & Keefer 1950)

175 (shake flask-UV, Klevens 1950)

208* (shake flask-UV, measured range 0.4 – $42.8^{\circ}C$, Bohon & Claussen 1951)

165 (shake flask-UV, Morrison & Billett 1952)

159 (shake flask-GC, McAuliffe 1963)

152 (shake flask-GC, McAuliffe 1966)

177* (shake flask-GC, Polak & Lu 1973)

180* (shake flask-GC, measured range 4.5 – $20.1^{\circ}C$, Brown & Wasik 1974)

203 (shake flask-UV, Vesala 1974)

161 (shake flask-GC, Sutton & Calder 1975)

131 (shake flask-GC, Price 1976)

131 (shake flask-GC, Krzyzanowska & Szeliga 1978)

203, 212 (10 , $20^{\circ}C$, shake flask-UV, Ben-Naim & Wiff 1979)

208*, 184* ($20^{\circ}C$, elution chromatography, shake flask-UV, measured range 10 – $30^{\circ}C$, Schwarz & Miller 1980)

181* (vapor saturation-UV, measured range 15 – $45^{\circ}C$, Sanemasa et al. 1981)

169* (vapor saturation-UV, measured range 15 – $45^{\circ}C$, Sanemasa et al. 1982)

172 (generator column-HPLC/UV, Tewari et al. 1982a)

187 (generator column-HPLC/UV, Tewari et al. 1982c)

166 (HPLC- k' correlation, converted from γ_w , Hafkenscheid & Tomlinson 1983a)

187 (generator column-HPLC/UV, Wasik et al. 1983)

172 (vapor saturation-UV, Sanemasa et al. 1984)

- 192* (generator column-HPLC/UV, measured range 10–45°C, Owens et al. 1986)
 172 (shake flask-purge and trap-GC, Coutant & Keigley 1988)
 169* (IUPAC recommended value, temp range 0–100°C, Shaw 1989b)
 170* (30°C, equilibrium flow cell-GC, measured range 30–100°C, Chen & Wagner 1994c)
 $\ln x = 11.59 - 20.52 \cdot (T_r/K)^{-1} + 4.750 \cdot (T_r/K)^{-2}$; $T_r = T/T_c$, the reduced temp, system temp T divided by critical temp T_c , temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994c)
 $\ln x = -30.799 + 3986.26/(T/K) + 7.9095 \times 10^{-5} \cdot (T/K)^2$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
 170* (vapor absorption technique-HPLC/UV, measured range 0.5–55°C, Dohányosová et al. 2001)
 170* (shake flask-UV, measured range 0–50°C, Sawamura et al. 2001)
 $\ln x = -263.220 + 11024.75/(T/K) + 37.8858 \cdot \ln (T/K)$; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 209.3* (0°C, mercury manometer, measured range –11.6 to 0°C, Linder 1931)
 1546* (30°C, Hg manometer, measured range 10–50°C, Rintelen 1937)
 $\log (P/\text{mmHg}) = 22.90283 - 2847.75/(T/K) - 5 \cdot \log (T/K)$; temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)
 6277* (56.589°C, ebulliometry, measured range 56.589–137.124°C, Willingham et al. 1945)
 $\log (P/\text{mmHg}) = 6.94998 - 1419.315/(212.611 + t/^\circ\text{C})$; temp range 56.6–137.1°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
 1333* (25.9°C, summary of literature data, Stull 1947)
 8399* (63.3°C, static-Hg manometer, measured range 63.3–135.9°C, Buck et al. 1949)
 6398* (56.689°C, ebulliometry, measured range 56.689–137.16°C, Forziati et al. 1949)
 $\log (P/\text{mmHg}) = 6.95904 - 1425.464/(213.345 + t/^\circ\text{C})$; temp range 56.7–137.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
 $\log (P/\text{mmHg}) = -3225/(T/K) - 7.553 \cdot \log (T/K) + 30.49$; temp range 80–120°C (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)
 1276(extrapolated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 6.95719 - 1424.255/(213.206 + t/^\circ\text{C})$, temp range: 45–190°C (Antoine eq. for liquid state, Dreisbach 1955)
 133800* (146.85°C, ebulliometry, measured range 146.85–326.85°C, Ambrose et al. 1967)
 1270* (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = 6.95719 - 1424.255/(213.206 + t/^\circ\text{C})$; temp range 25.88–163.47°C (Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = [-0.2185 \times 9303.3/(T/K)] + 7.809470$; temp range –9.8 to 326.5°C, (Antoine eq., Weast 1972–73)
 9585* (66.031°C, comparative ebulliometry, measured range 66.031–176.953°C, Osborn & Scott 1980)
 $\log (P/\text{atm}) = (1 - 409.229/T) \times 10^{(0.859833 - 6.85948 \times 10^{-4} \cdot T + 5.94439 \times 10^{-7} \cdot T^2)}$; T in K, temp range 243.2–615.0 K (Cox vapor pressure eq., Chao et al. 1983)
 1270, 1265 (extrapolated-Antoine eq., Boublik et al. 1984; quoted, Howard 1989)
 $\log (P/\text{kPa}) = 6.08206 - 1425.305/(213.415 + t/^\circ\text{C})$, temp range: 25.88–92.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.0785 - 1421.653/(212.816 + t/^\circ\text{C})$; temp range 56.6–137.12°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
 1268 (interpolated-Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 6.95719 - 1424.255/(213.21 + t/^\circ\text{C})$; temp range 26–164°C (Antoine eq., Dean 1985, 1992)
 1300 (selected value., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.09280 - 1431.71/(214.099 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 1266 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.06991 - 1416.922/(-69.716 + T/K)$; temp range 298–420 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.10898 - 1445.262/(-57.128 + T/K)$; temp range 409–459 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.36656 - 1665.991/(-26.716 + T/\text{K})$; temp range 457–554 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.49119 - 3056.747/(159.496 + T/\text{K})$; temp range 549–617 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

1280, 283 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 36.1998 - 3.3402 \times 10^3/(T/\text{K}) - 9.7970 \cdot \log (T/\text{K}) - 1.1467 \times 10^{-11} \cdot (T/\text{K}) + 2.5758 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 178–617 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

559.1* (20.06°C, headspace-GC, Brown & Wasik 1974)

757 (calculated-bond contribution, Hine & Mookerjee 1975)

879 (calculated as $1/K_{AW} \cdot C_W/C_A$, reported as exptl., Hine & Mookerjee 1975)

854 (batch stripping-GC, Mackay et al. 1979; quoted, Howard 1989)

734* (vapor-liquid equilibrium-GC, Sanemasa et al. 1981)

797* (vapor-liquid equilibrium.-GC, Sanemasa et al. 1982)

653 (gas stripping-GC, Warner et al. 1987)

798* (EPICS-GC/FID, Ashworth et al. 1988)

$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 11.92 - 4994/(T/\text{K})$, temp range 10–30°C, EPICS measurements, Ashworth et al. 1988)

815 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

756 (infinite activity coeff. γ^∞ in water determined by inert gas stripping-GC, Li et al. 1993)

660* (equilibrium headspace-GC, Perlinger et al. 1993)

788* (static headspace-GC, Robbins et al. 1993)

397 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)

669* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)

302, 838 (6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35‰, Dewulf et al. 1995)

$\ln K_{AW} = -4567/(T/\text{K}) + 0.01047 \cdot Z + 14.001$; with Z salinity 0–35.5‰, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)

602 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

895 (vapor-liquid equilibrium.-GC, Turner et al. 1996)

629 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

943.2 (modified EPICS method-GC, Ryu & Park 1999)

583 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 6.541 - 2100/(T/\text{K})$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

1173–1273 (27°C, equilibrium headspace-GC, solute concn 0.43–18.66 mg/L, measured range 300–315 K, Cheng et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C:

3.15 (shake flask-UV, Hansch et al. 1968; Hansch & Leo 1979; Hansch & Leo 1985)

3.13 (calculated-fragment const., Rekker 1977)

3.12 (HPLC- k' correlation, Hanai et al. 1981)

3.12 (HPLC- k' correlation, D'Amboise & Hanai 1982)

3.26 (HPLC- k' correlation, Hammers et al. 1982)

3.15 (generator column-HPLC/UV, Tewari et al. 1982a)

3.13 (generator column-HPLC/UV, Tewari et al. 1982c)

3.16 (HPLC- k' correlation, Miyake & Terada 1982)

3.24 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983b)

3.13 (generator column-HPLC/UV, Wasik et al. 1983)

3.13 (generator column-RP-LC, Schantz & Martire 1987)

3.13, 3.21 (RP-HPLC capacity factor correlations, Sherblom & Eganhouse 1988)

3.15 (recommended, Sangster 1989, 1993)

3.15 (recommended, Hansch et al. 1995)

3.32, 3.32, 3.53, 3.51 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovsakya et al. 1995)

3.05 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated

- 3.85, 3.62, 3.41, 3.24 (20.29, 30.3, 40.4, 50.28°C, from GC-determined γ^∞ in octanol, Gruber et al. 1997)
 3.72, 3.698 (interpolated value from exptl value of Gruber et al. 1997, calculated using measured γ^∞ in pure octanol by Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 0.67 (clams, exposed to water-soluble fraction of crude oil, Nunes & Benville 1979; selected, Howard 1989)
 2.16 (fish, calculated, Lyman et al. 1982; quoted, Howard 1989)
 2.67 (microorganisms-water, calculated- K_{OW} , Mabey et al., 1982)
 1.19 (goldfish, Ogata et al. 1984)
 1.20, 1.19 (fish: calculated, correlated, Sabljic 1987b)
 2.31 (*S. capricornutum*, Herman et al. 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 1.98 (soil, sorption isotherm, Chiou et al. 1983)
 2.41 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
 2.30 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)
 2.03 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.83, 2.61 (organic cations treated Marlette soil A horizon: HDTMA treated OC 10.03%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.13 (untreated Marlette soil B_t horizon, organic carbon OC 0.30%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 3.23, 3.12, 2.58 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.26, 2.38 (untreated soils: St. Clair soil B_t horizon OC 0.44%; Oshtemo soil B_t horizon OC 0.11%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 3.37, 3.19 (organic cations HDTMA treated soils: St. Clair soil B_t horizon OC 3.25%; Oshtemo soil B_t horizon OC 0.83%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.27, 2.05 (Riddles soil: top layer pH 5.0, below top layer pH 5.3, batch equilibrium, Boyd et al. 1990)
 2.52, 2.47 (RP-HPLC- k' correlation, humic acid-silica column, Szabo et al. 1990a,b)
 2.35, 2.40, 2.42 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
 2.51, 2.51 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 2.32 (HPLC-screening method, Müller & Kördel 1996)
 2.49, 2.73, 2.65, 2.73, 2.77, 2.73 2.74 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon f_{OC} = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)
 2.04, 2.18, 1.90 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, $0.1 \leq$ OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM} :

- 1.98 (Woodburn silt loam soil, 1.9% organic matter, equilibrium isotherm-GC, Chiou et al. 1983)
 1.04 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 1.89, 1.81 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.53, 2.46, 2.08 (organic cations treated Marlette soil B_t horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil B_t horizon OM 4.38%; Oshtemo soil B_t horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k, or Half-lives, $t_{1/2}$:

- Volatilization: rate constants: $k = 0.035 \text{ d}^{-1}$ with $t_{1/2} = 20 \text{ d}$ in spring at 8–16°C, $k = 0.331 \text{ d}^{-1}$ with $t_{1/2} = 2.1 \text{ d}$ in summer at 20–22°C, $k = 0.054 \text{ d}^{-1}$ with $t_{1/2} = 13 \text{ d}$ in winter at 3–7°C for the periods when volatilization

appears to dominate, and $k = 0.097 \text{ d}^{-1}$ with $t_{1/2} = 7.1 \text{ d}$ with HgCl_2 in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);

$t_{1/2} \sim 3.1 \text{ h}$ of evaporation from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s at 20°C (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982).

Oxidation: rate constant k ; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

$k_{\text{OH}} = (4.8 \pm 1.0) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 4.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.24\text{--}24 \text{ h}$ (Darnall et al. 1976)

$t_{1/2} \approx 15 \text{ h}$ in water, probably not important as aquatic fate (Callahan et al. 1979)

$k_{\text{OH}} = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and residence time of 1.4 d, loss of 51% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $720 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 radical (Mabey et al. 1982)

$k_{\text{OH}} = 4.4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 1.3 \text{ d}$ in the atmosphere (Mill 1982)

$k_{\text{O}_3} = 340 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k = (14 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 100 mM *t*-BuOH as scavenger at pH 2.0 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{\text{OH}} = 7.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 8.56\text{--}85.6 \text{ h}$ (Atkinson 1985)

$k_{\text{OH}} = 6.47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Ohta & Ohshima 1985)

$k_{\text{OH}}(\text{calc}) = 6.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 7.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}} = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $\sim 298 \text{ K}$ (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 6.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: not aquatically significant (Callahan et al. 1979);

no hydrolyzable functional groups (Mabey et al. 1982)

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of $1.36 \times 10^{-6} \text{ L/L}$ (Jamison et al. 1976)

$t_{1/2}(\text{aq. aerobic}) = 72\text{--}240 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life and seawater dieaway test data (Van der Linden 1978; Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 4224\text{--}5472 \text{ h}$, based on anaerobic groundwater die-away test data (Wilson et al. 1986; Howard et al. 1991)

$k = 0.5 \text{ d}^{-1}$, significant degradation under favourable conditions in an aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2} \sim 2 \text{ d}$ degradation by established microorganisms depending on body of water and its temperature (Howard 1989)

$k = 0.07 \text{ yr}^{-1}$ with $t_{1/2} = 37 \text{ d}$ (Olsen & Davis 1990).

Biotransformation: $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982).

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}24 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976); photodecomposition $t_{1/2} = 5.0 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976); residence time of 1.4 d, loss of 51% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

summer daylight lifetime $\tau = 20 \text{ h}$ due to reaction with OH radical (Altshuller 1991);

$t_{1/2} = 8.56\text{--}85.6 \text{ h}$, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991).

Surface Water: $t_{1/2} = 5\text{--}6 \text{ h}$ (Callahan et al. 1979), based on the estimated evaporative loss of toluene at 25°C and 1 m depth of water (Mackay & Leinonen 1975);

$t_{1/2} = 20 \text{ d}$ in spring at $6\text{--}16^\circ\text{C}$, $t_{1/2} = 2.1 \text{ d}$ in summer at $20\text{--}22^\circ\text{C}$, $t_{1/2} = 13 \text{ d}$ in winter at $3\text{--}7^\circ\text{C}$ and $t_{1/2} = 7.1 \text{ d}$ with HgCl_2 in marine mesocosm experiments (Wakeham et al. 1983);

$t_{1/2} = 72\text{--}240 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Howard et al. 1991).

Ground water: $t_{1/2} = 144\text{--}5472 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life and seawater dieaway test data (Van der Linden 1978; Howard et al. 1991);

$t_{1/2} \sim 0.3 \text{ yr}$ from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981).

Soil: $t_{1/2} = 72\text{--}240$ h, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Howard et al. 1991);
 $t_{1/2} < 10$ d (Ryan et al. 1988).

Biota:

TABLE 3.1.1.3.1
Reported aqueous solubilities of ethylbenzene at various temperatures

1.

Bohon & Claussen 1951		Polak & Lu 1973		Brown & Wasik 1974		Ben-Naim & Wiffb 1979	
shake flask-UV		shake flask-GC		headspace-GC		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0.4	219	0	197	4.5	196	10	203
5.2	213	25	177	6.3	192	20	212
20.7	207			7.1	186		
21.2	207			9	187		
25	208			11.8	181		
25.6	209			12.1	183		
30.2	211			15.1	180		
34.9	221			17.9	184		
42.8	231			20.1	180		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 11.9$			
25°C	1.6			at 25°C			
2°C	-3.98						
7°C	-2.74						
12°C	-1.63						
17°C	-0.343						
22°C	-0.167						
27°C	1.97						
32°C	3.615						
37°C	7.36						

2.

Schwarz & Miller 1980		Sanemasa et al. 1981		Owens et al. 1986		Shaw 1989b (IUPAC)	
shake flask-UV		vapor saturation-UV		generator column-HPLC/UV		recommended values	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	180	15	176	10	197	0	200
20	184	25	181	14	192	10	180
		35	194	17	189	20	181
elution chromatography		45	215	18	183	25	169
10	211			19	178	30	190
20	208	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.60$		20	188	40	200
		at 25°C		21	183	50	220
				22	182	60	250
		Sanemasa et al. 1982		23.5	186	70	280
		vapor saturation-UV		25	192	80	330
		t/°C S/g·m⁻³		25.8	186	90	390
				28	185.5	100	460
				30	188.7		
				35	193		
		15	160			$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.1$	
		25	169				

TABLE 3.1.1.3.1 (Continued)

Schwarz & Miller 1980		Sanemasa et al. 1981		Owens et al. 1986		Shaw 1989b (IUPAC)	
shake flask-UV		vapor saturation-UV		generator column-HPLC/UV		recommended values	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
		35	176	40	205	at 25°C	
		45	196	45	211.4		
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.90$ at 25°C		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.30$ 25°C			
3.							
Chen & Wagner 1994c		Dohányosová et al. 2001		Sawamura et al. 2001			
equil. flow cell-GC		vapor abs-HPLC/UV		shake flask-UV			
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³		
30	170	0.5	169	0	190.8		
40	172	5	167	5	182		
50	198	15	167	10	175		
60	240	25	170	15	170		
70	291	35	177	20	169		
80	353	45	188	25	170		
90	410	55	213.5	30	173.8		
100	504			35	179.8		
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.0$		40	188.1		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.30$		at 25°C		45	196.9		
at 25°C				50	208		

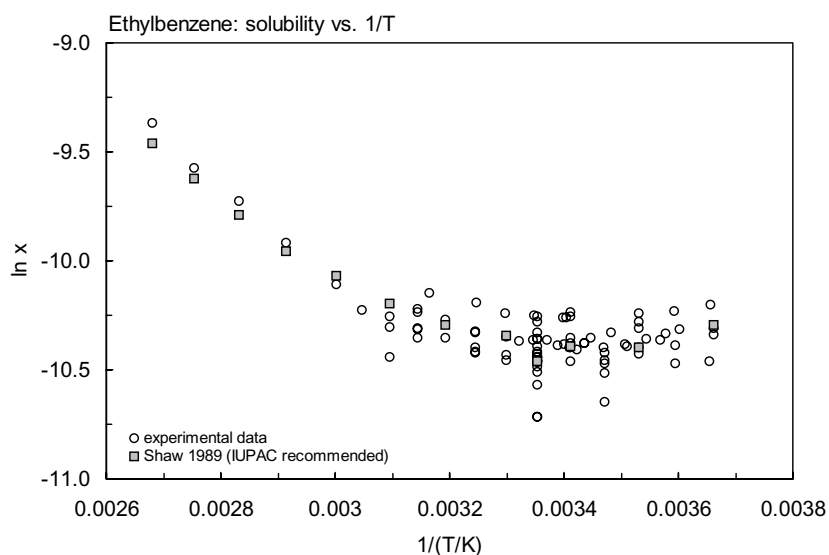
FIGURE 3.1.1.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for ethylbenzene.

TABLE 3.1.1.3.2 (Continued)

Forziati et al. 1949		Ambrose et al. 1967		Zwolinski & Wilhoit 1971		Osborn & Scott 1980	
ebulliometry		ebulliometry		selected values		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
79.791	16633	266.85	1321500	68.596	10666	84.587	19933
83.619	19944	286.85	1751100	74.105	13332	90.869	25023
89.09	23474	306.85	2279100	84.687	19998	97.199	31177
95.074	28978	326.85	2924900	92.68	26664	103.575	38565
100.675	34925			99.182	33331	110.001	47375
107.21	43360	eq. 5	P/bar	104.703	39997	116.474	57817
114.046	53698	A	21.956	113.823	53329	122.998	70120
121.331	66796	B	2923.84	121.266	66661	129.571	84532
129.234	83749	C	5.67301	127.603	79993	136.193	101325
134.815	97645	D	1772	133.152	93326	142.863	120790
135.413	99235			134.185	95991	149.587	143240
135.969	100725			135.196	98659	156.356	169020
136.602	102462			135.164	101325	163.174	198490
137.16	103999			25	1266.6	170.038	232020
						176.953	270030
eq. 2	P/mmHg			eq. 2	P/mmHg		
A	6.959			A	6.95719	data fitted to 4-constant vapor pressure eq.	
B	1425.46			B	1424.255		
C	213.345			C	213.206		
bp/°C	136.186			bp/°C	136.186		
				$\Delta H_v/(\text{kJ mol}^{-1})$			
				at 25°C	42.25		
				at bp	35.56		

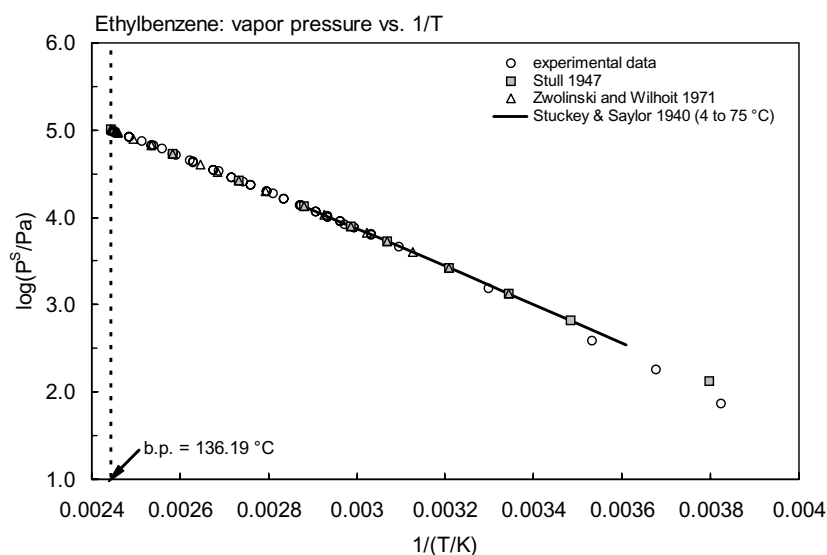


FIGURE 3.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for ethylbenzene.

TABLE 3.1.1.3.3

Reported Henry's law constants of ethylbenzene at various temperatures and temperature dependence equations

$$\begin{aligned} \ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) & (4) & \ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K) & (4a) \\ K_{AW} &= A - B\cdot(T/K) + C\cdot(T/K)^2 & (5) & & \end{aligned}$$

1.

Brown & Wasik 1974		Sanemasa et al. 1981		Sanemasa et al. 1982		Ashworth et al. 1988	
head space-GC		vapor-liquid equilibrium		vapor-liquid equilibrium		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
4.5	187.5	15	459	15	418	10	330
6.33	217.2	25	797	25	734	15	457
7.06	235.1	35	1339	35	1211	20	609
8.96	265	45	1436	45	1436	25	798
11.75	329					30	1064
12.1	333.6						
15.1	409.7					eq. 4a	H/(atm m ³ /mol)
17.93	480.2					A	11.92
20.06	559.1					B	4994

2.

Robbins et al. 1993		Perlinger et al. 1993		Dewulf et al. 1995	
static headspace-GC		equilibrium headspace-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
25	788	10	306	2	180
30	1034	15	428	6	194
40	1662	20	583	10	257
		25	660	18.2	497
eq. 4	H/(Pa m ³ /mol)	30	1044	25	669
A	7.14				
B	3689			eq 1	K _{AW}
				A	14.001
				B	4567

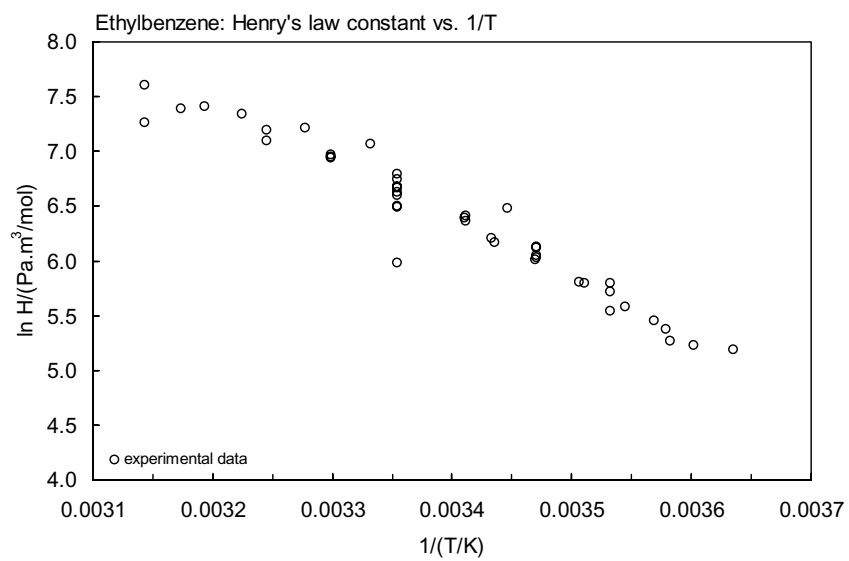
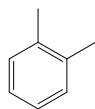


FIGURE 3.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for ethylbenzene.

3.1.1.4 *o*-Xylene

Common Name: *o*-Xylene

Synonym: 1,2-dimethylbenzene, *o*-xylol, 2-methyltoluene

Chemical Name: *o*-xylene

CAS Registry No: 95-47-6

Molecular Formula: C_8H_{10} , $C_6H_4(CH_3)_2$

Molecular Weight: 106.165

Melting Point ($^{\circ}C$):

−25.2 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

144.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8802 (Weast 1982–83)

Molar Volume (cm^3/mol):

120.6 ($20^{\circ}C$, calculated-density)

140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

43.434, 36.82 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

13.6 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$)

55.23 (Yalkowsky & Valvani 1980)

54.9, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated *, are compiled at the end of this section):

204	(shake flask-UV, Andrews & Keefer 1949)
175	(shake flask-GC, McAuliffe 1963)
175	(shake flask-GC, McAuliffe 1966)
176	(shake flask-GC, Hermann 1972)
213*	(shake flask-GC, Polak & Lu 1973)
170.5	(shake flask-GC, Sutton & Calder 1975)
167	(shake flask-GC, Price 1976)
167	(shake flask-GC, Krzyzanowska & Szeliga 1978)
240*	($20^{\circ}C$, shake flask-UV, Ben-Naim & Wiff 1979)
179*	(vapor saturation-UV spec., measured range 15 – $45^{\circ}C$, Sanemasa et al. 1982)
221	(generator column-HPLC/UV, Tewari et al. 1982c)
221	(generator column-HPLC/UV, Wasik et al. 1983)
176	(shake flask-purge and trap-GC, Coutant & Keigley 1988)
173*	(IUPAC recommended value, temp range 0 – $45^{\circ}C$, Shaw 1989b)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

146.7*	($0.60^{\circ}C$, mercury manometer, measured range -17 to $0.60^{\circ}C$, Linder 1931)
767*	($20^{\circ}C$, Hg manometer, Kassel 1936)
$\log (P/mmHg) = -2830.0/(T/K) - 5 \cdot \log (T/K) + 22.7480$; temp range 0 – $80^{\circ}C$ (vapor pressure eq. from Hg manometer measurements, Kassel 1936)	
987*	($30^{\circ}C$, Hg manometer, measured range 10 – $50^{\circ}C$, Rintelen et al. 1937)

$\log (P/\text{mmHg}) = -2908.07/(T/K) - 5 \cdot \log (T/K) + 22.95279$; temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)

880* (Hg manometer measurements, Pitzer & Scott 1943)

$\log (P/\text{mmHg}) = -3327.16/(T/K) - 8.0 \log (T/K) + 31.7771$; temp range 0–60°C (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)

6354* (63.460°C, ebulliometry, measured range 63.460–145.367°C, Willingham et al. 1945)

6401* (63.608°C, ebulliometry, measured range 63.608–145.400°C, Forziati et al. 1949)

$\log (P/\text{mmHg}) = 6.99937 - 1474.969/(213.714 + t/^\circ\text{C})$; temp range 63.5–145.4°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

266.6* (20.2°C, summary of literature data, Stull 1947)

$\log (P/\text{mmHg}) = 6.99891 - 1474.679/(213.686 + t/^\circ\text{C})$; temp range 63.6–145.4°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

892 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/\text{mmHg}) = 6.99891 - 1474.679/(213.686 + t/^\circ\text{C})$; temp range 50–200°C (Antoine eq. for liquid state, Dreisbach 1955)

1333* (32.155°C, compiled data, temp range 32.155–172.095°C, Bond & Thodos 1960)

108000* (146.85°C, ebulliometry, measured range 146.85–346.85°C, Ambrose et al. 1967)

882* (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 6.99891 - 1474.679/(213.686 + t/^\circ\text{C})$; temp range 32.14–172.07°C (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 9998.5/(T/K)] + 8.147551$; temp range –3.8 to 144.4°C (Antoine eq., Weast 1972–73)

$\log (P/\text{atm}) = (1 - 417.496/T) \times 10^{(0.855257 - 6.48662 \times 10^4 \cdot T + 5.53883 \times 10^7 \cdot T^2)}$; T in K, temp range: 253.2–631.64 K (Cox vapor pressure eq., Chao et al. 1983)

882, 885 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.12699 - 1476.753/(213.911 + t/^\circ\text{C})$; temp range 63.46–145.4°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.9422 - 1387.336/(206.409 + t/^\circ\text{C})$; temp range 0–50°C (Antoine eq. from reported exptl. data of Pitzer & Scott 1943, Boublik et al. 1984)

882 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.99891 - 1474.679/(213.69 + t/^\circ\text{C})$; temp range 32–172°C (Antoine eq., Dean 1985, 1992)

880 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.13072 - 1479.82/(214.315 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

885 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.13132 - 1480.155/(-58.804 + T/K)$; temp range 333–419 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15921 - 1502.949/(-55.725 + T/K)$; temp range 416–473 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.46119 - 1772.963/(-18.84 + T/K)$; temp range 471–571 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.91427 - 3735.582/(229.953 + T/K)$; temp range 567–630 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 37.2413 - 3.4573 \times 10^3/(T/K) - 10.126 \cdot \log (T/K) + 9.0676 \times 10^{-11} \cdot (T/K) + 2.6123 \times 10^{-6} \cdot (T/K)^2$, temp range 248–630 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

542, 506 (calculated as $1/K_{AW}$, calculated-bond contribution, Hine & Mookerjee 1975)

647 (vapor liquid equilibrium-concentration ratio, Leighton & Calo 1981)

526* (vapor-liquid equilibrium, Sanemasa et al. 1982)

594 (20°C, EPICS-GC, Yurteri et al. 1987)

493* (EPICS-GC/FID, Ashworth et al. 1988)

$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 5.541 - 3220/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

424 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

592 (concentration ratio, Anderson 1992)

1067* (40°C, equilibrium headspace-GC, Kolb et al. 1992)

$\ln (1/K_{AW}) = -7.61 + 2647/(T/K)$, temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

485 (infinite activity coeff. γ^∞ in water determined by inert gas stripping-GC, Li et al. 1993)

506* (static headspace-GC, Robbins et al. 1993)

372 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)

429* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)

189, 496 (6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35‰ Dewulf et al. 1995)

$\ln K_{AW} = -4232/(T/K) + 0.01115 \cdot Z + 12.400$; with Z salinity 0–35.5‰, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)

412 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

731 (vapor-liquid equilibrium-GC, Turner et al. 1996)

464.4 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

390 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 5.064 - 1719/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C:

3.15 (calculated- π substituent constant, Hansch et al. 1968)

2.73 (shake flask-LSC, Banerjee et al. 1980)

3.19 (HPLC- k' correlation, Hammers et al. 1982)

3.13 (generator column-HPLC/UV, Tewari et al. 1982b,c)

3.13 (generator column-HPLC/UV, Wasik et al. 1983)

3.13; 3.14, 3.14, 3.06, 3.16, 3.42 (quoted exptl.; calculated- π const., f const., MW, MCI χ , TSA, Doucette & Andren 1988)

3.25, 3.35 (RP-HPLC- k' capacity factor correlations, Sherblom & Eganhouse 1988)

3.12 (recommended, Sangster 1989)

3.18 (normal phase HPLC- k' correlation, Govers & Evers 1992)

3.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.80* (30.3°C, from GC-determined γ^∞ in octanol, measured range 30.3–50.28°C, Gruber et al. 1997)

3.72 (calculated-measured γ^∞ in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

1.33 (eels, Ogata & Miyake 1978)

0.79 (clams, Nunes & Benville 1979)

1.15 (goldfish, Ogata et al. 1984)

2.34 (*S. capricornutum*, Herman et al. 1991)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C:

1.68–1.83 (Nathwani & Philip 1977)

2.35 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)

2.73 (HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)

2.37, 2.40 (RP-HPLC- k' correlation, humic acid-silica column, Szabo et al. 1990a,b)

3.13 (average of 5 soils, sorption isotherms by batch equilibrium method, Xing et al. 1994)

2.36, 2.65, 2.65 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)

2.45, 2.45 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

2.40, 2.70, 2.58, 2.68, 2.73, 2.69, 2.68 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 5.61$ h from water depth of 1 m (Mackay & Leinonen 1975; Haque et al. 1980);

$t_{1/2} \sim 3.2$ h of evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s (Lyman et al. 1982);

$t_{1/2} \sim 31\text{--}125$ h of evaporation from a typical river or pond (Howard 1990).

Photolysis: $k = 7.46 \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO^- in the gas (Dilling et al. 1988).

Oxidation: rate constant k ; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

$k_{\text{OH}} = (7.7 \pm 2.3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$; $k_{\text{O(}^3\text{P)}} = (1.05 \pm 0.11) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ with O(^3P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{\text{OH}} = (15.3 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O(}^3\text{P)}} = (1.74 \pm 0.18) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction of O(^3P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{\text{OH}} = 8.4 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.24\text{--}24$ h (Darnall et al. 1976)

$k_{\text{OH}}^* = (14.3 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured over temp range $296\text{--}473$ K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{\text{OH}} = (12.9, 13.0, 12.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{\text{OH}} = 13.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and residence time of 0.8 d, loss of 71.3% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K with a calculated lifetime $\tau > 2300$ d, and a calculated lifetime of 0.8 d due to reaction with OH radical at room temp. (Atkinson et al. 1982)

$k_{\text{O}_3} = 950 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k_{\text{OH}} = (5.9\text{--}12) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.47\text{--}1.0$ d (Mill 1982)

$k = (90 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH $1.7\text{--}5.0$ and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{\text{NO}_3} = 1.1 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 13.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 4.4\text{--}44$ h (Atkinson 1985)

$k_{\text{OH}} = 12.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Ohta & Ohyama 1985)

$k_{\text{OH}} = 12.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 24.2°C , with a calculated atmospheric lifetime of 0.93 d (Edney et al. 1986)

$k_{\text{OH}}(\text{calc}) = 6.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 14.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship] Atkinson 1987)

$k_{\text{OH}} = 1.47 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 3.74 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} = 1.47 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 3.7 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson & Aschmann 1988)

$k_{\text{OH}}^* = 1.37 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ independent over $296\text{--}320$ K (recommended, Atkinson 1989)

$k_{\text{OH}} = 13.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}}(\text{calc}) = 6.92 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 14.75 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}}(\text{calc}) = 6.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{exptl}) = 13.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of $1.62 \times 10^{-6} \text{ L/L}$ (Jamison et al. 1976);

$t_{1/2}(\text{aq. Aerobic}) = 168\text{--}672$ h, estimated based on aqueous screening test data (Bridie et al. 1979; Howard et al. 1991) and soil column study simulating an aerobic river/ground-water infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 4320\text{--}8640$ h, estimated based on acclimated grab sample data for anaerobic soil from a groundwater aquifer receiving landfill leachate (Wilson et al. 1986) and a soil column study simulating an anaerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$k = 0.06 \text{ yr}^{-1}$ with $t_{1/2} = 32$ d (Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 7$ d, $t_{1/2}(\text{anaerobic}) = 180$ d in natural waters (Capel & Larson 1995)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976);

residence time of 0.8 d, loss of 71.3% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

calculated lifetimes $\tau > 2300$ d and 0.8 d due to reactions with O_3 and OH radical respectively at room temp. (Atkinson et al. 1982);

$t_{1/2} = 4.4\text{--}44$ h, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);

summer daylight lifetime $\tau = 10$ h due to reaction with OH radical (Altshuller 1991);

calculated lifetime $\tau = 0.93$ d due to reaction with OH radical (Edney et al. 1986).

Surface Water: photooxidation $t_{1/2} = 3.9 \times 10^5\text{--}2.7 \times 10^8$ h in water, based on estimated rate data for alkoxy radical in aqueous solution (Hendry et al. 1974);

$t_{1/2} = 5.18$ h, based on evaporative loss at 25°C and 1 m depth of water (Mackay & Leinonen 1975; Haque et al. 1980);

$t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

$t_{1/2} = 1\text{--}5$ d, volatilization to be the dominant removal process (Howard 1990).

$t_{1/2}(\text{aerobic}) = 7$ d, $t_{1/2}(\text{anaerobic}) = 180$ d in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 336\text{--}8640$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Wilson et al. 1986; Howard et al. 1991);

$t_{1/2} \sim 0.3$ yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981).

Soil: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991).

Biota: $t_{1/2} = 2$ d to eliminate from eels in seawater (Ogata & Miyake 1978).

TABLE 3.1.1.4.1

Reported aqueous solubilities of *o*-xylene at various temperatures

Polak & Lu 1973		Ben-Naim & Wiff 1979		Sanemasa 1982		Shaw 1989b (IUPAC)	
shake flask-GC		shake flask-UV		vapor saturation-UV		recommended values	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	142	10	212.4	15	168	0	140
25	213	20	240	25	179	15	170
				35	198	25	173
				45	214	35	200
						45	210

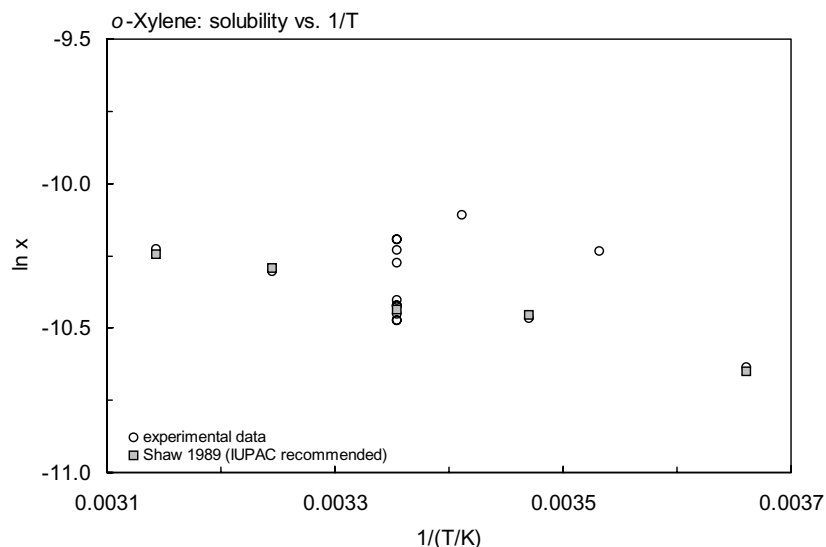


FIGURE 3.1.1.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *o*-xylene.

TABLE 3.1.1.4.2

Reported vapor pressures of *o*-xylene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) + D \cdot P/(T/K)^2 & (5) & & \end{array}$$

1.

Kassel 1936		Rintelen et al. 1937		Stuckey & Saylor 1940		Pitzer & Scott 1943	
mercury manometer		mercury manometer		mercury manometer		mercury manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	215	10	213	measured 4–75°C		0	173
10	417	30	987	eq. 4	P/mmHg	12.5	400
20	767	50	3346	A	22.95279	25.0	880
30	1347			B	908.07	37.5	1800
40	2280	bp 144.0–144.1°C		C	5.0	50	3400
50	3680					60	5413
60	5826	Linder 1931		bp/°C	144.39–144.41		
70	8892	mercury manometer				eq. 4	P/mmHg
80	13186	t/°C	P/Pa			A	31.7771
		–17	26.66			B	3327.16
eq. 4	P/mmHg	–10.7	56.0			C	8.0
A	23.7480	0	141.3				
B	2830.06	0.60	146.7				
C	5.0						
							$\Delta H_v/(\text{kJ mol}^{-1}) = 43.806$ at 25°C

2.

Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Bond & Thodos 1960	
ebulliometry		summary of literature data		ebulliometry		compiled data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
63.460	6354	–3.80	133.3	63.608	6401	32.155	1333
67.746	7654	20.2	266.6	67.852	7693	63.48	6354
71.481	8963	32.1	1333	71.548	8991	74.87	10303
74.857	10303	45.1	2666	74.916	10331	112.46	39997
77.993	11699	59.5	5333	78.048	11722	141.35	93326
82.242	13819	68.8	7999	82.285	13843	172.095	199984
87.081	16621	81.3	13332	87.101	16635		
91.987	19924	100.2	26664	92.015	19945	eq. 5	P/mmHg
96.541	23450	121.7	53329	96.568	23475	A	25.82849
102.632	28954	144.4	101325	102.657	28979	B	3040.72
108.227	34897			198.250	34926	C	5.94175
114.965	43322	mp/°C	–25.2	114.988	43362	D	2.61456
121.909	53654			121.935	53700		
129.318	66756			129.333	66797	bp/°C	144.426
137.346	83717			137.356	83750		
143.007	97604			143.619	97647		
143.614	99200			143.626	99236		
144.176	100692			144.190	87395		
144.809	102385			144.832	90465		

(Continued)

TABLE 3.1.1.4.2 (Continued)

Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Bond & Thodos 1960	
ebulliometry		summary of literature data		ebulliometry		compiled data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
145.367	103905			145.400	104000		
eq. 2	P/mmHg			eq. 2	P/mmHg		
A	6.99937			A	6.99891		
B	1474.967			B	1474.679		
C	144.414			C	213.686		
bp/°C	144.414			bp/°C	144.411		

3.

Ambrose et al. 1967		Zwolinski & Wilhoit 1971			
ebulliometry		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
146.85	108000	32.14	1333	145.395	103991
166.85	177200	45.13	2666	146.359	106658
186.85	276700	53.38	4000	150.912	119990
206.85	413900	59.56	5333	155.08	13322
226.85	598300	64.558	6666	162.53	159987
246.85	839100	68.778	7999	172.07	199984
266.85	1146500	75.704	10666	25.0	879.9
286.85	1532100	81.314	13332		
306.85	2009000	92.085	19998	eq. 2	P/mmHg
326.85	2592500	100.217	26664	A	6.99891
346.85	3304100	106.829	33331	B	1474.679
		112.441	39997	C	213.686
eq. 5	P/bar	121.708	53329		
A	20.79970	129.267	66661	bp/°C	144.411
B	2921.11	135.700	79993		
C	5.26888	141.332	93326	ΔH_v /(kJ mol ⁻¹)	
D	1672	142.380	95991	at 25°C	43.43
		143.407	98659	at bp	36.82
1 bar = 1×10 ⁵ Pa		144.411	101325		

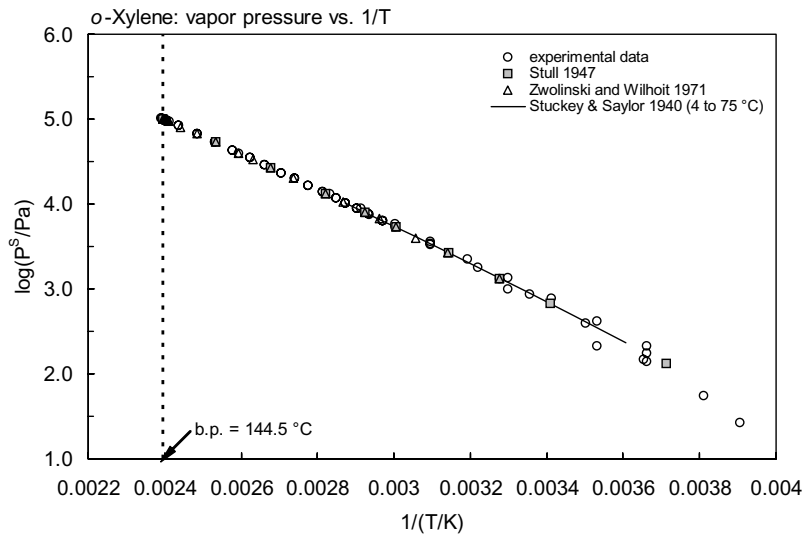


FIGURE 3.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for *o*-xylene.

TABLE 3.1.1.4.3
Reported Henry’s law constants of *o*-xylene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)				
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)				
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)							
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)				
$K_{AW} = A - B (T/K) + C (T/K)^2$		(5)							
Sanemasa et al. 1982		Ashworth et al. 1988		Kolb et al. 1992		Robbins et al. 1993		Dewulf et al. 1995	
vapor-liquid equilibrium		EPICS-GC		headspace-GC		static headspace-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
15	299	10	289	40	1067	25	506	2	133
25	526	15	366	60	2114	30	637	6	118
35	844	20	480	70	2825	40	1104	10	155
45	1323	25	493	80	2966	45	1074	18	325
		30	634			50	1175	25	429
		eq. 4a		eq. 2	K _{AW}	eq. 4		eq 1	K _{AW}
		H/(atm m ³ /mol)		A	761	H/(Pa m ³ /mol)		A	12.4
		A	5.541	B	2647/R	A	17.67818	B	4243
		B	3220			B	3397.97		

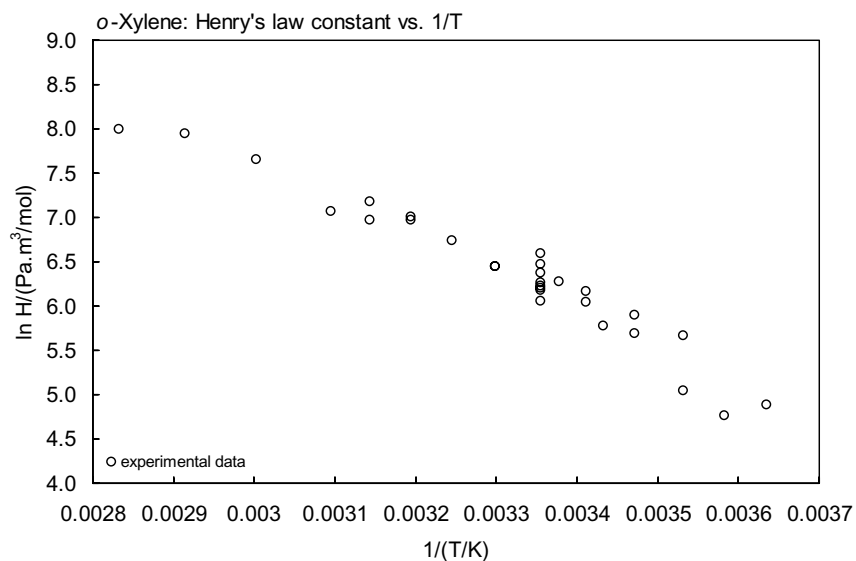
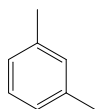


FIGURE 3.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for *o*-xylene.

TABLE 3.1.1.4.4
Reported octanol-air partition coefficients of *o*-xylene at various temperatures

Gruber et al. 1997

GC det'd activity coefficient	
$t/^\circ\text{C}$	$\log K_{\text{OA}}$
20.29	-
30.3	3.80
40.4	3.59
50.28	3.38

3.1.1.5 *m*-Xylene

Common Name: *m*-Xylene

Synonym: 1,3-dimethylbenzene, *m*-xylol, 3-methyltoluene

Chemical Name: *m*-xylene

CAS Registry No: 108-38-3

Molecular Formula: C_8H_{10} , $C_6H_4(CH_3)_2$

Molecular Weight: 106.165

Melting Point ($^{\circ}C$)

−47.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

139.12 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8842 (Weast 1982–83)

Molar Volume (cm^3/mol):

120.1 ($20^{\circ}C$, calculated-density)

140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

42.656, 36.36 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

11.57 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

51.88 (Yalkowsky & Valvani 1980)

51.4, 45.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$, or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

173 (shake flask-UV, Andrews & Keefer 1949)

196* (shake flask-UV, measured range 0.4 – $39.6^{\circ}C$, Bohon & Claussen 1951)

157 (shake flask-GC, Hermann 1972)

162* (shake flask-GC, Polak & Lu 1973)

206 (shake flask-UV, Vesala 1974)

146 (shake flask-GC, Sutton & Calder 1975)

160* (synthetic method-GC, measured range 20 – $70^{\circ}C$, Chernoglazova & Simulin 1976)

134 (shake flask-GC, Price 1976)

134 (shake flask-GC, Krzyzanowska & Szeliga 1978)

162* (vapor saturation-UV spec., measured range 15 – $45^{\circ}C$, Sanemasa et al. 1982)

159 (generator column-HPLC/UV, Tewari et al. 1982c)

160 (generator column-HPLC/UV, Wasik et al. 1983)

160* (IUPAC recommended value, temp range 0 – $70^{\circ}C$, Shaw 1989b)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1812.7* ($-2.80^{\circ}C$, mercury manometer, measured range -8.40 to $-2.80^{\circ}C$, Linder 1931)

833* ($20^{\circ}C$, Hg manometer, Kassel 1936)

$\log (P/mmHg) = -2876.3/(T/K) - 5 \cdot \log (T/K) + 22.9425$; temp range 0 – $80^{\circ}C$ (vapor pressure eq. from Hg manometer measurements, Kassel 1936)

1213* ($30^{\circ}C$, Hg manometer, measured range 10 – $50^{\circ}C$, Rintelen et al. 1937)

- $\log (P/\text{mmHg}) = -2870.38/(T/K) - 5 \cdot \log (T/K) + 22.92341$; temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)
- 1113* (Hg manometer, measured range 0–60°C, Pitzer & Scott 1943)
- $\log (P/\text{mmHg}) = -2871.66/(T/K) - 5.0 \log (T/K) + 22.9270$; temp range 0–60°C (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)
- 6355* (59.203°C, ebulliometry, measured range 59.203–140.041°C, Willingham et al. 1945)
- $\log (P/\text{mmHg}) = 7.00343 - 1458.214/(214.609 + t/^\circ\text{C})$; temp range 59.2–140.0°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
- 266.6* (16.8°C, summary of literature data, temp range –6.9 to 139.1°C, Stull 1947)
- 6400* (59.335°C, ebulliometry, measured range 59.335–140.078°C, Forziati et al. 1949)
- $\log (P/\text{mmHg}) = 8.00849 - 1461.925/(215.073 + t/^\circ\text{C})$; temp range 59.3–140.1°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
- 1115 (extrapolated-Antoine eq., Dreisbach 1955)
- $\log (P/\text{mmHg}) = 7.00908 - 1462.266/(215.105 + t/^\circ\text{C})$; temp range 45–195°C (Antoine eq. for liquid state, Dreisbach 1955)
- 124200* (146.85°C, ebulliometry, measured range 146.85–316.85°C, Ambrose et al. 1967)
- 1100* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
- $\log (P/\text{mmHg}) = 7.00908 - 1462.266/(215.105 + t/^\circ\text{C})$; temp range 28.24–166.39°C (Antoine eq., Zwolinski & Wilhoit 1971)
- $\log (P/\text{mmHg}) = [-0.2185 \times 9904.2/(T/K)] + 8.167049$; temp range –6.9 to 139.1°C (Antoine eq., Weast 1972–73)
- $\log (P/\text{atm}) = (1 - 3412.335/T) \times 10^{(0.859841 - 6.73249 \times 10^4 \cdot T + 5.87438 \times 10^7 \cdot T^2)}$; T in K, temp range 243.2–619.2 K (Cox vapor pressure eq., Chao et al. 1983)
- 1104, 1142 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.13232 - 1460.805/(214.895 + t/^\circ\text{C})$; temp range 59.2–140.4°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.4729 - 1641.628/(230.899 + t/^\circ\text{C})$; temp range: 0–60°C (Antoine eq. from reported exptl. data of Pitzer & Scott 1943, Boublik et al. 1984)
- 1106 (extrapolated-Antoine eq., Dean 1985, 1992)
- $\log (P/\text{mmHg}) = 7.00908 - 1462.266/(215.11 + t/^\circ\text{C})$; temp range: 28–166°C (Antoine eq., Dean 1985, 1992)
- 1100 (selected lit. value., Riddick et al. 1986)
- $\log (P/\text{kPa}) = 6.13785 - 1465.39/(215.512 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
- 1110 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.14083 - 1457.244/(-57.442 + T/K)$; temp range 331–414 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.76037 - 1292.22/(-72.052 + T/K)$; temp range 267–301 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.17035 - 1490.184/(-54.184 + T/K)$; temp range 412–462 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.42535 - 1710.901/(-24.591 + T/K)$; temp range 461–554 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 7.59221 - 3163.74/(165.278 + T/K)$; temp range 550–617 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- $\log (P/\text{mmHg}) = 34.6803 - 3.2981 \times 10^3/(T/K) - 9.2570 \cdot \log (T/K) - 4.3563 \times 10^{-10} \cdot (T/K) + 2.4103 \times 10^{-6} \cdot (T/K)^2$, temp range 226–617 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

- 731* (vapor-liquid equilibrium, Sanemasa et al. 1982)
- 754* (EPICS-GC/FID, Ashworth et al. 1988)
- $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 6.280 - 3337/(T/K)$; temp range: 10–30°C (EPICS measurements, Ashworth et al. 1988)
- 675 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 665 (infinite activity coeff. γ^∞ in water determined by inert gas stripping-GC, Li et al. 1993)
- 739* (static headspace-GC, same as *p*-xylene, Robbins et al. 1993)
- 615* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)

- 297, 771 (6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35%, Dewulf et al. 1995)
 $\ln K_{AW} = -4026/(T/K) + 0.00846 \cdot Z + 12.123$; with Z salinity 0–35.5%, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)
 590 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 658.5 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 561 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 5.204 - 1713/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C:

- 3.20 (Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
 3.18 (generator column-HPLC/UV, Wasik et al. 1981)
 3.29 (HPLC- k' correlation, Hammers et al. 1982)
 3.13 (generator column-HPLC/UV, Tewari et al. 1982b,c)
 3.20 (generator column-HPLC/UV, Wasik et al. 1983)
 3.28 (HPLC-RV retention volume correlation, Garst & Wilson 1984)
 3.37 (HPLC- k' correlation, Haky & Young 1984)
 3.33, 3.45 (RP-HPLC- k' capacity factor correlations, Sherblom & Eganhouse 1988)
 3.20 (recommended, Sangster 1989, 1993)
 3.31 (normal phase HPLC- k' correlation, Govers & Evers 1992)
 3.20 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.69* (30.3°C, from GC-determined γ^∞ in octanol, measured range 30.3–50.28°C, Gruber et al. 1997)
 3.79 (calculated-measured γ^∞ in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 1.37 (eels, Ogata & Miyake 1978)
 0.78 (clams, Nunes & Benville 1979)
 1.17 (goldfish, Ogata et al. 1984)
 2.40 (*S. capricornutum*, Herman et al. 1991)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C:

- 2.11, 2.48, 2.20 (forest soil pH 5.6, forest soil pH 4.2, agricultural soil pH 7.4, Seip et al. 1986)
 2.37, 2.40 (RP-HPLC- k' correlation, Szabo et al. 1990a,b)
 2.62, 2.63 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 2.06, 2.33 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 3.1$ h for evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s (Lyman et al. 1982);
 $t_{1/2} \sim 27$ –135 h for evaporation from a typical river or pond (Howard 1990).

Photolysis:

Oxidation: rate constant k ; for gas-phase second-order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

photooxidation $t_{1/2} = 4.8 \times 10^6 - 2.4 \times 10^8$ h in water, based on estimated rate data for alkoxy radical in aqueous solution (Hendry et al. 1974)

$k_{OH} = (14 \pm 1) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.83$ h; $k_{O(3P)} = (2.12 \pm 0.21) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ with O(³P) atom at room temp. (relative rate method, Doyle et al. 1975)

$k_{OH} = 1.4 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$ with an initial concn of $2.0 \times 10^{-10} \text{ mol L}^{-1}$ at 300 K (Doyle et al. 1975)

$k_{OH} = (23.6 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{O(3P)} = (3.52 \pm 0.35) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction of O(³P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = (12.9 \pm 2.6) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at 305 ± 2 K (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 14.1 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ (Darnall et al. 1976)

$k_{\text{OH}}^* = (24.0 \pm 2.5) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{\text{OH}} = (15.6 - 21.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishanakara et al. 1978)

$k_{\text{OH}} = 23.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and residence time of 0.5 d, loss of 86.5% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{O}_3} < 0.005 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau > 1150 \text{ d}$ and a lifetime $\tau = 0.5 \text{ d}$ due to reaction with OH radical at room temp. (Atkinson et al. 1982)

$k_{\text{O}_3} = 780 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with ozone at 300 K (Lyman et al. 1982)

$k_{\text{OH}} = (5.9\text{--}12) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.47\text{--}1.0 \text{ d}$ for xylenes (Mill 1982)

$k = (94 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{NO}_3} = 7.1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 23.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 2.6\text{--}26 \text{ h}$ in air (Atkinson 1985; Howard et al. 1991)

$k_{\text{OH}} = 22.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Ohta & Ohyama 1985)

$k_{\text{OH}} = 22.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 23.5°C, with a calculated atmospheric lifetime $\tau = 0.51 \text{ d}$ (Edney et al. 1986)

$k_{\text{OH}}(\text{calc}) = 14 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 24.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = 2.49 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} = 2.45 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{OH}}^* = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 1.45 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 17.47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}} = (1.81 \pm 0.40) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $(2.03 \pm 0.10) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Phouongphouang & Arey 2002)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of $3.28 \times 10^{-6} \text{ L/L}$ (Jamison et al. 1976)

$t_{1/2}(\text{aq. aerobic}) = 168\text{--}672 \text{ h}$, based on aqueous screening test data (Bridie et al. 1979; Howard et al. 1991) and soil column study simulating an aerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2} = 0.03 \text{ d}$ (Olsen & Davis 1990)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.83 \text{ h}$, based on rate of disappearance for the reaction with OH radical in ambient LA basin air at 300 K (Doyle et al. 1975);

photodecomposition $t_{1/2} = 2.9 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976); estimated lifetime $\tau = 1.5 \text{ h}$ under photochemical smog conditions in S.E. England (Brice & Derwent 1978) and (Perry et al. 1977);

residence time of 0.5 d, loss of 86.5% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

calculated lifetimes $\tau > 1150 \text{ d}$ and 0.5 d due to reactions with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982);

$t_{1/2} = 2.6\text{--}26 \text{ h}$, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);

calculated atmospheric lifetime $\tau = 0.51 \text{ d}$ due to reaction with OH radical (Edney et al. 1986);

summer daylight lifetime $\tau = 5.9 \text{ h}$ due to reaction with OH radical (Altshuller 1991);

calculated lifetimes of 5.9 h, 200 d and $> 4.5 \text{ yr}$ for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

Surface Water: $t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

volatilization appears to be dominant removal process with $t_{1/2} = 1\text{--}5.5 \text{ d}$ (Howard 1990).

Ground water: $t_{1/2} = 336\text{--}8640$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

$t_{1/2} \sim 0.3$ yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981);

abiotic hydrolysis or dehydro-halogenation $t_{1/2} = 377$ months (Olsen & Davis 1990).

Soil: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991).

Biota: $t_{1/2} = 2$ d, half-life to eliminate from eels in seawater (Ogata & Miyake 1978).

TABLE 3.1.1.5.1

Reported aqueous solubilities of *m*-xylene at various temperatures

Bohon & Claussen 1951		Polak & Lu 1973		Sanemasa et al. 1982		Shaw 1989b (IUPAC)	
shake flask-UV		shake flask-GC		vapor saturation-UV		recommended values	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0.4	209	0	196	15	158	0	203
5.2	201	25	162	25	162	10	200
14.9	192			35	168	20	170
21	196			45	186	25	160
25	196					30	180
25.6	196					40	220
30.3	198					50	230
34.9	203					60	320
39.6	218					70	350
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$		Chernoglazova & Simulin		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.60$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.9$	
		1976		at 25°C			
		synthetic method-GC					
		$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$				
25 $^{\circ}\text{C}$	2.8						
2 $^{\circ}\text{C}$	-5.506						
7 $^{\circ}\text{C}$	-3.828						
12 $^{\circ}\text{C}$	-1.59	20	160				
17 $^{\circ}\text{C}$	0	40	220				
22 $^{\circ}\text{C}$	1.22	70	380				
27 $^{\circ}\text{C}$	1.99						
32 $^{\circ}\text{C}$	3.92						
37 $^{\circ}\text{C}$	8.87						
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 11.9$					
		between 127–239 $^{\circ}\text{C}$					

(calc from Van't Hoff eq.)

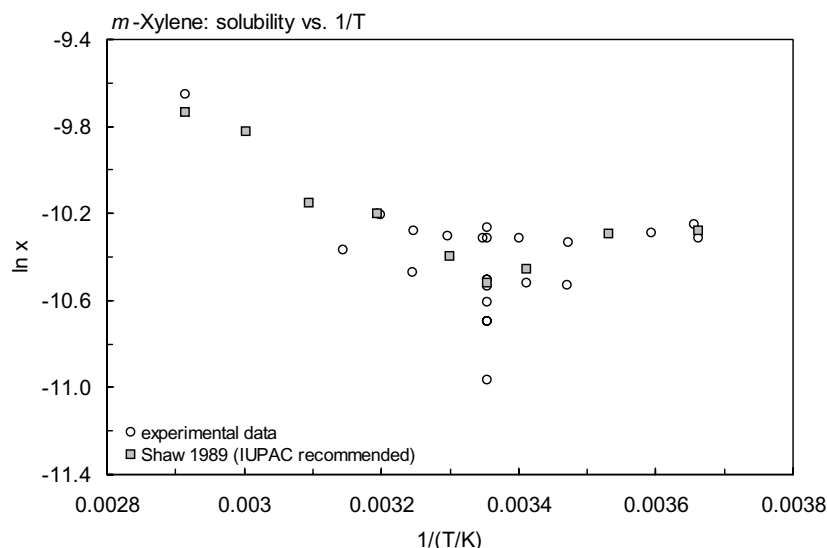
FIGURE 3.1.1.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *m*-xylene.

TABLE 3.1.1.5.2 (Continued)

Stull 1947		Forziati et al. 1949		Ambrose et al. 1967		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
55.3	5333	73.601	11720	226.85	671500	60.269	6666
64.4	7999	77.778	13842	246.85	937400	64.437	7999
76.8	13332	81.527	16633	266.85	1276300	71.277	10666
95.5	26664	87.387	19945	268.86	1700900	76.818	13332
116.7	53329	91.874	23474	306.85	2226600	87.454	19998
139.1	101325	97.887	28979	316.85	2872100	95.483	26664
		103.412	34925			102.01	33331
mp/°C	-47.9	110.067	43360	eq. 5	P/bar	107.55	39997
		116.923	53700	A	21.9924	116.69	53329
		124.226	66796	B	2957.79	124.15	66661
		132.144	83749	C	5.66789	130.58	79993
		137.731	97647	D	1776	136.06	93326
		138.329	99235			137.1	95991
		138.887	100726			138.112	98659
		129.52	102464			138.1	101325
		140.078	104000			25	1106.6
		eq. 2	P/mmHg			eq. 2	p/mmHg
		A	7.00849			A	7.00908
		B	1461.925			B	1462.266
		C	215.073			C	215.105
		bp/°C	139.104			bp/°C	139.103
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	42.66
						at bp	36.36

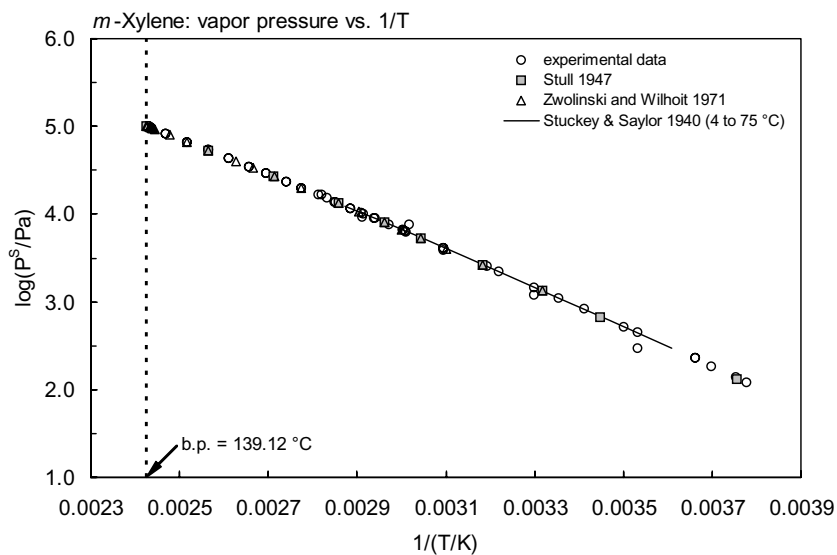
FIGURE 3.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for *m*-xylene.

TABLE 3.1.1.5.3

Reported Henry's law constants of *m*-xylene at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

$$\log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

Sanemasa et al. 1982		Ashworth et al. 1988		Robbins et al. 1993		Dewulf et al. 1995	
vapor-liquid equilibrium		EPICS-GC		static headspace-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
15	405	10	416	25	739	2	209
25	731	15	503	30	900	6	204
35	1329	20	606	40	1489	10	264
45	1872	25	754	45	1591	18.2	472
		30	899	50	1652	25	615
		eq. 4a	H/(atm m ³ /mol)	eq. 4	H/(Pa m ³ /mol)	eq 1	K _{AW}
		A	6.28	A	17.83472	A	12.13
		B	3337	B	3337.45	B	4026

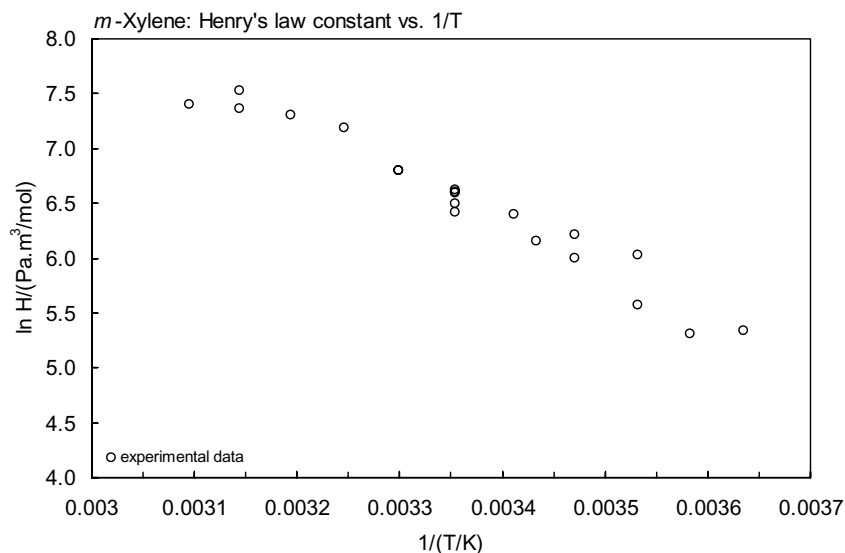


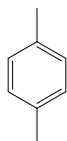
FIGURE 3.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for *m*-xylene.

TABLE 3.1.1.5.4

Reported octanol-air partition coefficients of *m*-xylene at various temperatures

Gruber et al. 1997

GC det'd activity coefficient	
t/°C	log K _{OA}
20.29	-
30.3	3.69
40.4	3.51
50.28	3.30

3.1.1.6 *p*-XyleneCommon Name: *p*-XyleneSynonym: 1,4-dimethylbenzene, *p*-xylol, 4-methyltolueneChemical Name: *p*-xylene

CAS Registry No: 106-42-3

Molecular Formula: C_8H_{10} , $C_6H_4(CH_3)_2$

Molecular Weight: 106.165

Melting Point ($^{\circ}C$):

13.25 (Lide 2003)

Boiling Point ($^{\circ}C$):

138.37 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8611 (Weast 1982–83)

Molar Volume (cm^3/mol):123.3 ($20^{\circ}C$, calculated-density)

140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):42.376, 35.98 ($25^{\circ}C$, bp, Riddick et al. 1986)Enthalpy of Fusion ΔH_{fus} (kJ/mol):

17.113 (Tsonopoulos & Prausnitz 1971; Riddick et al. 1986)

17.11 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

59.413 (Tsonopoulos & Prausnitz 1971; Yalkowsky & Valvani 1980)

59.77, 45.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

200 (shake flask-UV, Andrews & Keefer 1949)

198* (shake flask-UV, measured range 0.4 – $85^{\circ}C$, Bohon & Claussen 1951)

185* (shake flask-GC, Polak & Lu 1973)

156 (shake flask-GC, Sutton & Calder 1975)

163 (shake flask-GC, Hermann 1972)

157 (shake flask-GC, Price 1976)

157 (shake flask-GC, Krzyzanowska & Szeliga 1978)

191* ($20^{\circ}C$, shake flask-UV, Ben-Naim & Wiff 1979)163* (vapor saturation-UV spec., measured range 15 – $45^{\circ}C$, Sanemasa et al. 1982)

214.5 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982c)

182 (HPLC- k' correlation, converted from reported γ_w , Hafkenscheid & Tomlinson 1983a)

214 (generator column-HPLC, Wasik et al. 1983)

215 (generator column-GC/ECD, Miller et al. 1985)

190 (shake flask-radiometric, Lo et al. 1986)

180* (IUPAC recommended value, temp range 0 – $90^{\circ}C$, Shaw 1989b)169* ($30^{\circ}C$, equilibrium flow cell-GC, measured range 30 – $100^{\circ}C$, Chen & Wagner 1994c)

$\ln x = 11.79 - 20.89 \cdot (T/K)^{-1} + 4.892 \cdot (T/K)^{-2}$; $T_r = T/T_c$, the reduced temp, system temp T divided by critical temp T_c , temp range 303.15 – $373.15\ K$ (equilibrium flow cell-GC, Chen & Wagner 1994c)

$\ln x = -27.937 + 3230.3/(T/K) + 7.595 \times 10^{-5} \cdot (T/K)^2$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

154.7* (0.2°C, mercury manometer, Linder 1931)

787* (20°C, Hg manometer, Kassel 1936)

$\log (P/\text{mmHg}) = -2930.0/(T/K) - 5 \cdot \log (T/K) + 23.1000$; temp range 0–80°C (vapor pressure eq. from Hg manometer measurements, Kassel 1936)

1437* (30°C, Hg manometer, measured range 10–50°C, Rintelen et al. 1937)

$\log (P/\text{mmHg}) = -2851.90/(T/K) - 5 \cdot \log (T/K) + 22.88436$; temp range 4–75°C (vapor pressure eq. from manometer measurement, Stuckey & Saylor 1940)

1187* (Hg manometer, Pitzer & Scott 1943)

$\log (P_s/\text{mmHg}) = -3141.33/(T/K) + 11.6092$; temp range 0–13.23°C (manometer, solid, two-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)

$\log (P_L/\text{mmHg}) = -3080.31/(T/K) - 6.7 \log (T/K) + 27.8581$; temp range 13.23–60°C (manometer, liquid, three-constant eq. from exptl. data, Pitzer & Scott 1943)

6354* (58.288°C, ebulliometry, measured range 58.288–139.289°C, Willingham et al. 1945)

$\log (P/\text{mmHg}) = 6.98648 - 1491.548/(207.171 + t/^\circ\text{C})$; temp range 58.3–139.8°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

1333* (27.3°C, summary of literature data, Stull 1947)

6398* (58.419°C, ebulliometry, measured range 58.419–139.329°C, Forziati et al. 1949)

$\log (P/\text{mmHg}) = 6.99184 - 1454.328/(215.411 + t/^\circ\text{C})$; temp range 58.4–139.3°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

1175 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/\text{mmHg}) = 6.99052 - 1453.430/(215.307 + t/^\circ\text{C})$; temp range 45–190°C (Antoine eq. for liquid state, Dreisbach 1955)

126500* (146.85°C, ebulliometry, measured range 146.85–316.85°C, Ambrose et al. 1967)

1170* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 6.9052 - 1453.430/(215.307 + t/^\circ\text{C})$; temp range 27.32–165.73°C (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 9809.9/(T/K)] + 8.124805$; temp range –8.1 to 138.3°C (Antoine eq., Weast 1972–73)

880.3* (20.015 °C, inclined-piston gauge, measured range –26.043 to 20.015, Osborn & Douslin 1974)

$\log (P/\text{atm}) = (1 - 411.503/T) \times 10^4(0.847730 - 6.39489 \times 10^4 \cdot T + 5.59094 \times 10^7 \cdot T^2)$; T in K, temp range 290.0–618.2 K (Cox vapor pressure eq., Chao et al. 1983)

1170 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.11376 - 1452.215/(215.518 + t/^\circ\text{C})$, temp range 58.3–139.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.11513 - 1453.812/(215.242 + t/^\circ\text{C})$; temp range 99.17–179.23°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1974, Boublik et al. 1984)

1167 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.90052 - 1453.430/(215.31 + t/^\circ\text{C})$; temp range 27–166°C (Antoine eq., Dean 1985, 1992)

1200; 1160 (quoted lit.; calculated-Antoine eq., Riddick et al. 1986; quoted, Howard 1990)

$\log (P/\text{kPa}) = 6.11140 - 1451.39/(215.148 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

1180 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 15.50091 - 6327.014/(115.724 + T/K)$; temp range 247–286 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14779 - 1475.767/(-55.241 + T/K)$; temp range 286–453 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14049 - 1472.773/(-55.342 + T/K)$; temp range 411–463 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.44333 - 1735.196/(-19.846 + T/K)$; temp range 460–553 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.84182 - 3543.356/(208.522 + T/K)$; temp range 551–616 K (liquid, Antoine eq.-V, Stephenson & Malanowski 1987)

1165* (McLeod gauge, measured range 20.0–50.07, Smith 1990)

$\log (P/\text{mmHg}) = 60.0531 - 4.1059 \times 10^3/(T/K) - 19.441 \cdot \log (T/K) + 8.2881 \times 10^{-3} \cdot (T/K) - 2.3647 \times 10^{-12} \cdot (T/K)^2$, temp range 286–616 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 762* (vapor-liquid equilibrium, measured range $15\text{--}45^\circ\text{C}$, Sanemasa et al. 1982)
 754*; 752 (EPICS-GC/FID; batch air stripping-GC, Ashworth et al. 1988)
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 6.931 - 3520/(T/K)$; temp range $10\text{--}30^\circ\text{C}$ (EPICS measurements, Ashworth et al. 1988)
 614 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 856, 1189, 1576 ($27, 35.8, 46^\circ\text{C}$, EPICS-GC, Hansen et al. 1993)
 $\ln [H/(\text{kPa}\cdot\text{m}^3/\text{mol})] = -3072/(T/K) + 10.0$; temp range $27\text{--}46^\circ\text{C}$ (EPICS measurements, Hansen et al. 1993)
 696 (infinite activity coeff. γ^∞ in water determined by inert gas stripping-GC, Li et al. 1993)
 739* (static headspace-GC, same as *m*-xylene, Robbins et al. 1993)
 595 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
 575* (EPICS-GC/FID, measured range $2\text{--}25^\circ\text{C}$, Dewulf et al. 1995)
 318, 763 ($6.0, 25^\circ\text{C}$, EPICS-GC/FID, natural seawater with salinity of 35‰ , Dewulf et al. 1995)
 $\ln K_{\text{AW}} = -4479/(T/K) + 0.01196\cdot Z + 13.597$; with *Z* salinity $0\text{--}35.5\text{‰}$, temp range $2\text{--}25^\circ\text{C}$ (EPICS-GC/FID, Dewulf et al. 1995)
 641 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)
 678.6 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 669.1 (modified EPICS method-GC, Ryu & Park 1999)
 604 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 4.900 - 1615/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C :

- 3.15 (Leo et al. 1971; Hansch & Leo 1985)
 3.20 (Hansch & Leo 1979)
 3.10 (HPLC- k' correlation, Hanai et al. 1981)
 3.28 (HPLC- k' correlation, Hammers et al. 1982)
 3.18 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982b,c)
 3.29 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983b)
 3.18 (generator column-HPLC/UV, Wasik et al. 1983)
 3.29 (HPLC-RV correlation, Garst 1984)
 3.36, 3.48 (RP-HPLC- k' capacity factor correlations; Sherblom & Eganhouse 1988)
 3.15 (recommended, Sangster 1989, 1993)
 3.35 (normal phase HPLC- k' correlation, Govers & Evers 1992)
 3.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.68* (30.3°C , from GC-determined γ^∞ in octanol, measured range $30.3\text{--}50.28^\circ\text{C}$, Gruber et al. 1997)
 3.79 (calculated-measured γ^∞ in pure octanol of Gruber et al. 1997, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.37 (eels, Ogata & Miyake 1978)
 1.17 (goldfish, Ogata et al. 1984)
 2.41 (*S. capricornutum*, Herman et al. 1991)

Sorption Partition Coefficient, $\log K_{\text{OC}}$ at 25°C or as indicated:

- 2.52 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)
 2.42 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
 2.24 (aquifer material with f_{OC} of 0.006 and measured partition coeff. $K_p = 1.04 \text{ mL/g.}$, Abdul et al. 1990)
 1.87, 2.22 (Webster soil, Webster soil HP, batch equilibrium, Pennell et al. 1992)
 3.53, 2.63 (sorbent: Silica gel, kaolinite, batch equilibrium, Pennell et al. 1992)
 2.72, 2.17 (Captina silt loam pH 4.97, McLaurin sandy loam pH 4.43, Walton et al. 1992)
 2.43, 2.44 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

- 2.37 (HPLC-screening method, Müller & Kördel 1996)
 2.49, 2.75, 2.65, 2.76, 2.79, 2.76, 2.78 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)
 2.27, 2.31, 2.21 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 3.1$ h for evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s h (Lyman et al. 1982);
 $t_{1/2} \sim 27$ –135 h for evaporation from a typical river or pond (Howard 1990).

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

photooxidation $t_{1/2} = 2.8 \times 10^6$ – 1.4×10^8 h, based on estimated rate data for alkoxy radical in aqueous solution (Hendry 1974)

$k_{OH} = (7.4 \pm 1.5) \times 10^9$ L mol⁻¹ s⁻¹; $k_{O(3P)} = (1.09 \pm 0.11) \times 10^8$ L mol⁻¹ s⁻¹ with O(³P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (12.2 \pm 1.2) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹; $k_{O(3P)} = (1.81 \pm 0.18) \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ for the reaction of O(³P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 7.45 \times 10^9$ L mol⁻¹ s⁻¹ with $t_{1/2} = 0.24$ –2.4 h (Darnall et al. 1976)

$k_{OH}^* = (15.3 \pm 1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH} = (8.8$ – $10.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{OH} = 12.3 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ and residence time of 0.9 d, loss of 67% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH} = 950$ cm³ mol⁻¹ s⁻¹ at 300 K (Lyman et al. 1982)

$k_{OH} = (5.9$ – $12) \times 10^9$ M⁻¹ s⁻¹ with $t_{1/2} = 0.47$ –1.0 d for xylenes (Mill 1982)

$k = (140 \pm 30)$ M⁻¹ s⁻¹ for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{NO_3} = 1.4 \times 10^{-16}$ cm³ molecule⁻¹ s⁻¹ at 296 K (Atkinson et al. 1984)

$k_{OH} = 14.1 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with half-life of 4.2–42 h (Atkinson 1985; Howard et al. 1991)

$k_{OH} = 12.9 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 25°C (Ohta & Ohya 1985)

$k_{OH} = 13.6 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 22.8°C, with a calculated atmospheric lifetime $\tau = 0.84$ d (Edney et al. 1986)

$k_{OH}(\text{calc}) = 6.9 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(\text{obs.}) = 15.2 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{NO_3} = 4.50 \times 10^{-16}$ cm³ molecule⁻¹ s⁻¹, $k_{OH} = 1.52 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{OH}^* = 1.43 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ over temp range at 296–335 K (recommended, Atkinson 1989)

$k_{OH} = 14.3 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1990)

$k_{OH}(\text{calc}) = 6.92 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{OH}(\text{calc}) = 17.40 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1993)

$k_{OH}(\text{calc}) = 6.51 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(\text{exptl}) = 14.3 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982)

$t_{1/2} = 1150$ months, abiotic hydrolysis or dehydro-halogenation half-life (Olsen & Davis 1990).

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of 1.03×10^{-6} L/L (Jamison et al. 1976)

$t_{1/2}(\text{aq. aqueous}) = 168$ –672 h, based on aqueous screening test data (Bridie et al. 1979) and soil column study simulating an aerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 672$ –2688 h, based on unacclimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2} = 0.03$ d (Olsen & Davis 1990).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976)
residence time of 0.9 d, loss of 67% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

photodecomposition $t_{1/2} = 3.1$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976)

$t_{1/2} = 4.2\text{--}42$ h, based on photooxidation half-life (Howard et al. 1991);

calculated atmospheric lifetime $\tau = 0.84$ d due to reaction with OH radical (Edney et al. 1986);

summer daylight lifetime $\tau = 10$ h due to reaction with OH radical (Altshuller 1991).

Surface Water: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 336\text{--}8640$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991);

$t_{1/2} \sim 0.3$ yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981);

abiotic hydrolysis or dehydro-halogenation $t_{1/2} = 1150$ months (Olsen & Davis 1990).

Soil: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

disappearance $t_{1/2} = 2.2$ d from test soils (Anderson et al. 1991).

Biota: $t_{1/2} = 2.6$ d, half-life to eliminate from eels in seawater (Ogata & Miyake 1978).

TABLE 3.1.1.6.1

Reported aqueous solubilities of *p*-xylene at various temperatures

1.

Bohon & Claussen 1951		Polak & Lu 1973		Shaw 1989b (IUPAC)		Chen & Wagner 1994c	
shake flask-UV		shake flask-GC		recommended values		equilibrium flow cell-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0.4	156	0	164	0	160	30	169
10	188	25	185	10	200	30	188
10	197			20	180	50	102
21	195			25	180	60	230
25	198			30	190	70	289
25.6	199	Ben-Naim & Wiff 1979		40	220	80	337
30.2	201	shake flask-UV		50	280	90	395
30.3	204	t/°C S/g·m ⁻³		60	320	100	516
34.9	207	10	189	70	360		
35.2	207	20	191	80	420	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.48$	
42.8	222			90	480	at 25°C	
42.8	256						
54.4	310			$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 6.90$			
61.7	340	Sanemasa et al. 1982		at 25°C			
73.9	387	vapor saturation-UV					
85	459	t/°C S/g·m ⁻³					
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$		15	157				
25°C	3.9	25	163				
7°C	-0.422	35	176				
12°C	-1.34	45	178				
17°C	0.515						
22°C	1.36						
27°C	2.29	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.20$					
32°C	4.23	at 25°C					
37°C	7.36						

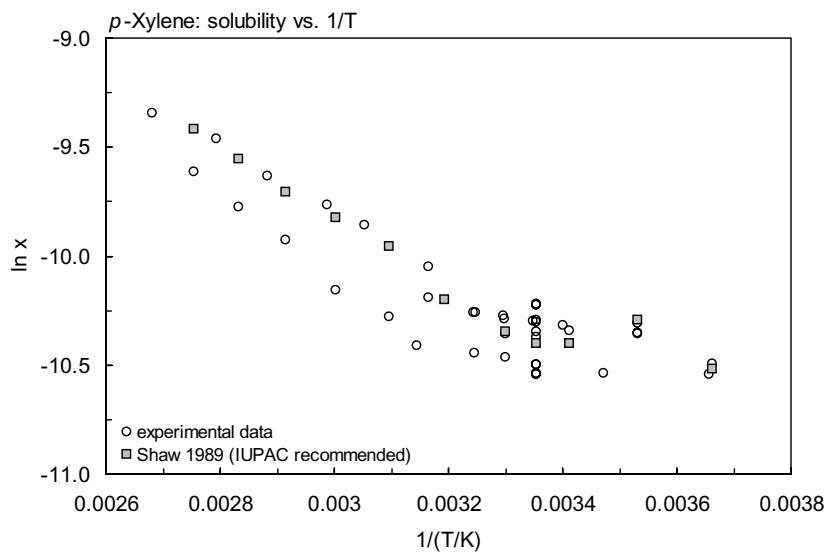


FIGURE 3.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *p*-xylene.

TABLE 3.1.1.6.2
Reported vapor pressures of *p*-xylene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$

(1)

$\ln P = A - B/(T/K)$

(1a)

$\log P = A - B/(C + t/^{\circ}C)$

(2)

$\ln P = A - B/(C + t/^{\circ}C)$

(2a)

$\log P = A - B/(C + T/K)$

(3)

$\log P = A - B/(T/K) - C \cdot \log (T/K)$

(4)

$\log P = A - B/(T/K) - C \cdot \log (T/K) + D(T/K)^2$

(5)

1.

Kassel 1936		Rintelen et al. 1937		Pitzer & Scott 1943		Willingham et al. 1945	
mercury manometer		mercury manometer		mercury manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	208	10	307	0	178	58.288	6354
10	415	30	1427	12.5	540	62.523	7657
20	787	50	4306	25	1187	66.216	8966
30	1427	bp 138.27–138.37°C		37.7	2333	69.549	10306
40	2453			50	4346	72.657	11696
50	4093			60	6846	76.832	13822
60	6573					81.636	16623
70	10226					86.488	18725
80	15452					0–13.23°C solid	90.990
eq. 4	P/mmHg			eq. 1	P/mmHg	97.013	28956
				A	11.6092	102.546	34901
				B	3141.33	109.211	43326
						116.083	53656
						123.049	66756
A	23.100			13.23–60°C liquid		123.049	66756
				eq. 4	P/mmHg	131.355	83717
				A	27.8581	136.956	97605
				B	3080.31	137.558	99201
B	2930.0						
C	5.0						

TABLE 3.1.1.6.2 (Continued)

Kassel 1936		Rintelen et al. 1937		Pitzer & Scott 1943		Willingham et al. 1945	
mercury manometer		mercury manometer		mercury manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
Linder 1931		Stuckey & Saylor 1940		C	6.7	138.114	100694
mercury manometer		mercury manometer		$\Delta H_v/(\text{kJ mol}^{-1}) = 42.30$ at 298 K		138.742	102392
t/°C	P/Pa	t/°C	P/Pa			139.289	103906
–9.5	44.0	measured 4–75°C				eq. 2	P/mmHg
–2.5	116	eq. 4	P/mmHg			A	6.98648
0	126.7	A	22.88436			B	1450.688
0.2	154.7	B	2851.90			C	214.990
		C	5.0				
		bp/°C 138.33–138.38				bp/°C	138.348
		mp/°C 13.20–12.95					

2.

Stull 1947		Forziati et al. 1949		Ambrose et al. 1967		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–8.10	133.3	58.419	6398	146.85	126500	27.32	1333
15.5	266.6	62.419	7690	166.85	205200	40.15	2666
27.3	1333	66.280	8990	186.85	317100	48.31	4000
40.1	2666	69.605	10330	206.85	470900	54.42	5333
54.4	5333	72.684	11720	226.85	675800	59.363	6666
63.5	7999	76.885	13842	246.85	941900	63.535	7999
75.9	13332	81.658	16633	266.85	1280800	70.383	10666
94.6	26664	86.506	19944	286.85	1705700	75.931	13332
115.9	53323	91.017	23474	306.85	2232400	86.583	19998
138.3	101325	97.032	28978	316.85	2880400	94.626	26664
		102.573	34925			101.167	33331
mp/°C	13.3	109.240	43360	eq. 5	P/bar	106.719	39997
		123.431	66796	A	21.14250	115.887	53329
		131.371	83749	B	2892.27	123.366	66661
		137.574	99235	C	5.40051	129.372	79993
		138.132	100726	D	1759	135.304	93326
		138.768	102462			136.341	95991
		139.329	104000			137.347	98659
						138.351	101325
		eq. 2	P/mmHg			25.0	1173.2
		A	6.99184				
		B	1454.328			eq. 2	P/mmHg
		C	215.411			A	6.99052
						B	1453.430
						C	215.307
		bp/°C	138.351			bp/°C	138.351
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	42.38
						at bp	35.98

(Continued)

TABLE 3.1.1.6.2 (Continued)

3.

Osborn & Douslin 1974				Smith 1990	
inclined-piston gauge		ebulliometry		McLeod gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−26.043	11.60	67.795	9590	20.0	865.3
−21.164	19.60	70.881	10892	25.0	1165
−16.277	33.20	73.978	12344	30.0	1541
−10.403	60.79	77.086	13960	35.24	2075
−4.995	103.86	80.206	15752	40.0	2645
−0.006	170.5	83.339	17737	44.27	3306
4.912	272.4	86.483	19933	50.07	4374
9.838	429.2	92.804	25023		
12.483	544.4				
13.285	581.7			eq. 2a	P/mmHg
15.004	648.9			A	16.19136
17.474	755.4			B	3371.18
20.015	880.3			C	215.367
				$\Delta H_v/(\text{kJ mol}^{-1}) = 42.98$	
				at 25°C	
				$\Delta S_v/(\text{J mol}^{-1} \text{ K}^{-1}) = 107.0$	
				at 25°C	

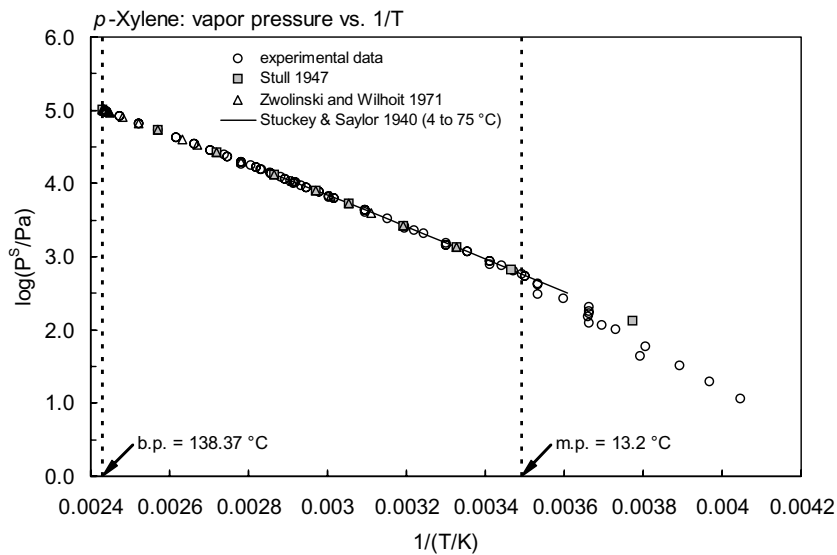


FIGURE 3.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for *p*-xylene.

TABLE 3.1.1.6.3
Reported Henry's law constants of *p*-xylene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)				
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)				
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)							
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)				
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)							
Sanemasa et al. 1982		Ashworth et al. 1988		Robbins et al. 1993		Hansen et al. 1993		Dewulf et al. 1995	
vapor-liquid equil		EPICS-GC		static headspace-GC		EPICS-GC		EPICS-GC	
t/°C	H/Pa m³/mol	t/°C	H/Pa m³/mol	t/°C	H/Pa m³/mol	t/°C	H/Pa m³/mol	t/°C	H/Pa m³/mol
15	430	10	426	25	739	27	856	2	176
25	762	15	489	30	900	35.8	1189	6	158
35	1265	20	654	40	1489	46	1576	10	252
45	2052	25	754	45	1591			18.2	468
		30	958	50	1652			25	575
		eq. 4a		eq. 4		eq. 4		eq 1	
		H/(atm m³/mol)		H/(Pa m³/mol)		H/(kPa m³/mol)		K _{AW}	
		A	6.931	A	17.83472	A	10.1	A	13.597
		B	3520	B	3337.45	B	3072	B	4479

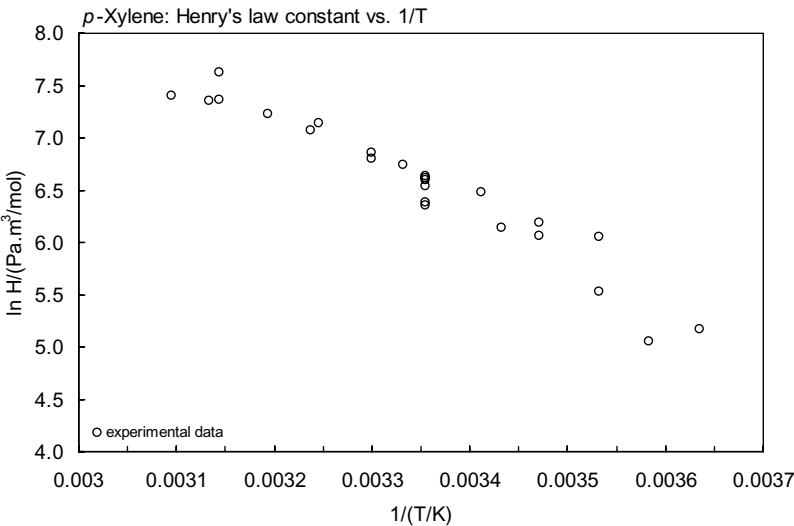
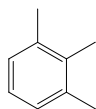


FIGURE 3.1.1.6.3 Logarithm of Henry's law constant versus reciprocal temperature for *p*-xylene.

TABLE 3.1.1.6.4
Reported octanol-air partition coefficients of *p*-xylene at various temperatures

Gruber et al. 1997	
GC det'd activity coefficient	
t/°C	log K _{OA}
20.29	-
30.3	3.68
40.4	3.48
50.28	3.29

3.1.1.7 1,2,3-Trimethylbenzene



Common Name: 1,2,3-Trimethylbenzene

Synonym: hemimellitene

Chemical Name: 1,2,3-trimethylbenzene

CAS Registry No: 526-73-8

Molecular Formula: C_9H_{12} , $C_6H_3(CH_3)_3$

Molecular Weight: 120.191

Melting Point ($^{\circ}C$):

−25.4 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

176.1 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8944 (Weast 1982–83)

Molar Volume (cm^3/mol):

134.4 ($20^{\circ}C$, calculated-density)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

0.66, 1.33, 8.18; 10.17 (−54.45, −42.85, −25.35 $^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

41.81, 46.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

75.2 (shake flask-GC, Sutton & Calder 1975)

62.7* (vapor saturation-UV spec., measured range 15–45 $^{\circ}C$, Sanemasa et al. 1982)

65.5 (generator column-HPLC/UV, Tewari et al. 1982c)

69* (IUPAC recommended value, temp range 15–45 $^{\circ}C$, Shaw 1989b)

$\ln x = -39.5173 + 5289.13/(T/K) + 1.149 \times 10^{-4} \cdot (T/K)^2$; temp range 5–50 $^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (16.8 $^{\circ}C$, summary of literature data, Stull 1947)

6417* (90.332 $^{\circ}C$, ebulliometry, measured range 90.332–177.126 $^{\circ}C$, Forziati et al. 1949)

$\log (P/mmHg) = 7.04082 - 1593.958/(207.078 + t/^{\circ}C)$; temp range 90.3–177.1 $^{\circ}C$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

206 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.04082 - 1593.958/(207.078 + t/^{\circ}C)$; temp range 75–230 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

198* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 7.04082 - 1593.958/(207.078 + t/^{\circ}C)$; temp range 56.79–205.36 $^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = [-0.2185 \times 10781.9/(T/K)] + 8.154069$; temp range 16.8–176 $^{\circ}C$ (Antoine eq., Weast 1972–73)

217 (calculated-bp, Mackay et al. 1982; Eastcott et al. 1988)

$\log (P/atm) = (1 - 449.175/T) \times 10^{(0.869047 - 6.33423 \times 10^4 \cdot T + 5.14963 \times 10^7 \cdot T^2)}$; T in K, temp range 290.0–660.0 K (Cox vapor pressure eq., Chao et al. 1983)

157 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.16365 - 1592.422/(206.905 + t/^{\circ}\text{C})$; temp range 90.33–177.1 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

198.4 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.04082 - 1593.958/(207.08 + t/^{\circ}\text{C})$; temp range 57–205 $^{\circ}\text{C}$ (Antoine eq., Dean 1985, 1992)

199 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 6.16477 - 1593.776/(-66.032 + T/\text{K})$; temp range 363–456 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 2.7492 - 2.6428 \times 10^3/(T/\text{K}) + 3.6120 \cdot \log (T/\text{K}) - 1.0213 \times 10^{-2} \cdot (T/\text{K}) + 5.0553 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 248–665 K (vapor pressure eq., Yaws 1994)

$\log (P/\text{kPa}) = 6.17303 - 1593.958/[(T/\text{K}) - 66.072]$; temp range 5–50 $^{\circ}\text{C}$ (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

441* (vapor-liquid equilibrium-GC, measured range 15–45 $^{\circ}\text{C}$, Sanemasa et al. 1982)

364 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.66 (Hansch & Leo 1979)

3.66 (HPLC- k' correlation, Hammers et al. 1982)

3.55 (generator column-HPLC/UV, Tewari et al. 1982b, 1982c)

3.70, 3.86 (RP-HPLC- k' correlation, Sherblom & Eganhouse 1988)

3.63 (recommended, Sangster 1989, 1993)

3.55, 3.59, 3.66 (quoted lit. values, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.80 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k ; for gas-phase second-order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = (14 \pm 3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$; $k_{\text{O}(^3\text{P})} = (6.9 \pm 0.7) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ with O(^3P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{\text{OH}} = (26.4 \pm 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}(^3\text{P})} = 11.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction of O(^3P) atom at room temp (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{\text{OH}} = 14.9 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ (Darnall et al. 1976)

$k_{\text{OH}}^* = (33.3 \pm 4.5) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence Perry et al. 1977)

$k_{\text{OH}} = (15\text{--}30) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.2\text{--}0.4 \text{ d}$ for trimethylbenzenes (Mill 1982)

$k = (400 \pm 100) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.7 and 20–23 $^{\circ}\text{C}$ (Hoigné & Bader 1983)

$k_{\text{NO}_3} = 5.6 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 3.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}} = 2.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Ohta & Ohyama 1985)

$k_{\text{OH}}(\text{calc}) = 1.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 3.33 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = 1.85 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} = 3.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{OH}} = 3.27 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 1.78 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 3.99 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biotransformation:

Biodegradation:

Bioconcentration:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

estimated lifetime $\tau = 1.5 \text{ h}$ under photochemical smog conditions in S.E. England (Brice & Derwent 1978) and (Perry et al. 1977);

summer daylight lifetime $\tau = 4.2 \text{ h}$ due to reaction with OH radical (Altshuller 1991)

TABLE 3.1.1.7.1
Reported aqueous solubilities and Henry's law constants of 1,2,3-trimethylbenzene at various temperatures

Aqueous solubility				Henry's law constant	
Sanemasa et al. 1982		Shaw 1989b (IUPAC)		Sanemasa et al. 1982	
vapor saturation-UV		recommended values		vapor-liquid equilibrium	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)
15	75.2	15	60	15	241.2
25	65.5	25	69	25	441
35	72.2	35	72	35	706
45	85.2	45	85	45	1058

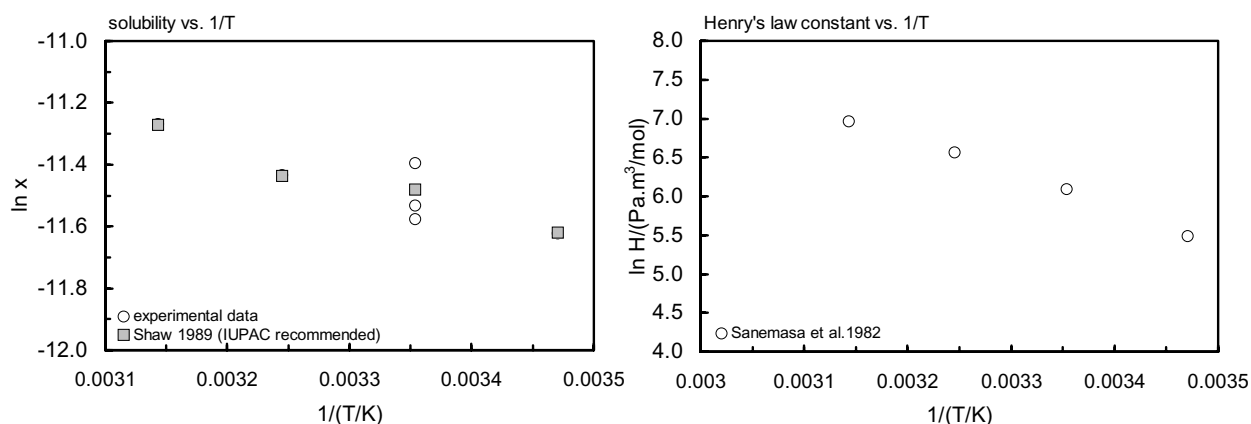
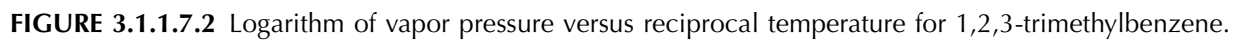


FIGURE 3.1.1.7.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1,2,3-trimethylbenzene.

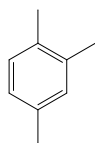
TABLE 3.1.1.7.2

Reported vapor pressures of 1,2,3-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log(T/K)$		(4)			
Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
16.8	133.3	90.332	6417	56.79	1333
42.9	666.6	94.826	7697	70.62	2666
55.9	1333	98.77	8993	79.41	4000
69.9	2666	102.336	10328	86	5333
85.4	5333	105.663	11720	91.313	6666
95.3	7999	110.157	13840	95.802	7999
1088	13332	115.287	16640	103.168	10666
129	26664	120.504	19944	109.132	13332
152	53329	125.333	23474	120.578	19998
176.1	101325	131.8	28978	129.215	26664
		137.737	34918	136.214	33331
mp/ $^{\circ}\text{C}$	-25.5	144.882	43351	142.191	39997
		152.26	53692	152.022	53329
		160.106	66792	160.037	66661
		168.614	83750	166.856	79993
		174.606	97644	172.823	93326
		175.252	99237	173.934	95992
		175.852	100732	175.02	98659
		176.527	102453	176.084	101325
		177.126	103985		
				eq. 2	P/mmHg
				A	7.04082
		eq. 2	P/mmHg	B	1593.958
		A	7.04082	C	207.078
		B	1593.958	bp/ $^{\circ}\text{C}$	176.084
		C	207.078	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				at 25 $^{\circ}\text{C}$	49.06
		bp/ $^{\circ}\text{C}$	176.084	at bp	40.04



3.1.1.8 1,2,4-Trimethylbenzene



Common Name: 1,2,4-Trimethylbenzene

Synonym: pseudocumene

Chemical Name: 1,2,4-trimethylbenzene

CAS Registry No: 95-63-6

Molecular Formula: C_9H_{12} , $C_6H_3(CH_3)_3$

Molecular Weight: 120.191

Melting Point ($^{\circ}C$):

−43.77 (Lide 2003)

Boiling Point ($^{\circ}C$):

169.38 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8758 (Weast 1982–83)

Molar Volume (cm^3/mol):

137.2 ($20^{\circ}C$, calculated-density)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

13.19 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

57.53, 46.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

57 (shake flask-GC, McAuliffe 1966)

59.0 (shake flask-GC, Sutton & Calder 1975)

51.9 (shake flask-GC, Price 1976)

51.9 (shake flask-GC, Krzyzanowska & Szeliga 1978)

56.5* (vapor saturation-UV spec., measured range 15 – $45^{\circ}C$, Sanemasa et al. 1982)

56* (IUPAC recommended, temp range 15 – $45^{\circ}C$, Shaw 1989b)

$\ln x = -8.760 - 868.70/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($13.6^{\circ}C$, summary of literature data, Stull 1947)

6417* ($84.804^{\circ}C$, ebulliometry, measured range 84.804 – $170.377^{\circ}C$, Forziati et al. 1949)

$\log (P/mmHg) = 7.04393 - 1573.267/(208.564 + t/^{\circ}C)$; temp range 84.8 – $170.4^{\circ}C$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

280 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.04383 - 1573.267/(208.564 + t/^{\circ}C)$; temp range 70 – $220^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

2666* ($65.405^{\circ}C$, compiled data, temp range 65.405 – $198.215^{\circ}C$, Bond & Thodos 1960)

$\log (P/mmHg) = 23.2393 - 3301.19/(T/K) - 6.21412 \cdot \log (T/K) + 3.15835[P(mmHg)/(T/K)^2]$, temp range 65.4 – $198^{\circ}C$ (Bond & Thodos 1960)

271* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981; Eastcott et al. 1988)

$\log (P/mmHg) = 7.04383 - 1573.267/(208.564 + t/^{\circ}C)$; temp range 51.75 – $198.2^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 10710.2/(T/K)] + 8.209013$; temp range 13.6–169.2°C (Antoine eq., Weast 1972–73)
 $\log (P/\text{atm}) = (1 - 442.537/T) \times 10^{(0.846724 - 5.41424 \times 10^4/T + 4.22211 \times 10^7/T^2)}$; T in K, temp range 253.0–645.0 K (Cox vapor pressure eq., Chao et al. 1983)
 270 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.16282 - 1569.06/(208.089 + t/^\circ\text{C})$; temp range 84.8–170.4°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 7.04383 - 1573.83/(208.56 + t/^\circ\text{C})$; temp range 52–198°C (Antoine eq., Dean 1985, 1992)
 $\log (P_L/\text{kPa}) = 6.16695 - 1572.687/(-64.593 + T/K)$; temp range 357–450 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 2.1667 - 2.6318 \times 10^3/(T/K) + 4.0350 \cdot \log (T/K) - 1.1776 \times 10^{-2} \cdot (T/K) + 6.0956 \times 10^{-6} \cdot (T/K)^2$, temp range 229–649 K (vapor pressure eq., Yaws 1994)
 $\log (P/\text{kPa}) = 6.16866 - 1573.267/[(T/K) - 64.586]$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

619* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1982)
 475 (20°C, EPICS-GC, Yurteri et al. 1987)
 571 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 704, 1135, 1591 (27, 35, 45°C, EPICS-GC, Hansen et al. 1993)
 $\ln [H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -4298/(T/K) + 14.0$; temp range 27–45°C (EPICS-GC, Hansen et al. 1993)
 529 (20°C, selected from literature experimentally measured data, Staudinger & Roberts, 1996, 2001)
 $\log K_{AW} = 5.125 - 1697/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.65 (calculated- π substituent constant, Hansch et al. 1968)
 3.63 (shake flask-HPLC/UV both phases, Wasik et al. 1981)
 3.78 (HPLC- k' correlation, Hammers et al. 1982)
 3.82, 4.00 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
 3.63 (recommended value, Sangster 1989)
 3.78 (normal phase HPLC- k' correlation, Govers & Evers 1992)
 3.70 (recommended, Sangster 1993)
 3.83, 3.78 (quoted lit., Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

3.28 (computed- K_{OW} , Kollig 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Photolysis: rate constant $k = 2.686 \times 10^{-2} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).
 no photolyzable functional groups (Howard et al. 1991).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = (2.0 \pm 0.3) \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.58 \text{ h}$; $k_{O(3P)} = (6.0 \pm 0.6) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ with O(³P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (33.5 \pm 3.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{NO_3} = 10.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction of O(³P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 20 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ (Darnall et al. 1976)

$k_{OH}^* = (40.0 \pm 4.5) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence Perry et al. 1977)

photooxidation $t_{1/2} = 1056\text{--}43000$ h in water, based on measured rate data with hydroxy radical in aqueous solution (Güsten et al. 1981)

$k_{\text{OH}} = 33.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and residence time of 0.3 d, loss of 96.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}} = (1.5\text{--}30) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.2\text{--}0.4$ d for trimethylbenzenes (Mill 1982)

$k_{\text{NO}_3} = 5.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{\text{OH}} = 38.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 1.6\text{--}16$ h (Atkinson 1985)

$k_{\text{OH}} = 31.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C (Ohta & Ohyama 1985)

$k_{\text{OH}}(\text{calc}) = 18 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = 1.80 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}} = 3.84 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{\text{OH}} \approx 32.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1990)

$k_{\text{OH}}(\text{calc}) = 1.78 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{\text{OH}}(\text{calc}) = 39.72 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 168\text{--}672$ h, based on aqueous screening studies (Marion & Malaney 1964; Kitano 1978; Van der Linden 1978; Tester & Harker 1981; Trzilova & Horska 1988; Howard et al. 1991);

anaerobic aqueous biodegradation $t_{1/2} = 672\text{--}2688$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Half-Lives in the Environment:

Air: $t_{1/2} = 0.58$ h estimated from the rate of disappearance for the reaction with OH radical (Doyle et al. 1975)

$t_{1/2} = 0.24\text{--}2.4$ h (Darnall et al. 1976);

residence time of 0.3 d, loss of 96.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 1.6\text{--}16$ h, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);

summer daylight lifetime $\tau = 4.3$ h due to reaction with OH radical (Altshuller 1991);

calculated lifetimes of 4.3 h, 26 d and > 4.5 yr for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

Surface Water: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-lives (Kitano 1978; Van der Linden 1978; Tester & Harker 1981; Trzilova & Horska 1988; Marion & Melaney 1964; Howard et al. 1991);

photooxidation $t_{1/2} = 1056\text{--}43000$ h, based on measured rate data with OH radical in aqueous solution (Güsten et al. 1981; Howard et al. 1991).

Ground water: $t_{1/2} = 336\text{--}1344$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Soil: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biota:

TABLE 3.1.1.8.1

Reported aqueous solubilities and Henry's law constants of 1,2,4-trimethylbenzene at various temperatures

Aqueous solubility				Henry's law constant			
Sanemasa et al. 1982		Shaw 1989b (IUPAC)		Sanemasa et al. 1982		Hansen et al. 1993	
vapor saturation-UV		recommended values		vapor-liquid equilibrium		EPICS-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
15	52.3	15	52	15	377	27	704
25	56.5	25	56	25	619	35	1135
35	62.1	35	62	35	1042	45	1591
45	69.3	45	69	45	1663		

$\ln [H/(\text{kPa m}^3/\text{mol})] =$
 $A - B/(T/K)$
 $A \quad 14.0$
 $B \quad 4298$

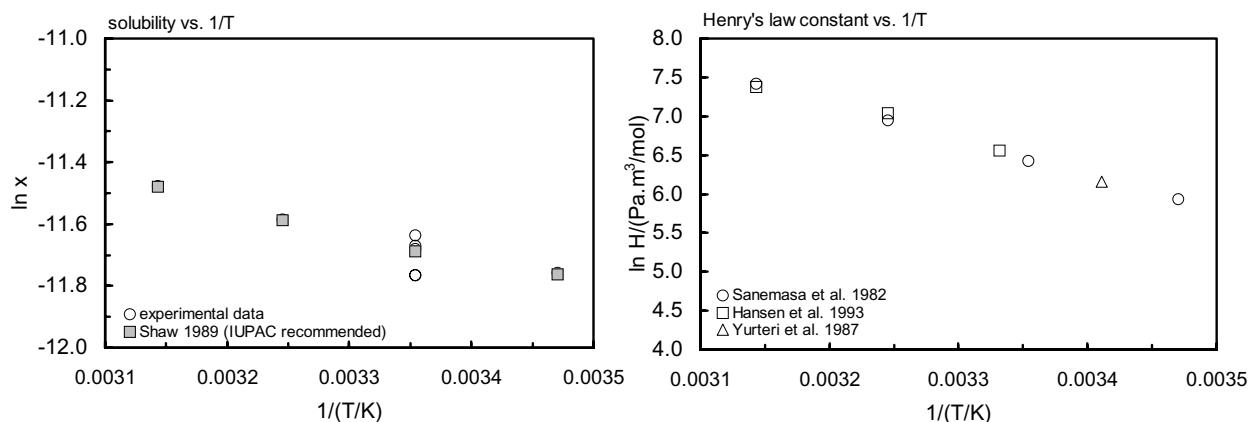


FIGURE 3.1.1.8.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1,2,4-trimethylbenzene.

TABLE 3.1.1.8.2

Reported vapor pressures of 1,2,4-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\log P = A - B/(T/K) - C \cdot \log (T/K) + D \cdot P/(T/K)^2$	(5)						
Stull 1947	Forziati et al. 1949	Bond & Thodos 1960	Zwolinski & Wilhoit 1971				
summary of literature data	ebulliometry	summary of literature data	selected values				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
13.6	133.3	84.804	6417	65.405	2666	51.75	1333
38.4	666.6	89.259	7697	97.49	10666	65.39	2666
50.7	1333	93.155	8991	153.55	66661	74.05	4000
64.5	2666	96.65	10328	180.505	133322	80.54	5333

TABLE 3.1.1.8.2 (Continued)

Stull 1947		Forziati et al. 1949		Bond & Thodos 1960		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		summary of literature data		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
79.8	5333	99.94	11720	198.215	199984	85.787	6666
89.5	7999	104.369	13840			90.214	7999
102.8	13332	109.418	16640	bp/°C	169.366	97.475	10666
122.7	26664	114.572	19944			103.355	13332
145.4	53329	119.328	23474	eq. 5	P/mmHg	114.639	19998
169.2	101325	125.694	28978	A	23.2393	123.153	26664
		131.556	34918	B	3301.19	130.072	33331
mp/°C	-44.1	138.599	43351	C	6.21412	135.944	39997
		145.867	53692	D	3.15835	145.634	53329
		153.604	66792			153.534	66661
		161.991	83750			160.256	79993
		167.896	97644			166.137	93326
		168.534	99237			167.231	95992
		169.121	100732			168.302	98659
		169.788	102453			169.351	101325
		170.377	103985				
		eq. 2	P/mmHg			eq. 2	P/mmHg
		A	7.04383			A	7.04383
		B	1573.267			B	1573.267
		C	208.564			C	208.564
						bp/°C	169.351
						$\Delta H_v/(kJ\ mol^{-1}) =$	
						at 25°C	47.94
						at bp	39.25

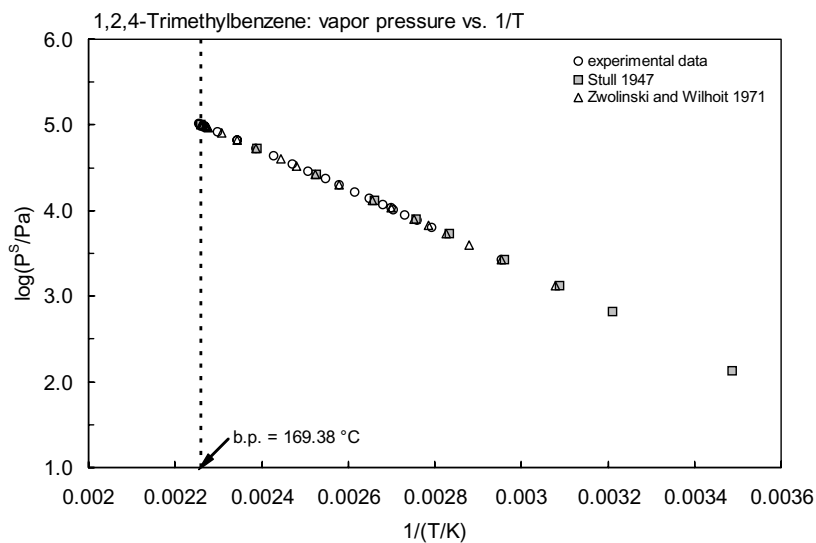
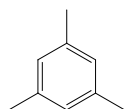


FIGURE 3.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4-trimethylbenzene.

3.1.1.9 1,3,5-Trimethylbenzene



Common Name: 1,3,5-Trimethylbenzene

Synonym: mesitylene

Chemical Name: 1,3,5-trimethylbenzene

CAS Registry No: 108-67-8

Molecular Formula: C_9H_{12} , $C_6H_3(CH_3)_3$

Molecular Weight: 120.191

Melting Point ($^{\circ}C$):

-44.7 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

164.74 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.880 (Weast 1982–83)

Molar Volume (cm^3/mol):136.6 ($20^{\circ}C$, calculated-density)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):47.48, 39.04 ($25^{\circ}C$, bp, Riddick et al. 1986)

51.85 (calculated-bp, Govers & Evers 1992)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

9.514 (Riddick et al. 1986)

9.51 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

41.66, 46.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

173 (residue-volume method, Booth & Everson 1948)

97 (shake flask-UV, Andrews & Keffer 1950)

39.4 (shake flask-UV, Vesala 1974)

48.2 (shake flask-GC, Sutton & Calder 1975)

49.5* (vapor saturation-UV, temp range 15 – $45^{\circ}C$, Sanemasa et al. 1981)50* (vapor saturation-UV, temp range 15 – $45^{\circ}C$, Sanemasa et al. 1982)49.5 (HPLC- k' correlation, converted from reported γ_w , Hafkenscheid & Tomlinson 1983)48.9* (recommended, temp range 15 – $45^{\circ}C$, Shaw 1989b)64* ($30^{\circ}C$, equilibrium flow cell-GC, measured range 30 – $100^{\circ}C$, Chen & Wagner 1994c)

$\ln x = 26.26 - 35.26 \cdot (T_r/K)^{-1} + 7.905 \cdot (T_r/K)^{-2}$; $T_r = T/T_c$, the reduced temp, system temp T divided by critical temp T_c , temp range 303.15 – $373.15\ K$ (equilibrium flow cell-GC, Chen & Wagner 1994c)

$\ln x = -9.533 - 678.83/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

121.3* ($10.6^{\circ}C$, mercury manometer, Linder 1931)248* ($20^{\circ}C$, mercury manometer, Kassel 1936)

$\log (P/mmHg) = -3104.5/(T/K) - 5 \cdot \log (T/K) + 23.1929$; temp range 0 – $80^{\circ}C$ (vapor pressure eq. from Hg manometer measurements, Kassel 1936)

507* ($30^{\circ}C$, mercury manometer, measured range 10 – $50^{\circ}C$, Rintelen et al. 1937)

- log (P/mmHg) = $-3122.45/(T/K) - 5 \cdot \log (T/K) + 22.23680$; temp range 4–75°C (manometer, vapor pressure eq. from exptl. data, Stuckey & Saylor 1940)
- 133.3* (9.6°C, summary of literature data, Stull 1947)
- 6415* (81.488°C, ebulliometry, measured range 81.488–165.725°C, Forziati et al. 1949)
- log (P/mmHg) = $7.07437 - 1569.622/(209.578 + t/^\circ\text{C})$; temp range 81.5–165.7°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
- 331 (extrapolated-Antoine eq., Dreisbach 1955)
- log (P/mmHg) = $7.07436 - 1569.622/(209.578 + t/^\circ\text{C})$; temp range 70–210°C (Antoine eq. for liquid state, Dreisbach 1955)
- 328* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981; Eastcott et al. 1988)
- log (P/mmHg) = $7.07435 - 1569.622/(209.578 + t/^\circ\text{C})$; temp range 48.82–193.07°C (Antoine eq., Zwolinski & Wilhoit 1971)
- log (P/mmHg) = $[-0.2185 \times 10516.8/(T/K)] + 8.161663$; temp range 9.6–164.7°C (Antoine eq., Weast 1972–73)
- 366 (calculated-bp, Mackay et al. 1982)
- log (P/atm) = $(1 - 437.769/T) \times 10^{(0.872945 - 6.55508 \times 10^4 \cdot T + 5.47586 \times 10^7 \cdot T^2)}$; T in K, temp range 253.0–635.0 K (Cox vapor pressure eq., Chao et al. 1983)
- 323 (extrapolated-Antoine eq., Boublik et al. 1984)
- log (P/kPa) = $6.20212 - 1571.575/(209.79 + t/^\circ\text{C})$; temp range 81.488–165.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 322 (extrapolated-Antoine eq., Dean 1985)
- 330 (selected lit., Riddick et al. 1986)
- log (P/kPa) = $6.21017 - 1577.80/(210.526 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
- log (P/mmHg) = $7.07436 - 1569.622/(209.58 + t/^\circ\text{C})$; temp range 49–193°C (Antoine eq., Dean 1985, 1992)
- 330 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.19762 - 1569.749/(-63.565 + T/K)$; temp range 354–445 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.62312 - 1810.653/(-43.307 + T/K)$; temp range 249–356 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
- 360 (computed-expert system SPARC, Kollig 1995)
- log (P/kPa) = $6.18965 - 1569.622/[(T/K) \pm 63.572]$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 929* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1981)
- 887* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1982)
- 682; 849 (EPICS; batch stripping, Ashworth et al. 1988)
- 682* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
- ln [H/(atm m³/mol)] = $7.241 - 3628/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
- 803 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 704 (infinite activity coeff. γ^∞ in water determined by inert gas stripping-GC, Li et al. 1993)
- 597 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
- log K_{AW} = $4.329 - 1448/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

- 3.42 (Leo et al. 1971; Hansch & Leo 1979)
- 3.78 (HPLC-k' correlation, Hammers et al. 1982)
- 3.82 (HPLC-k' correlation, Hafkenscheid & Tomlinson 1983)
- 3.42 (HPLC-RV correlation, Garst 1984)
- 3.89 (normal phase HPLC-k' correlation, Govers & Evers 1992)
- 3.42 (recommended value, Sangster 1993)
- 3.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.82 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)
- 2.77 (soil, calculated-MCI χ , Sabljic 1987a)
- 2.75 (soil, calculated-MCI χ , Sabljic 1987b)
- 2.85 (soil, calculated-MCI χ , Bahnick & Doucette 1988)
- 2.82 (soil, calculated-QSAR- χ , Sabljic et al. 1995)
- 3.37 (computed- K_{OW} , Kollig 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 1.606 \times 10^{-2} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with $\text{HO}\cdot$ in the gas (Dilling et al. 1988).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O_3} < 60 \text{ L mol}^{-1} \text{ s}^{-1}$ for vapor phase reaction with ozone at 30°C (Bufalini & Altshuller 1965)

$k_{OH} = (31 \pm 4) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$; $k_{O(3P)} = (16.8 \pm 2.0) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ with $\text{O}(^3\text{P})$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (47.2 \pm 4.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O(3P)} = (27.9 \pm 3.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction of $\text{O}(^3\text{P})$ atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 29.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ (Darnall et al. 1976)

$k_{OH}^* = (62.4 \pm 7.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

photooxidation in water, $t_{1/2} = 3208\text{--}1.28 \times 10^5 \text{ h}$, based on measured rate constant for reaction with hydroxyl radical in water (Mill et al. 1980)

$k_{OH} = 49.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and residence time of 0.2 d, loss of 99.3% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{O_3} = 4200 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with ozone at 300 K (Lyman et al. 1982)

$k_{OH} = (15\text{--}30) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.2\text{--}0.4 \text{ d}$ for trimethylbenzenes (Mill 1982)

$k = (700 \pm 200) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.7 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{NO_3} = 2.4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{OH} = 60.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{OH} = 38.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Ohta & Ohyama 1985)

$k_{NO_3} = 7.91 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{OH} = 6.05 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985; Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{OH}(\text{calc}) = 38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 62.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH}^* = 57.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}(\text{calc}) = 3.72 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{OH}(\text{calc}) = 54.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: unacclimated aerobic aqueous biodegradation $t_{1/2} = 48\text{--}192 \text{ h}$, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 192\text{--}768 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Bioconcentration:

Half-Lives in the Environment:

Air: $0.24\text{--}2.4 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

estimated lifetime under photochemical smog conditions in S.E. England is 0.7 h (Brice & Derwent 1978; Perry et al. 1977 and Darnall et al. 1976);

residence time of 0.2 d, loss of 99.3% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 9.72\text{--}97.2$ h, based on estimated photooxidation half-life in air (Atkinson 1987).

Surface Water: $t_{1/2} = 48\text{--}192$ h, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991);

$t_{1/2} = 1$ d in surface waters in case a first order reduction process may be assumed (estimated, Zoeteman et al. 1980).

Ground water: $t_{1/2} = 96\text{--}384$ h, based on a soil column study in which aerobic ground water was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991).

Soil: $t_{1/2} = 48\text{--}192$ h, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991).

Biota:

TABLE 3.1.1.9.1

Reported aqueous solubilities of 1,3,5-trimethylbenzene at various temperatures

Sanemasa et al. 1981		Sanemasa et al. 1982		Shaw 1989b (IUPAC)		Chen & Wagner 1994c	
vapor saturation-UV		vapor saturation-UV		recommended values		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	45.6	15	46	15	46	30	64
25	49.5	25	50	25	48.9	40	67.8
35	54.2	35	54.9	35	54	50	74.12
45	56.5	45	58.9	45	57	60	90.82
						70	111
						80	140
						90	164
						100	194
						$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 4.49$	
						at 25°C	

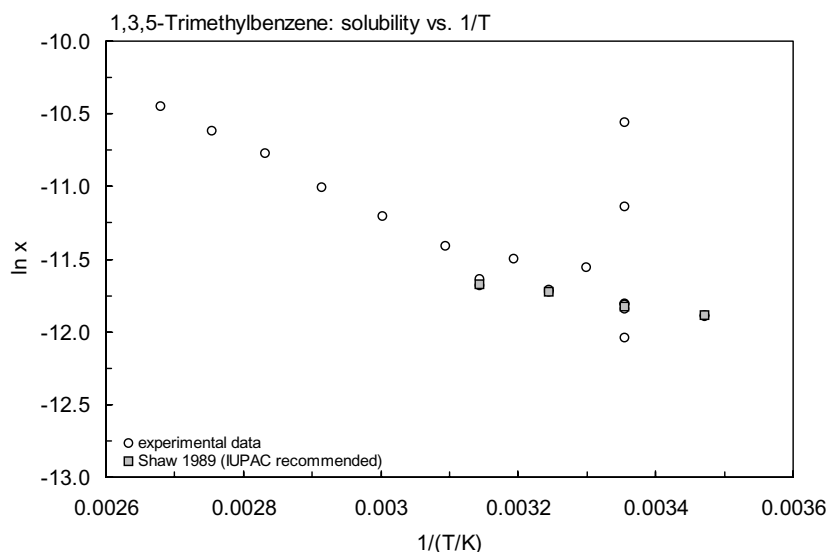


FIGURE 3.1.1.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,3,5-trimethylbenzene.

TABLE 3.1.1.9.2

Reported vapor pressures of 1,3,5-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

1.

Linder 1931		Kassel 1936		Rintelen et al. 1937		Stull 1947	
Hg manometer		mercury manometer		mercury manometer		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-1.7	45.3	0	58.7	10	80	9.6	133.3
0	50	10	124	30	507	34.7	266.6
2.3	66.7	20	248	50	1523	47.4	1333
3.2	70.7	30	521	Stuckey & Saylor 1940		61	2666
-2.75	38.66	40	844	mercury manometer		76.1	5333
-1.20	44	50	1467	t/°C	P/Pa	85.8	7999
1.5	57.3	60	2440	measured 4–75°C		98.9	13332
10.6	121.3	70	3933	eq. 4	P/mmHg	118.6	26664
-4.20	37.33	80	6133	A	23.2367	141	53323
2.7	66.66	90	9319	B	3122.45	164.7	101325
10.2	121.32	100	13786	C	5	mp/°C	44.8
		eq. 4	P/mmHg	bp/°C	164.54		
		A	22.1929				
		B	3104.5				
		C	5.0				

2.

Forziati et al. 1949				Zwolinski & Wilhoit 1971			
ebulliometry				selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
81.488	6415	163.911	99244	48.82	1333	161.556	93326
85.857	7697	164.489	100733	62.3	2666	162.632	95991
89.662	8991	165.146	102454	70.85	4000	163.686	98659
93.131	10328	165.725	103987	77.25	5333	164.716	101325
96.386	11722			82.424	6666		
100.747	13840	eq. 2	P/mmHg	86.789	7999	eq. 2	P/mmHg
105.716	16641	A	7.07437	93.949	10666	A	7.07436
110.789	19944	B	1573.267	99.746	13332	B	1569.622
115.498	23474	C	208.564	110.866	19998	C	209.578
121.765	28979			119.254	26664		
134.464	43352	bp/°C	164.716	126.068	33331	bp/°C	164.716
141.618	53692			131.849	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
149.238	66792			141.387	53329	at 25°C	47.48
157.477	83752			149.161	66661	at bp	39.04
163.289	97644			155.772	79993		

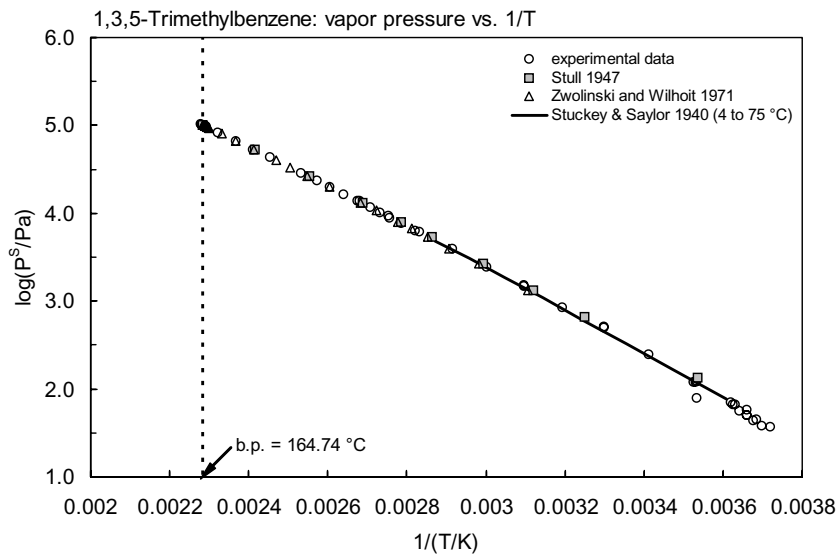


FIGURE 3.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trimethylbenzene.

TABLE 3.1.1.9.3
Reported Henry’s law constants of 1,3,5-trimethylbenzene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Sanemasa et al. 1981		Sanemasa et al. 1982		Ashworth et al. 1988	
vapor-liquid equilibrium		vapor-liquid equilibrium		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
15	547	15	511	10	408
25	929	25	887	15	466
35	1501	35	1365	20	477
45	2466	45	2394	25	682
				30	976
				eq. 4a	
				H/(atm m ³ /mol)	
				A	7.241
				B	3628

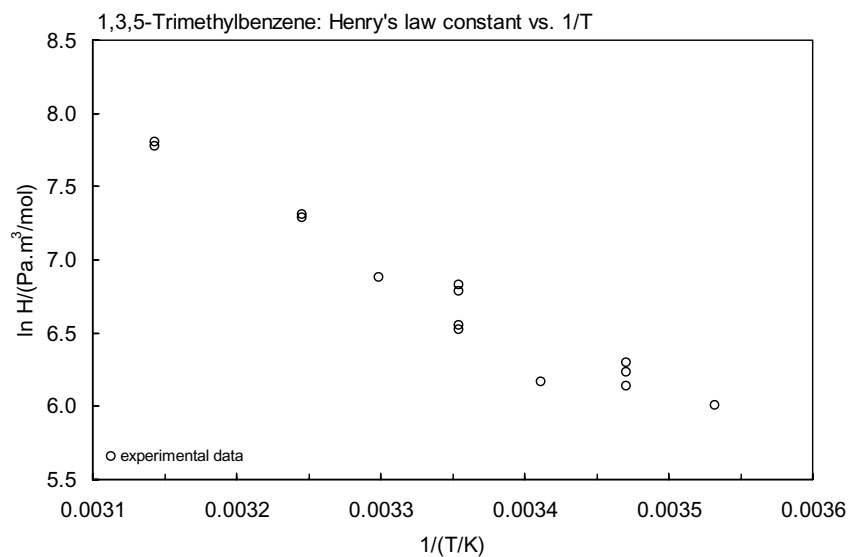
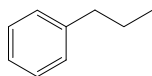


FIGURE 3.1.1.9.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,3,5-trimethylbenzene.

3.1.1.10 *n*-Propylbenzene

Common Name: *n*-Propylbenzene

Synonym: 1-phenylpropane, propylbenzene

Chemical Name: *n*-propylbenzene

CAS Registry No: 103-65-1

Molecular Formula: C₉H₁₂, C₆H₅(CH₂)₂CH₃

Molecular Weight: 120.191

Melting Point (°C):

−99.6 (Lide 2003)

Boiling Point (°C):

159.24 (Lide 2003)

Density (g/cm³ at 20°C):

0.862 (Weast 1982–83)

Molar Volume (cm³/mol):

139.4 (20°C, calculated-density)

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

9.27 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} (J/mol K):

53.39, 59.3 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

60 (15°C, volumetric, Fühner 1924; quoted, Chiou et al. 1982; Chiou 1985)

120 (shake flask-turbidimetric, Stearns et al. 1947)

55 (shake flask-UV, Andrews & Keffer 1950)

120 (shake flask-UV, Klevens 1951)

60 (shake flask-GC, Hermann 1972)

70 (shake flask-GC, Krasnoshchekova & Gubergrits 1975)

66.4 (shake flask-UV spec., Ben-Naim & Wiff 1979)

51.9* (generator column-HPLC/UV, 15–30°C, DeVoe et al. 1981)

51.0* (vapor saturation-UV spec., measured range 15–45°C, Sanemasa et al. 1982)

47.1 (generator column-HPLC/UV, Tewari et al. 1982a)

52.2 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982c)

59.5 (HPLC-k' correlation, converted from reported γ_w, Hafkenscheid & Tomlinson 1983a)

52.1 (generator column-HPLC/UV, Wasik et al. 1983)

45.2 (vapor saturation-UV spec., Sanemasa et al. 1984)

51.7* (generator column-HPLC/UV, measured range 10–45°C, Owens et al. 1986)

55.0* (IUPAC recommended, temp range 15–45°C, Shaw 1989b)

48.2* (vapor absorption technique-HPLC/UV, measured range 0.5–55°C, Dohányosová et al. 2001)

55.0* (shake flask-UV, measured range 0–50°C, Sawamura et al. 2001)

ln *x* = −304.679 + 12774.71/(T/K) + 43.8994·ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations; *data at other temperatures are tabulated at end of section):

260* (13.9°C, mercury manometer, Linder 1931)

6353* (75.646°C, ebulliometry, measured range 75.646–160.202°C, Willingham et al. 1945)

- $\log (P/\text{mmHg}) = 6.95178 - 1649.548/(207.171 + t/^{\circ}\text{C})$; temp range 75.6–160.2°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
 667* (31.3°C, summary of literature data, Stull 1947)
 6402* (75.818°C, ebulliometry, measured range 75.818–160.239°C, Forziati et al. 1949)
 $\log (P/\text{mmHg}) = 6.95094 - 1490.963/(207.100 + t/^{\circ}\text{C})$; temp range 75.8–160.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
 458 (extrapolated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 6.95142 - 1491.297/(207.140 + t/^{\circ}\text{C})$; temp range 65–205°C (Antoine eq. for liquid state, Dreisbach 1955)
 449* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = 6.95142 - 1491.297/(207.140 + t/^{\circ}\text{C})$; temp range 43.33–187.87°C (Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = [-0.2185 \times 10424.1/(T/\text{K})] + 8.185880$; temp range 6.3–159.2°C (Antoine eq., Weast 1972–73)
 $\log (P/\text{atm}) = (1 - 432.321/T) \times 10^{(0.891023 - 6.89092 \times 10^4 \cdot T + 5.79948 \times 10^7 \cdot T^2)}$; T in K, temp range 280.0–635.0 K (Cox vapor pressure eq., Chao et al. 1983)
 450 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.08028 - 1493.914/(207.427 + t/^{\circ}\text{C})$; temp range 75.2–160.24°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 6.95142 - 1491.297/(207.14 + t/^{\circ}\text{C})$; temp range 43–188°C (Antoine eq., Dean 1985, 1992)
 449 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.07438 - 1490.61/(-66.029 + T/\text{K})$; temp range 348–433 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 39.8219 - 3.6978 \times 10^3/(T/\text{K}) - 10.962 \cdot \log (T/\text{K}) + 8.7429 \times 10^{-11} \cdot (T/\text{K}) + 2.6959 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 174–638 K (Yaws 1994)
 $\log (P/\text{kPa}) = 6.07625 - 1490.903/[(T/\text{K}) - 66.05]$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations; *data at other temperatures are tabulated at end of section):

- 1062* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1982)
 1094* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 7.835 - 3681/(T/\text{K})$, temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 1034 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 1102 (infinite activity coeff. γ^{∞} in water determined by inert gas stripping-GC, Li et al. 1993)
 1175* (equilibrium headspace-GC, measured range 10–30°C, Perlinger et al. 1993)
 902 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 4.587 - 1471/(T/\text{K})$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.68 (shake flask-UV, Iwasa et al. 1965; Hansch et al. 1968; 1972)
 3.57, 3.68 (Leo et al. 1971; Hansch & Leo 1979)
 3.66 (calculated-fragment const., Rekker 1977)
 3.44 (shake flask-HPLC, Nahum & Horvath 1980)
 3.691* (3.701, 3.72-HPLC/UV, DeVoe et al. 1981)
 3.71 (generator column-HPLC/UV both phases, Tewari et al. 1982a)
 3.63 (HPLC- k' correlation, Hammers et al. 1982)
 3.69 (generator column-HPLC/GC, Tewari et al. 1982b,c; Wasik et al. 1983)
 3.89 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
 3.69 (generator column-HPLC/UV, Wasik et al. 1983)
 3.69 (generator column-RP-HPLC, Schantz & Martire 1987)
 3.71, 3.88 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
 3.69 (recommended, Sangster 1989, 1993)
 3.69 (HPLC-RT correlation, Jenke et al. 1990)
 3.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

4.09 (calculated-measured γ^∞ in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

2.87 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
 2.83, 2.98 (RP-HPLC- k' correlation, humic acid-silica column, Szabo et al. 1990a,b)
 2.81, 2.84, 2.87 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: rate constants: $k = 0.037 \text{ d}^{-1}$, $t_{1/2} = 19 \text{ d}$ in spring at 8–16°C, $k = 0.539 \text{ d}^{-1}$, $t_{1/2} = 1.3 \text{ d}$ in summer at 20–22°C, $k = 0.065 \text{ d}^{-1}$, $t_{1/2} = 11 \text{ d}$ in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.086 \text{ d}^{-1}$, $t_{1/2} = 8.1 \text{ d}$ with HgCl_2 in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Photolysis: rate constant $k = 6.96 \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO in the gas (Dilling et al. 1988).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 3.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 2.4\text{--}24 \text{ h}$ (Darnall et al. 1976)

$k_{OH} = (3.7 \pm 0.8) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Lloyd et al. 1976)

$k_{OH} = (6.40, 5.86) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{OH} = 3.5 \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 1.6 \text{ d}$ (Mill 1982)

$k_{OH} = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{OH} = 6.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Ohta & Ohyama 1985)

$k_{OH}(\text{calc}) = 7.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH} = 6.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}(\text{calc}) = 5.99 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Bioconcentration

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

estimated lifetime $\tau = 6 \text{ h}$ under photochemical smog conditions in S.E. England (Brice & Derwent 1978; Darnall et al. 1976).

Surface water: $t_{1/2} = 19 \text{ d}$ in spring at 6–16°C, $t_{1/2} = 1.3 \text{ d}$ in summer at 20–22°C, $t_{1/2} = 11 \text{ d}$ in winter at 3–7°C when volatilization dominates and $t_{1/2} = 8.1 \text{ d}$ with HgCl_2 in marine mesocosm experiments (Wakeham et al. 1983)

TABLE 3.1.1.10.1

Reported aqueous solubilities of *n*-propylbenzene at various temperatures

1.

Sanemasa et al. 1982		DeVoe et al. 1981		Owens et al. 1986		Shaw 1989b (IUPAC)	
vapor saturation-UV		generator column-HPLC		generator column-HPLC		recommended values	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	46.1	23	51.32	10	53.73	15	47
25	51	15	51.21	15	52.29	25	55
35	55	20	51.09	20	54.33	35	55
45	64.1	25	51.93	25	52.25	45	64
		30	53.49	30	52.53		
				35	56.62		
				40	63.95		
				45	66.59		
				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.70$			
				25°C			

2.

Dohányosová et al. 2001		Sawamura et al. 2001	
vapor absorption-HPLC/UV		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0.5	46.5	0	60.2
5	45.8	5	57.8
15	44.8	10	55.96
25	48.2	15	54.96
35	52.2	20	54.5
45	62.4	25	54.96
55	74.4	30	56.2
		35	58.4
		40	61.3
		45	65.6
		50	90.6
$\Delta_{\text{sol}}H/(\text{kJ mol}^{-1}) = 6.20$			
25°C			

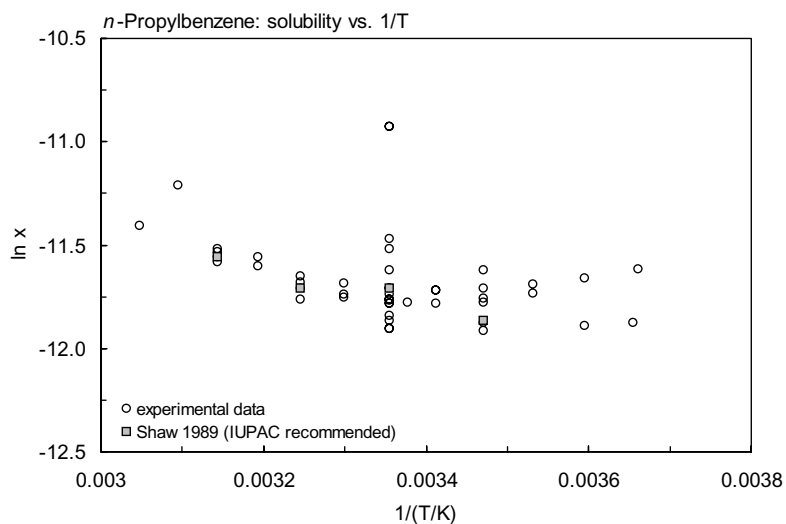
FIGURE 3.1.1.10.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *n*-propylbenzene.

TABLE 3.1.1.10.2

Reported vapor pressures of *n*-propylbenzene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)				
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)				
log P = A – B/(C + T/K)		(3)							
log P = A – B/(T/K) – C·log (T/K)		(4)							
Linder 1931		Willingham et al. 1945		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 71	
mercury manometer		ebulliometry		summary of lit. data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–6.8	46.7	75.646	6353	6.3	133.3	75.818	6402	43.44	1333
–0.7	77.3	80.064	7654	31.3	666.6	80.181	7694	56.79	2666
3.6	113.2	83.909	8965	43.4	1333	83.993	8993	65.28	4000
13.9	260	87.383	10304	56.8	2666	87.457	10332	71.64	5333
		90.622	11696	71.6	5333	90.688	11723	76.784	6666
		94.993	13820	81.1	7999	95.049	13844	81.13	7999
		99.986	16621	94	13332	100.02	16636	88.264	10666
		105.046	19924	113.5	66664	105.085	19946	94.046	13332
		109.744	23450	137.7	53329	109.781	23557	105.142	19998
		116.032	28955	159.2	101325	116.06	23982	113.542	26664
		121.807	34898			128.794	43364	120.367	33331
		128.764	43323	mp/°C	–99.5	135.972	53702	126.163	39997
		135.942	53654			143.625	66799	135.737	53329
		143.598	66757			151.921	83753	143.551	66661
		151.908	83718			157.779	97649	150.205	79993
		157.76	97607			158.408	99239	156.031	93326
		158.389	99203			158.991	100730	157.116	95992
		158.972	100694			159.654	102465	158.178	98659
		159.625	102386			160.239	104003	159.217	101325
		160.202	103910						
						eq. 2	P/mmHg	eq. 2	P/mmHg
		eq. 2	P/mmHg			A	6.95094	A	695142
		A	695178			B	1490.963	B	1491.297
		B	1491548			C	207.1	C	207.14
		C	207.171						
						bp/°C	159.218	bp/°C	159.217
		bp/°C	159.216					ΔH _v /(kJ mol ^{–1}) =	
								at 25°C	46.23
								at bp	38.24

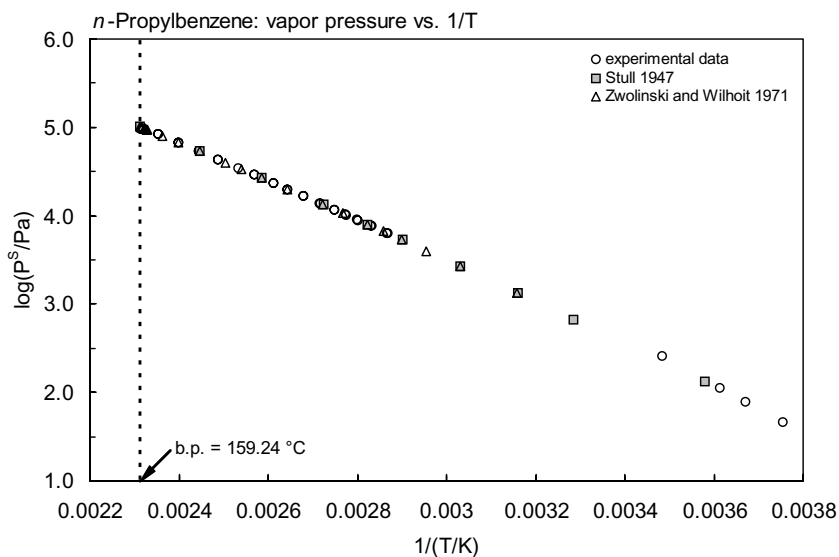


FIGURE 3.1.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-propylbenzene.

TABLE 3.1.1.10.3
Reported Henry's law constants and octanol-water partition coefficients of *n*-propylbenzene at various temperatures

Henry's law constant						log K_{OW}	
Sanemasa et al. 1982		Ashworth et al. 1988		Perlinger et al. 1993		DeVoe et al. 1981	
vapor-liquid equilibrium		EPICS-GC		equilibrium headspace-GC		generator column-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OW}
15	594	10	576	10	441	25	3.691
25	1062	15	741	15	629	25	3.701
35	1818	20	893	20	848	10	3.705
45	2754	25	1094	25	1175	20	3.735
		30	1388	30	1550	25	3.72
		ln H = A – B/(T/K) H/(atm m ³ /mol)				30	3.715
						35	3.682
		A	7.835			shake flask-GC	
		B	3681			ambient	3.734
						ambient	3.718
						ambient	3.711

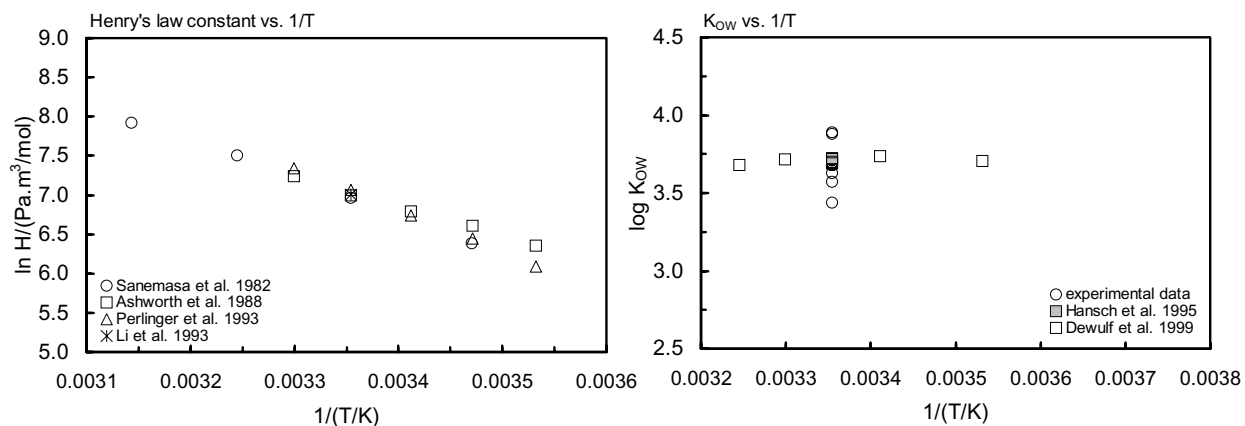
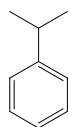


FIGURE 3.1.1.10.3 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for *n*-propylbenzene.

3.1.1.11 Isopropylbenzene



Common Name: Isopropylbenzene

Synonym: cumene, 2-phenylpropane, (1-methylethyl)benzene, cumol, *i*-propylbenzene

Chemical Name: isopropylbenzene

CAS Registry No: 98-82-8

Molecular Formula: C_9H_{12} , $C_6H_5CH(CH_3)_2$

Molecular Weight: 120.191

Melting Point ($^{\circ}C$):

−96.02 (Lide 2003)

Boiling Point ($^{\circ}C$):

152.41 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8618 (Weast 1982–83)

Molar Volume (cm^3/mol):

139.5 ($20^{\circ}C$, calculated-density)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.141, 37.53 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

7.786 (Riddick et al. 1986)

7.32 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

41.34, 46.3 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$; or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

170 (shake flask-turbidimetric, Stearns et al. 1947)

73 (shake flask-UV, Andrews & Keffer, 1950)

80.5* (shake flask-UV, measured range 25 – $80^{\circ}C$, Glew & Robertson 1956)

53 (shake flask-GC, McAuliffe 1963)

50 (shake flask-GC, McAuliffe 1966)

50 (shake flask-GC, Hermann 1972)

65.3 (shake flask-GC, Sutton & Calder 1975)

48.3 (shake flask-GC, Price 1976)

48.3 (shake flask-GC, Krzyzanowska & Szeliga 1978)

61.5* (vapor saturation-UV, measured range 15 – $45^{\circ}C$, Sanemasa et al. 1982)

56* (IUPAC recommended, temp range 15 – $80^{\circ}C$, Shaw 1989b)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

300* ($13.7^{\circ}C$, mercury manometer, measured range -8.2 – $13.7^{\circ}C$, Linder 1931)

$\log(P/mmHg) = -2175/(T/K) + 7.991$ (isotenoscope method, temp range not specified, Kobe et al. 1941)

6353* ($70.02^{\circ}C$, ebulliometry, measured range 70.02 – $153.367^{\circ}C$, Willingham et al. 1945)

$\log(P/mmHg) = 6.92929 - 1455.811/(207.202 + t/^{\circ}C)$; temp range 70.0 – $153.4^{\circ}C$ (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

666.6* ($31.3^{\circ}C$, summary of literature data, temp range 6.3 – $159.2^{\circ}C$, Stull 1947)

6401* ($70.16^{\circ}C$, ebulliometry, measured range 70.16 – $153.4^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 6.93958 - 1462.717/(207.993 + t/^{\circ}C)$; temp range 70.2 – $153.4^{\circ}C$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

- 621 (extrapolated-Antoine eq., Dreisbach 1955; quoted, Hine & Mookerjee 1975)
 $\log (P/\text{mmHg}) = 6.93666 - 1460.793/(207.777 + t/^{\circ}\text{C})$; temp range 60–200°C (Antoine eq. for liquid state, Dreisbach 1955)
- 609 (interpolated, Glew & Robertson 1956)
- 611* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = 6.93666 - 1460.793/(207.777 + t/^{\circ}\text{C})$; temp range 38.29–180.67°C (Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = [-0.2185 \times 10335.3/(T/\text{K})] + 8.231760$; temp range 2.9–152.4°C (Antoine eq., Weast 1972–73)
 $\log (P/\text{atm}) = (1 - 425.438/T) \times 10^{(0.877964 - 7.34971 \times 10^4 \cdot T + 6.06942 \times 10^7 \cdot T^2)}$; T in K, temp range 264.95–630.0 K (Cox vapor pressure eq., Chao et al. 1983)
- 610 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.0571 - 1457.715/(207.415 + t/^{\circ}\text{C})$; temp range 70.02–153.4°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.06528 - 1464.366/(208.235 + t/^{\circ}\text{C})$; temp range 56.39–151.69°C (Antoine eq. from reported exptl. data of Dreyer et al. 1955, Boublik et al. 1984)
- 610 (selected lit., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.06588 - 1464.17/(208.207 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P/\text{mmHg}) = 6.93666 - 1460.793/(207.78 + t/^{\circ}\text{C})$; temp range 39–181°C (Antoine eq., Dean 1985, 1992)
- 605 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.05949 - 1459.975/(-65.942 + T/\text{K})$; temp range 339–433 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = -0.9234 - 2.9558 \times 10^3/(T/\text{K}) + 7.1685 \cdot \log (T/\text{K}) - 2.5369 \times 10^{-2} \cdot (T/\text{K}) + 1.4858 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 177–631 K (Yaws 1994)
 $\log P/\text{kPa} = 6.06149 - 1460.793/[(T/\text{K}) - 65.373]$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1469 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 1323* (28°C, EPICS-GC, measured range 28–46.1°C, Hansen et al. 1993)
 $\ln [H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -3269/(T/\text{K}) + 11.0$; temp range 28–46.1°C (EPICS-GC, Hansen et al. 1993)
- 1126 (infinite activity coeff. γ^{∞} in water determined by inert gas stripping-GC, Li et al. 1993)
- 960 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
- 902 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 3.774 - 1256/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.43 (calculated- π substituent constant, Hansch et al. 1968)
- 3.66 (Leo et al. 1971; Hansch & Leo 1979)
- 3.63 (shake flask-GC, Chiou et al. 1977, 1982)
- 3.51 (headspace GC, Hutchinson et al. 1980)
- 3.52 (HPLC- k' correlation, Hanai et al. 1981)
- 3.52 (HPLC- k' correlation, D'Amboise & Hanai 1982)
- 3.40 (HPLC- k' correlation, Miyake & Terada 1982)
- 3.89, 4.07 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
- 3.66 (recommended, Sangster 1989, 1993)
- 3.82 (from measured activity coeff., Tse et al. 1994)
- 3.66 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C:

- 3.98 (calculated-measured γ^{∞} in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.55 (goldfish, Ogata et al. 1984)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 5.7$ h from water depth of 1 m (calculated, Mackay & Leinonen 1975).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (3.7 \pm 0.8) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Lloyd et al. 1976)

$k_{OH} = 3.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 2.4\text{--}24 \text{ h}$ (Darnall et al. 1976)

$k_{OH} = (7.79 \pm 0.40) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 200 torr He and 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{OH} = 4.6 \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 1.2 \text{ d}$ (Mill 1982)

$k = (11 \pm 3) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 100 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{OH} = 6.25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate method, Ohta & Ohyama 1985)

$k_{OH}(\text{calc}) = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH} = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}(\text{calc}) = 4.69 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Bioconcentration

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

estimated lifetime $\tau = 6 \text{ h}$ under photochemical smog conditions in S.E. England (Brice & Derwent 1978) and (Darnall et al. 1976).

Surface Water: $t_{1/2} = 5.79 \text{ h}$, calculated half-life based on evaporative loss at 25°C and 1 m depth of water (Mackay & Leinonen 1975).

TABLE 3.1.1.11.1

Reported aqueous solubilities and Henry's law constants of isopropylbenzene at various temperatures

		Aqueous solubility		Henry's law constant			
Glew & Robertson 1956		Sanemasa et al. 1982		Shaw 1989b (IUPAC)		Hansen et al. 1993	
shake flask-UV spec.		vapor equilibrium-UV spec.		recommended values		EPICS-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
24.936	80.47	15	59.5	15	60	28	1323
29.984	82.91	25	61.5	25	56	36	1547
34.918	85.64	35	68.7	30	74	46.1	2422
39.958	89.79	45	77.5	40	82		
44.905	94.57			50	90	$\ln H = A - B/(T/K)$	
49.902	100.4	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 5.10$		60	120	$H/(\text{kPa m}^3/\text{mol})$	
54.916	106.9	at 25°C		70	140	A	11
59.983	115			80	160	B	3299
65.165	124.4						
70.32	135.6						
75.097	147.3						
80.209	161.7						
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.57$							
at 25°C							

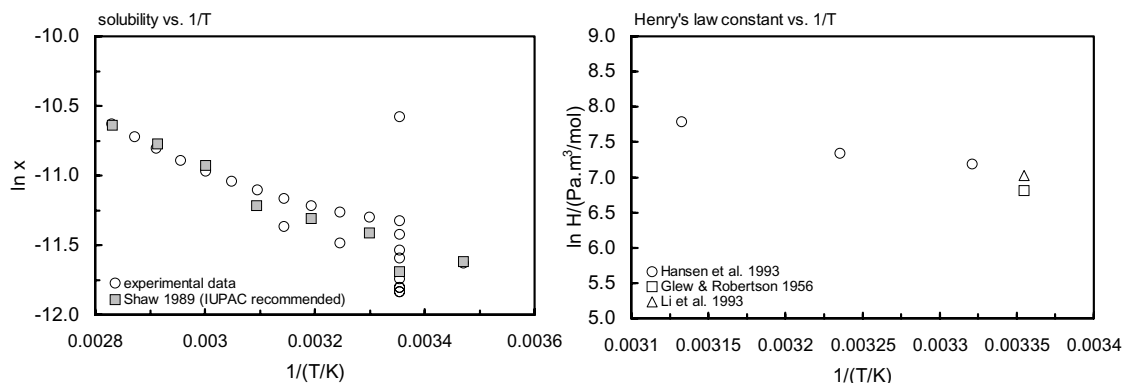


FIGURE 3.1.11.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for isopropylbenzene.

TABLE 3.1.1.11.2

Reported vapor pressures of isopropylbenzene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

$$\ln P = A - B/(T/K) \quad (1a)$$

$$\ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

Linder 1931		Willingham et al.1945		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
Hg manometer		ebulliometry		ebulliometry		selected values	
t/ [°] C	P/Pa	t/ [°] C	P/Pa	t/ [°] C	P/Pa	t/ [°] C	P/Pa
-8.2	57.3	70.02	6353	70.16	6401	36.29	1333
1.3	124	74.365	7654	74.47	7693	51.43	2666
13.7	300	78.155	8965	78.23	8993	59.79	4000
		81.579	10304	81.64	10331	66.06	5333
		84.768	11696	89.11	11722	71.123	6666
		89.077	13820	94.01	13843	75.407	7999
		93.991	16621	99	16636	82.433	10666
		98.975	19924	103.64	19946	88.13	13332
		103.604	23450	109.82	23477	99.076	19998
		109.802	28995	115.52	28980	107.346	26664
		115.495	34898	12.38	34928	114.076	33331
		122.353	43323	129.46	43363	119.789	39997
		129.433	53654	137.01	53701	129.23	53329
		136.983	66757	145.19	66799	136.937	66661
		145.176	83718	150.97	83752	143.501	79993
		150.956	97607	151.59	97649	149.249	93326
		151.576	99203	152.17	100730	150.319	95992
		152.152	100694	152.82	102465	151.367	98659
		152.798	102386	153.4	104003	152.392	101325
		153.367	103910				
		eq. 2	P/mmHg	eq. 2	P/mmHg	eq. 2	P/mmHg
		A	6.92929	A	6.93958	A	6.93666
		B	1455.81	B	1462.717	B	1460.793
		C	207.202	C	207.993	C	207.777
mp/ [°] C	-99.5	bp/ [°] C	152.393	bp/ [°] C	152.392	bp/ [°] C	152.392
							$\Delta H_v/(\text{kJ mol}^{-1}) =$
						at 25 [°] C	45.14
						at bp	37.53

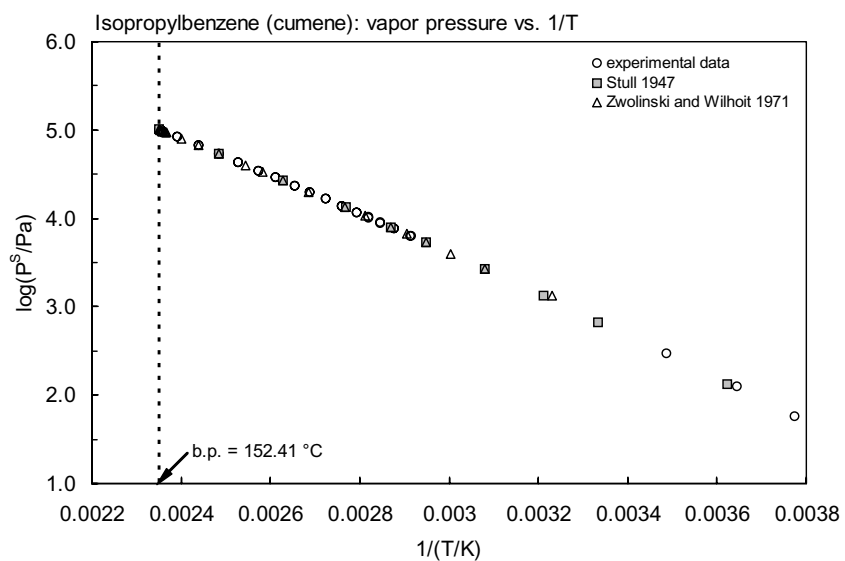
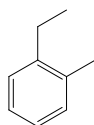


FIGURE 3.1.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for isopropylbenzene.

3.1.1.12 1-Ethyl-2-methylbenzene (*o*-Ethyltoluene)

Common Name: 1-Ethyl-2-methylbenzene

Synonym: 2-ethyltoluene, *o*-ethyltoluene

Chemical Name: 1-ethyl-2-methylbenzene, 1-methyl-2-ethylbenzene

CAS Registry No: 611-14-3

Molecular Formula: C_9H_{12} , $C_6H_4CH_3C_2H_5$

Molecular Weight: 120.191

Melting Point ($^{\circ}C$):

−79.83 (Lide 2003)

Boiling Point ($^{\circ}C$):

165.2 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8807 (Weast 1982–83)

Molar Volume (cm^3/mol):

136.5 ($20^{\circ}C$, calculated-density)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

40.0 (estimated from nomograph, Kabadi & Danner 1979)

93.05 (shake flask-GC, Mackay & Shiu 1981)

74.6 (generator column-HPLC/UV, Tewari et al. 1982c)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($9.4^{\circ}C$, summary of literature data, Stull 1947)

6417* ($81.146^{\circ}C$, ebulliometry, measured range 81.146 – $157.825^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 7.00314 - 1535.374/(207.300 + t/^{\circ}C)$; temp range 81.1 – $166.2^{\circ}C$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

336 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.00314 - 1535.374/(207.3 + t/^{\circ}C)$; temp range 70 – $215^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

330* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.00314 - 1535.374/(207.300 + t/^{\circ}C)$; temp range 48.46 – $193.89^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 10448.8/(T/K)] + 8.141032$; temp range 9.4 – $165.2^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 438.357/T) \times 10^{(0.863837 - 6.34917 \times 10^4 \cdot T + 5.19164 \times 10^7 \cdot T^2)}$; T in K, temp range 285.0 – 645.0 K (Cox vapor pressure eq., Chao et al. 1983)

328 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.11997 - 1529.684/(206.648 + t/^{\circ}C)$; temp range 81.146 – $166.2^{\circ}C$ (Antoine eq. from reported exptl. data Forziati et al. 1949, Boublik et al. 1984)

330 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.00314 - 1535.374/(207.30 + t/^{\circ}C)$; temp range 48 – $194^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.1129 - 1532.449/(-66.123 + T/K)$; temp range 353 – 443 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 15.1142 - 2.9821 \times 10^3/(T/K) - 1.2619 \cdot \log(T/K) - 6.3248 \times 10^{-3} \cdot (T/K) + 3.5155 \times 10^{-6} \cdot (T/K)^2$, temp range 192 – 651 K (Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

565 (EPICS-GC/FID, Ashworth et al. 1988)

$\ln [H/(\text{atm m}^3/\text{mol})] = 5.557 - 3179/(T/\text{K})$; temp range $10\text{--}30^\circ\text{C}$ (EPICS measurements, Ashworth et al. 1988)

426 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

512 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.63 (headspace GC, Hutchinson et al. 1980)

3.53 (generator column-HPLC/UV, DeVoe et al. 1981; Tewari et al. 1982a)

3.78, 3.95 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)

3.53 (recommended, Sangster 1989, 1993)

3.53 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (8.2 \pm 1.6) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 8.2 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with half-life of 0.24–2.4 h (Darnall et al. 1976)

$k_{\text{OH}} = 12.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}} = 12.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Ohta & Ohyama 1985)

$k_{\text{OH}} = 12.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 17.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);

summer daylight lifetime $\tau = 11 \text{ h}$ due to reaction with OH radical (Altshuller 1991).

Surface water: $t_{1/2} = 0.5 \text{ d}$ in surface water in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980).

TABLE 3.1.1.12.1

Reported vapor pressures of *o*-ethyltoluene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)	
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)	
log P = A – B/(C + T/K)		(3)				
log P = A – B/(T/K) – C·log (T/K)		(4)				
Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971		
summary of literature data		ebulliometry		selected values		
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	
9.4	133.3	81.146	6417	48.46	1333	eq. 2
34.8	666.6	85.618	7697	61.96	2666	A
47.6	1333	89.448	8993	70.54	4000	B
61.2	2666	92.949	10323	76.97	5333	C
76.4	5333	96.2	11720	82.165	6666	bp/°C
86	7999	100.584	13840	86.552	7999	ΔH _v /(kJ mol ⁻¹) =
99	13332	105.598	16641	93.751	10666	at 25°C
119	26664	110.711	19944	99.582	13332	at bp
141.4	53329	115.436	23473	110.777	19998	
165.1	101325	121.762	28978	119.29	26664	
		127.574	34920	126.1	33331	
mp/°C	–104.7	134.57	43351	131.933	39997	
		141.792	53693	141.563	53329	
		149.582	66792	149.418	66661	
		157.825	83749	156.103	79993	
				161.954	93326	
		eq. 2	P/mmHg	164.044	95992	
		A	7.00314	164.11	98659	
		B	1535.374	165.534	101325	
		C	207.3			
		bp/°C	165.153			

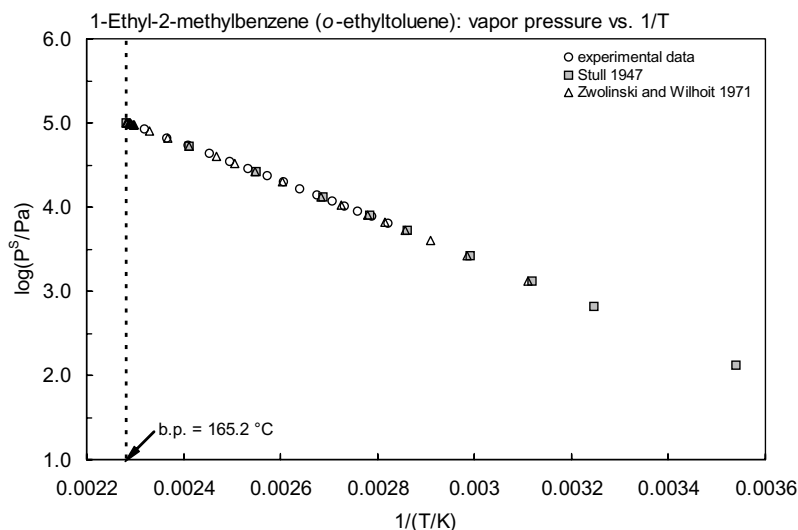
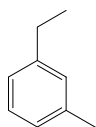


FIGURE 3.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for 1-ethyl-2-methylbenzene (*o*-ethyltoluene).

3.1.1.13 1-Ethyl-3-methylbenzene (*m*-Ethyltoluene)

Common Name: 1-Ethyl-3-methylbenzene

Synonym: 3-ethyltoluene, *m*-ethyl toluene

Chemical Name: 1-ethyl-3-methylbenzene, 1-methyl-3-ethylbenzene

CAS Registry No: 620-14-4

Molecular Formula: C_9H_{12} , $C_6H_4CH_3C_2H_5$

Molecular Weight: 120.191

Melting Point ($^{\circ}C$):

– 95.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

161.3 (Forziati et al. 1949, Weast 1982–83; Lide 2003)

Density (g/cm^3):

0.8645 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

139.0 ($20^{\circ}C$, calculated-density)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* ($32.3^{\circ}C$, summary of literature data, temp range 7.2 – $161.3^{\circ}C$, Stull 1947)

3066* ($62.1^{\circ}C$, mercury manometer, measured range 62.1 – $160.3^{\circ}C$, Buck et al. 1949)

6417* ($78.105^{\circ}C$, ebulliometry, measured range 78.105 – $154.053^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 7.01582 - 1529.784/(208.509 + t/^{\circ}C)$; temp range 78.1 – $162.3^{\circ}C$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

399 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.01582 - 1529.184/(208.509 + t/^{\circ}C)$; temp range 65 – $210^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

391* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.01582 - 1529.184/(208.509 + t/^{\circ}C)$; temp range 45.68 – $189.74^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 10416.6/(T/K)] + 8.152199$; temp range 7.2 – $161.3^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 434.538/T) \times 10^{(0.861399 - 6.30303 \times 10^4 \cdot T + 5.19848 \times 10^7 \cdot T^2)}$; T in K, temp range 280.0 – $635.0\ K$ (Cox vapor pressure eq., Chao et al. 1983)

394 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.12947 - 1531.584/(209.417 + t/^{\circ}C)$; temp range 78.3 – $163^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

391 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.01582 - 1529.184/(208.51 + t/^{\circ}C)$; temp range 46 – $190^{\circ}C$ (Antoine eq., Dean 1985, 1992)

391 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.13801 - 1527.983/(-64.715 + T/K)$; temp range 348 – $438\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 39.8909 - 3.6042 \times 10^3/(T/K) - 11.466 \cdot \log(T/K) + 3.5274 \times 10^{-2} \cdot (T/K) + 7.3492 \times 10^{-14} \cdot (T/K)^2$, temp range 178 – $637\ K$ (Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.88, 4.07 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
- 3.98 (lit. average value, Sangster 1993)
- 3.88 (quoted from Sherblom & Eganhouse 1988; Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.42 (aquifer material with f_{OC} of 0.006 and measured partition coeff. $K_{\text{p}} = 1.58 \text{ mL/g.}$, Abdul et al. 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (11.7 \pm 2.3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at $305 \pm \text{K}$ (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 11.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with estimated $t_{1/2} \sim 0.24\text{--}2.4 \text{ h}$ (Darnall et al. 1976)

$k_{\text{OH}} = (21.3 \pm 1.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate method, Ohta & Ohshima 1985; Atkinson 1989)

$k_{\text{OH}} = 1.92 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 20.93 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al 1976; Howard et al. 1991);

summer daylight lifetime $\tau = 7.2 \text{ h}$ due to reaction with OH radical (Altshuller 1991).

TABLE 3.1.1.13.1

Reported vapor pressures of *m*-ethyltoluene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Forziati et al. 1949		Buck et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		mercury manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
7.2	133.3	78.105	6417	62.1	3066	45.68	1333
32.3	666.6	82.525	7697	74	5386	59.07	2666
44.7	1333	86.293	8993	77.9	6293	67.58	4000
58.2	2666	89.793	10328	85.4	8693	73.95	5333
73.3	5333	93.022	11720	91.3	10879	79.102	6666
82.9	7999	97.368	13840	95.1	12772	83.45	7999
95.9	13332	102.326	16641	102.1	16772	90.584	10666
115.5	26664	107.383	19944	115.3	26398	96.363	13332
137.8	53329	112.074	23473	122.5	34264	107.456	19998
161.3	101325	118.338	28978	129.8	42397	115.829	26664
mp/°C	–104.7	124.082	34920	140.7	58262	122.635	33331
		131.027	43351	148.5	72527	128.412	39997
		138.178	53693	160.3	99592	137.949	53329
		145.795	66792			145.727	66661
		154.053	83749	eq. 4	P/mmHg	152.346	79993
				A	25.08	158.318	93326
		eq. 2	P/mmHg	B	3155	159.217	95992
		A	7.01582	C	5.663	160.272	98659
		B	1529.184			161.305	101325
		C	208.509				

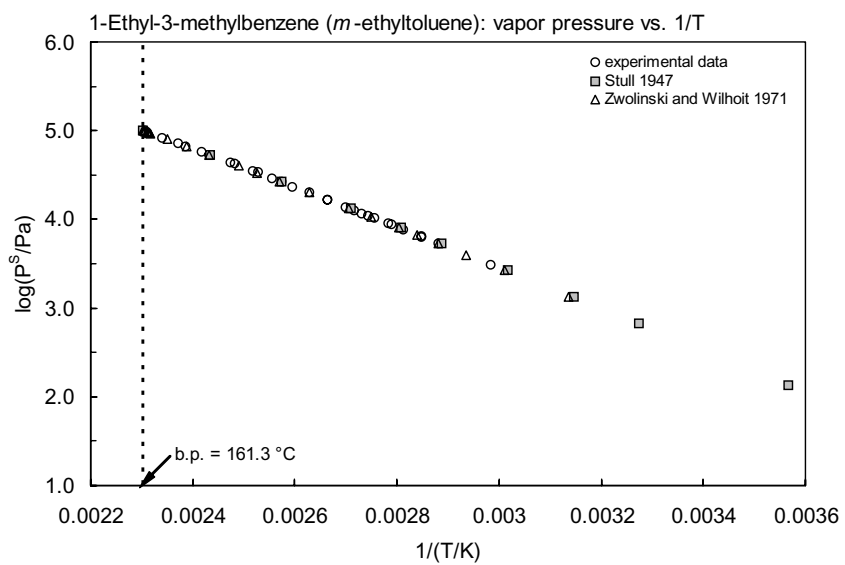
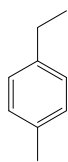


FIGURE 3.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for 1-ethyl-3-methylbenzene (*m*-ethyltoluene).

3.1.1.14 1-Ethyl-4-methylbenzene (*p*-Ethyltoluene)

Common Name: 1-Ethyl-4-methylbenzene

Synonym: 4-ethyltoluene, *p*-ethyl toluene

Chemical Name: 1-ethyl-4-methylbenzene, 1-methyl-4-ethylbenzene

CAS Registry No: 622-96-8

Molecular Formula: C_9H_{12} , $C_6H_4CH_3C_2H_5$

Molecular Weight: 120.191

Melting Point ($^{\circ}C$):

−62.35 (Lide 2003)

Boiling Point ($^{\circ}C$):

162 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8614 (Weast 1982–83)

Molar Volume (cm^3/mol):

139.5 ($20^{\circ}C$, calculated -density, Stephenson & Malanowski 1987)

162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

40.0 (estimated from nomograph, Kabadi & Danner 1979)

94.85 (shake flask-GC, Mackay & Shiu 1981)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* ($32.7^{\circ}C$, summary of literature data, temp range 7.6 – $162^{\circ}C$, Stull 1947)

3840* ($66.8^{\circ}C$, mercury manometer, measured range 66.8 – $161.1^{\circ}C$, Buck et al. 1949)

6417* ($78.396^{\circ}C$, ebulliometry, measured range 78.396 – $154.684^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 6.99801 - 1527.113/(208.921 + t/^{\circ}C)$; temp range 78.3 – $163.0^{\circ}C$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

402 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 6.99802 - 1527.113/(208.921 + t/^{\circ}C)$; temp range 65 – $210^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

393* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.99802 - 1527.113/(208.921 + t/^{\circ}C)$; temp range 45.68 – $190.64^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 10461.1/(T/K)] + 8.175267$; temp range 7.6 – $162^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 345.228/T) \times 10^{(0.856105 - 6.18307 \times 10^{-4} \cdot T + 5.08568 \times 10^{-7} \cdot T^2)}$; T in K, temp range 280.0 – 635.0 K (Cox vapor pressure eq., Chao et al. 1983)

393 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.99802 - 1527.113/(208.92 + t/^{\circ}C)$; temp range 46 – $191^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.11098 - 1519.486/(-65.035 + T/K)$; temp range 349 – 442 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 46.9026 - 3.8382 \times 10^3/(T/K) - 14.154 \cdot \log(T/K) + 4.9305 \times 10^{-3} \cdot (T/K) - 1.3901 \times 10^{-13} \cdot (T/K)^2$; temp range 211 – 640 K (Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 498 (calculated-P/C, Mackay & Shiu 1981, Eastcott et al. 1988)
- 498 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.63 (headspace GC, Hutchinson et al. 1980)
- 3.90, 4.09 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
- 3.63 (recommended, Sangster 1989, 1993)
- 3.90 (quoted from Sherblom & Eganhouse 1988, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (7.8 \pm 1.6) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = 7.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ (Darnall et al. 1976)

$k_{\text{OH}} = 12.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and residence time of 0.9 d, loss of 67% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}} = 11.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}} = 12.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Ohta & Ohshima 1985)

$k_{\text{OH}} = 12.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 21.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Half-Lives in the Environment:

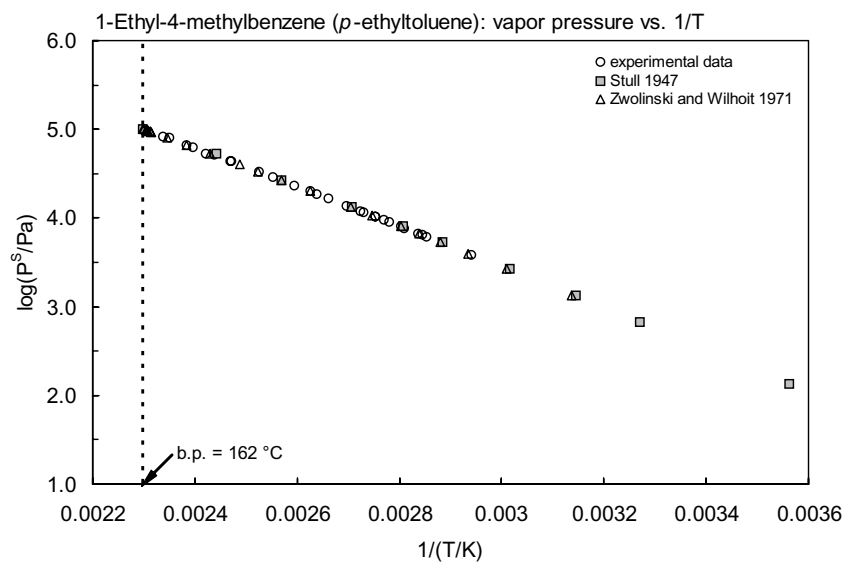
Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976)
residence time of 0.9 d, loss of 67% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

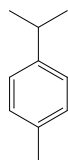
summer daylight lifetime $\tau = 11 \text{ h}$ due to reaction with OH radical (Altshuller 1991).

TABLE 3.1.1.14.1

Reported vapor pressures of *p*-ethyltoluene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Forziati et al. 1949		Buck et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		mercury manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
7.6	133.3	78.396	6417	66.8	3840	45.68	1333
32.7	666.6	82.701	7657	77.4	6106	59.14	2666
44.9	1333	86.523	8993	79.4	6586	67.68	4000
58.5	2666	89.988	10328	83.5	7999	74.09	5333
73.6	5333	93.252	11720	87.9	9466	79.265	6666
83.2	7999	97.63	13840	90.2	10399	83.637	7999
96.3	13332	102.619	16641	94	11999	90.811	10666
116.1	26664	107.71	19944	105.8	18638	96.623	13332
136.4	53329	112.422	23474	122.7	33197	107.781	19998
162	101325	118.727	28978	131.7	44130	116.205	26664
mp/°C	-	131.499	43351	136.9	51329	123.054	33331
		139.701	53693	144.2	63595	128.869	39997
		146.368	66792	152.5	79727	138.469	53329
		154.684	83750	161.1	100792	146.3	66661
						152.965	79993
		eq. 2	P/mmHg	eq. 4	P/mmHg	158.799	93326
		A	6.99801	A	21.27	159.885	95992
		B	1527.113	B	2939	160.948	98659
		C	208.921	C	4.406	161.989	101325
		bp/°C	161.989			eq. 2	P/mmHg
				A	6.99802		
				B	1527.113		
				C	208.921		
				bp/°C	161.989		
				ΔH _v /(kJ mol ⁻¹) =			
				at 25°C	46.61		
				at bp	38.41		



3.1.1.15 1-Isopropyl-4-methylbenzene (*p*-Cymene)

Common Name: 1-Isopropyl-4-methylbenzene

Synonym: *p*-cymene, *p*-isopropyltoluene, 1-methyl-4-isopropylbenzene

Chemical Name: 1-isopropyl-4-methylbenzene

CAS Registry No: 99-87-6

Molecular Formula: $C_{10}H_{14}$, $CH_3C_6H_4CH(CH_3)_2$

Molecular Weight: 134.218

Melting Point ($^{\circ}C$):

−67.94 (Lide 2003)

Boiling Point ($^{\circ}C$):

177.1 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8573 (Weast 1982–83)

Molar Volume (cm^3/mol):

156.6 ($20^{\circ}C$, calculated-density)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

9.66 (Dreisbach 1955)

9.67 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

47.33, 46.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

34.15 (residue volume method, Booth & Everson 1948)

23.35 (shake flask-LSC, Banerjee et al. 1980)

50.7 ± 2.3 (shake flask-HPLC/UV, Lun et al. 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

90.7* ($13.3^{\circ}C$, mercury manometer, Linder 1931)

$\log(P/mmHg) = 8.063 - 10670/(T/K)$ (isoteniscope method, measured range not specified, Kobe et al. 1941)

133.3* ($19^{\circ}C$, summary of literature data, Stull 1947)

212 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 6.9260 - 1538.00/(203.10 + t/^{\circ}C)$; temp range 80 – $215^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

12026* ($107.04^{\circ}C$, ebulliometry, measured range 107.04 – $178.42^{\circ}C$, McDonald et al. 1959)

204* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.9237 - 1537.06/(203.05 + t/^{\circ}C)$; temp range 56.4 – $207.1^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/atm) = (1 - 450.311/T) \times 10^{(0.875129 - 6.86627 \times 10^4 \cdot T + 5.61507 \times 10^7 \cdot T^2)}$; T in K, temp range 290.0 – 650.0 K (Cox vapor pressure eq., Chao et al. 1983)

$\log(P/mmHg) = 7.05074 - 1608.91/(208.72 + t/^{\circ}C)$; temp range 107 – $178^{\circ}C$ (Antoine eq., Dean 1985, 1992)

194 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.16214 - 1599.29/(-65.492 + T/K)$; temp range 380 – 452 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -5.5137 - 3.0256 \times 10^3/(T/K) + 8.9840 \cdot \log(T/K) - 2.5597 \times 10^{-2} \cdot (T/K) + 1.3823 \times 10^{-5} \cdot (T/K)^2$, temp range 205 – 653 K (Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

800	(calculated-P/C, Mackay & Shiu 1981)
942	(computed-expert system SPARC, Kollig 1995)

Octanol/Water Partition Coefficient, log K_{ow}:

4.10	(shake flask-LSC, Banerjee et al. 1980)
4.14	(calculated-UNIFAC activity coeff., Arbuckle 1983)
3.45	(calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
4.10	(recommended, Sangster 1989)
4.10	(recommended, Hansch et al. 1995)
4.0	(computed-expert system SPARC, Kollig 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

3.70	(computed-K _{ow} , Kollig 1995)
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Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: rate constant of $1.68 \times 10^{-2} \text{ h}^{-1}$ with H₂O₂ under photolysis at 25°C in F-113 solution and with HO· in the gas (Dilling et al. 1988).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:

k_{OH} = $0.92 \times 10^{11} \text{ M}^{-1} \text{ s}^{-1}$ at room temp. (estimated from structurally similar *p*-ethyltoluene, Winer et al. 1976)

k_{OH}(calc) = $1.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

k_{OH} = $1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Dilling et al. 1988)

k_{OH} = $(1.51 \pm 0.41) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a tropospheric lifetime $\tau = 1.0\text{--}1.4 \text{ d}$; k_{NO₃} = $(9.9 \pm 1.6) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a tropospheric lifetime $\tau = 1.3 \text{ yr}$ and a calculated tropospheric lifetime $\tau > 330 \text{ d}$ due to reaction with O₃ at $295 \pm 2 \text{ K}$ (relative rate method, Corchnoy & Atkinson 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration

Half-Lives in the Environment:

Air: calculated tropospheric lifetimes of 1.0 d, > 330 d and 1.3 yr due to reactions with OH radical, O₃ and NO₃ radical, respectively (Corchnoy & Atkinson 1990)

TABLE 3.1.1.15.1

Reported vapor pressures of *p*-cymene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Linder 1931		Stull 1947		McDonald et al. 1959		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–3.5	18.67	19	133.3	107.04	12026	56.4	1333
–5.3	18.67	44.6	666.6	128.24	25189	70.3	2666
0	30.66	57.6	1333	151.9	51745	79.2	4000
0.8	33.33	71.5	2666	175.35	96965	85.8	5333
13.3	90.66	87	5333	176.46	99792	91.1	6666
		96.8	7999	177.36	101949	95.7	7999
		110.1	13332	178.42	104553	103.1	10666
		130	26664			109.3	13332
		151.8	53329	eq. 2	P/mmHg	120.7	19998
		175	101325	A	7.03724	129.5	26664
				B	1599.29	136.5	33331
		mp/°C		C	207.659	142.6	39997
						152.6	53329
				mp/°C	–67.98	108	66661
Kobe et al. 1941						167.7	79993
isoteniscope method						173.8	93326
t/°C	P/Pa					174.94	95992
						176.05	98659
						177.13	101325
data presented by							
eq. 1	P/mmHg					eq. 2	P/mmHg
A	8.063					A	6.9237
B	2332					B	1537.06
bp/°C	176.8					C	203.05
ΔH _v /(kJ mol ^{–1}) = 44.64						bp/°C	177.13
						ΔH _v /(kJ mol ^{–1}) =	
						at 25°C	50.29
						at bp	38.16

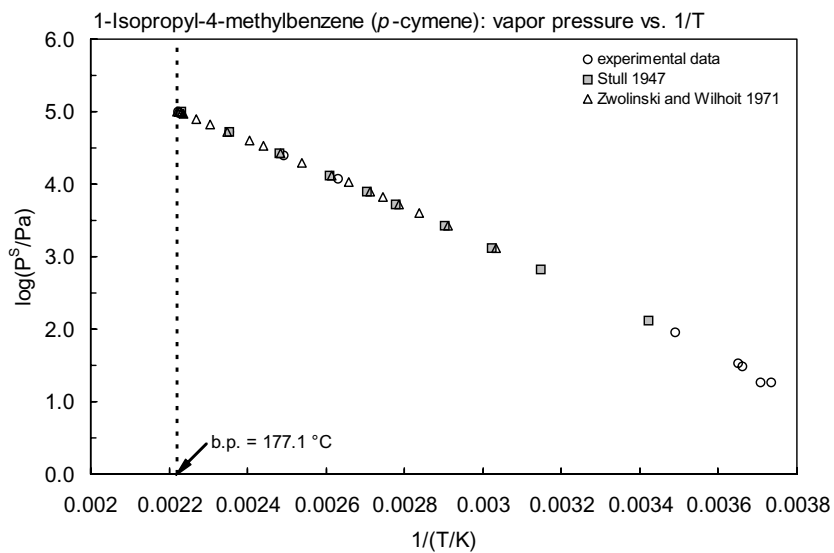
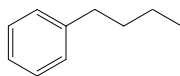


FIGURE 3.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for 1-isopropyl-4-methylbenzene (*p*-cymene).

3.1.1.16 *n*-Butylbenzene

Common Name: *n*-Butylbenzene

Synonym: butylbenzene

Chemical Name: *n*-butylbenzene

CAS Registry No: 104-51-8

Molecular Formula: $C_{10}H_{14}$, $C_6H_5(CH_2)_3CH_3$

Molecular Weight: 134.218

Melting Point ($^{\circ}C$):

−87.85 (Lide 2003)

Boiling Point ($^{\circ}C$):

183.31 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8601 (Weast 1982–83)

Molar Volume (cm^3/mol):

156.1 ($20^{\circ}C$, calculated-density)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

10.98 (Dreisbach 1955)

11.22 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

60.56, 66.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$; *data at other temperatures are tabulated at end of section):

12.6 (shake flask-UV, Andrews & Keefer 1950)

50.5 (shake flask-UV, Klevens 1950)

15.4 (estimated, Deno & Berkheimer 1960)

17.7 (shake flask-GC/ECD, Massaldi & King 1973)

11.8 (shake flask-GC, Sutton & Calder 1975)

12.6 (shake flask-GC, Mackay & Shiu 1981)

13.83 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982)

13.8 (generator column-HPLC/UV, Wasik et al. 1983)

13.76* (generator column-HPLC/UV, measured range 7 – $45^{\circ}C$, Owens et al. 1986)

15.0 (IUPAC recommended, Shaw 1989b)

16.7* ($30^{\circ}C$, equilibrium flow cell-GC, measured range 30 – $100^{\circ}C$, Chen & Wagner 1994c)

$\ln x = -43.2390 - 5720.35/(T/K) - 1.221 \times 10^{-4} \cdot (T/K)^2$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

12.25* (vapor absorption technique-HPLC/UV, measured range 0.5 – $55^{\circ}C$, Dohányosová et al. 2001)

$\ln x = -346.295 + 14524.83/(T/K) + 49.9130 \cdot \ln (T/K)$; temp range 290 – $400\ K$ (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations; *data at other temperatures are tabulated at end of section):

64* ($12.2^{\circ}C$, mercury manometer, Linder 1931)

133.3* ($22.7^{\circ}C$, summary of literature data, Stull 1947)

6415* ($96.233^{\circ}C$, ebulliometry, measured range 96.233 – $184.329^{\circ}C$, Forziati et al. 1949)

$\log (P/mmHg) = 6.98318 - 1577.965/(201.378 + t/^{\circ}C)$; temp range 96.2 – $184.2^{\circ}C$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

145 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 6.98317 - 1577.965/(201.378 + t/^{\circ}C)$; temp range 85 – $220^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

- 137* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = 6.98317 - 1577.965/(201.378 + t/^{\circ}\text{C})$; temp range 62.36–213.1 $^{\circ}\text{C}$ (Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = [-0.2185 \times 11052.1/(T/K)] + 8.194170$; temp range 22.7–183.1 $^{\circ}\text{C}$ (Antoine eq., Weast 1972–73)
 $\log (P/\text{atm}) = (1 - 456.368/T) \times 10^{(0.889482 - 7.01171 \times 10^4/T + 5.65027 \times 10^7/T^2)}$; T in K, temp range 295.0–660.0 K (Cox vapor pressure eq., Chao et al. 1983)
 138, 147 (extrapolated-Antoine equations, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.11624 - 1583.708/(202.013 + t/^{\circ}\text{C})$; temp range 96.2–184.3 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.22353 - 1660.274/(210.314 + t/^{\circ}\text{C})$; temp range 101.3–181.8 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 6.98317 - 1577.965/(201.378 + t/^{\circ}\text{C})$; temp range 62–213 $^{\circ}\text{C}$ (Antoine eq., Dean 1985, 1992)
 $\log (P_L/\text{kPa}) = 6.09809 - 1571.648/(-72.413 + T/K)$; temp range: 369–463 K (Antoine eq., Stephenson & Malanowski 1987)
 110 (20.51 $^{\circ}\text{C}$, static method, measured range 243.8–403.14 K, Kasehgari et al. 1993)
 $\log (P/\text{kPa}) = 6.41845 - 1779.018/(220.982 + t/^{\circ}\text{C})$; temp range 243.8–403.14 K (static method, Kasehgari et al. 1993)
 $\log (P/\text{mmHg}) = 49.9687 - 4.3981 \times 10^3/(T/K) - 14.352 \cdot \log (T/K) + 4.2054 \times 10^{-11} \cdot (T/K) + 3.4379 \times 10^{-6} \cdot (T/K)^2$, temp range 185–661 K (Yaws 1994)
 107 (20.16 $^{\circ}\text{C}$, static method, measured range 253.76–418.04 K, Mokbel et al. 1998)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$; *data at other temperatures are tabulated at end of section):

- 1300 (calculated-P/C, Mackay & Shiu 1981)
 1332 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 1502 (infinite activity coeff. γ^{∞} in water determined by inert gas stripping-GC, Li et al. 1993)
 1692* (equilibrium headspace-GC, Perlinger et al. 1993)
 1357.8 (modified EPICS method-GC, Ryu & Park 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 4.26 (Hansch & Leo 1979)
 4.19 (calculated-fragment const., Rekker 1977)
 3.86 (headspace GC, Hutchinson et al. 1980)
 4.26 (HPLC- k' correlation, Hammers et al. 1982)
 4.28 (generator column-HPLC/UV, Tewari et al. 1982c)
 4.21 (HPLC methods, Harnisch et al. 1983)
 4.28 (generator column-HPLC/UV, Wasik et al. 1983)
 4.29 (generator column-RP-LC, Schantz & Martire 1987)
 4.26, 4.50 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
 4.26 (recommended, Sangster 1989, 1993)
 4.377 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 4.38 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

- 3.39 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)
 3.40 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
 3.52 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)
 3.15, 3.32 (RP-HPLC- k' correlation, Szabo et al. 1990a,b)
 3.35, 3.38, 3.39 (RP-HPLC- k' correlation on different stationary phases, Szabo et al. 1995)

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 3.1.1.16.1

Reported aqueous solubilities and Henry's law constants of *n*-butylbenzene at various temperatures

Aqueous solubility						Henry's law constant	
Owens et al. 1986		Chen & Wagner 1994c		Dohányosová et al. 2001		Perlinger et al. 1993	
generator column-HPLC		equilibrium flow cell-GC		vapor abs.-HPLC/UV		equil. headspace-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)
7	13.34	30	16.7	0.5	11.5	10	543
10	12.98	40	17.82	5	11.5	15	828
12.5	13.14	50	20.3	15	11.3	20	1115
15	12.97	60	26.9	25	12.25	25	1692
17.5	13.14	70	32.06	35	14.5	30	2168
20	13.66	80	47.72	45	17.6		
25	13.76	90	61.14	55	21.2		
30	14.58	100	83.5				
35	15.4						
40	1763						
45	20.21						
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 6.60$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.29$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.29$			
at 25°C		at 25°C					

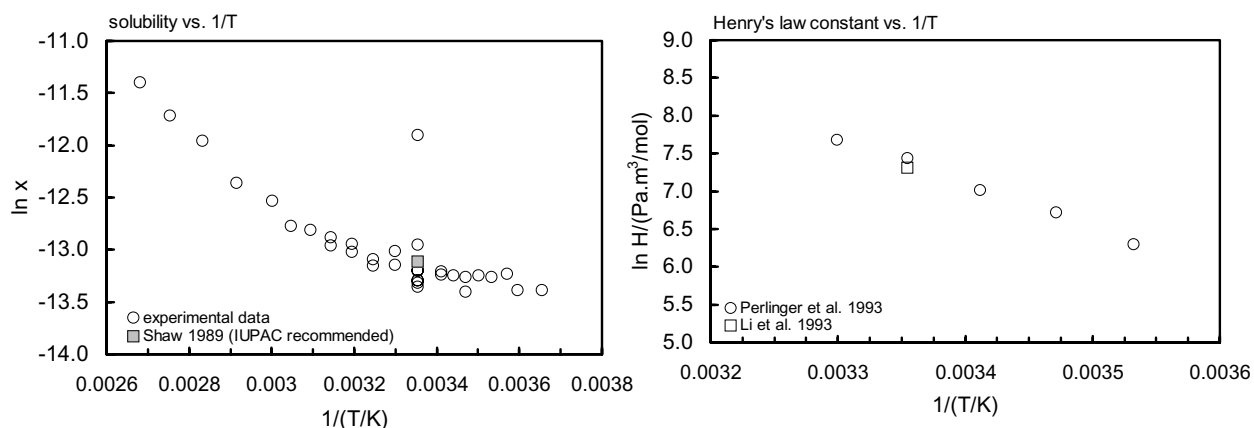
FIGURE 3.1.1.16.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for *n*-butylbenzene.

TABLE 3.1.1.16.2

Reported vapor pressures of *n*-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Linder 1931		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−4.7	13.3	22.7	133.3	96.233	6415	62.35	1333
5.5	33.3	48.8	666.6	100.814	7697	76.32	2666
12.2	64	63	1333	104.778	8991	85.21	4000
		76.3	2666	108.403	10328	91.86	5333
		92.4	5333	111.762	11722	97.241	6666
		102.6	7999	116.322	13840	101.785	7999
		116.2	13332	121.506	16640	109.243	10666
		136.9	26664	126.797	19945	115.286	13332
		159.2	53329	138.3	28979	126.89	19998
		183.1	101325	151.541	43352	135.853	26664
				159.032	53693	142.779	33331
		mp/°C	−82.1	167.011	66793	149.829	39997
				175.666	83753	158.82	53329
				181.767	97645	166.971	66661
				182.429	99245	173.91	79993
				183.636	100734	179.985	93326
				183.725	102456	181.116	95992
				184.329	103989	182.223	98659
						183.306	101325
				eq. 2	P/mmHg		
				A	6.98318	eq. 2	P/mmHg
				B	1577.965	A	6.9808
				C	201.378	B	1577.008
						C	201.331
				bp/°C	183.27		
						bp/°C	183.306
						$\Delta H_v/(\text{kJ mol}^{-1})$	
						at 25°C	50.12
						at bp	37.75

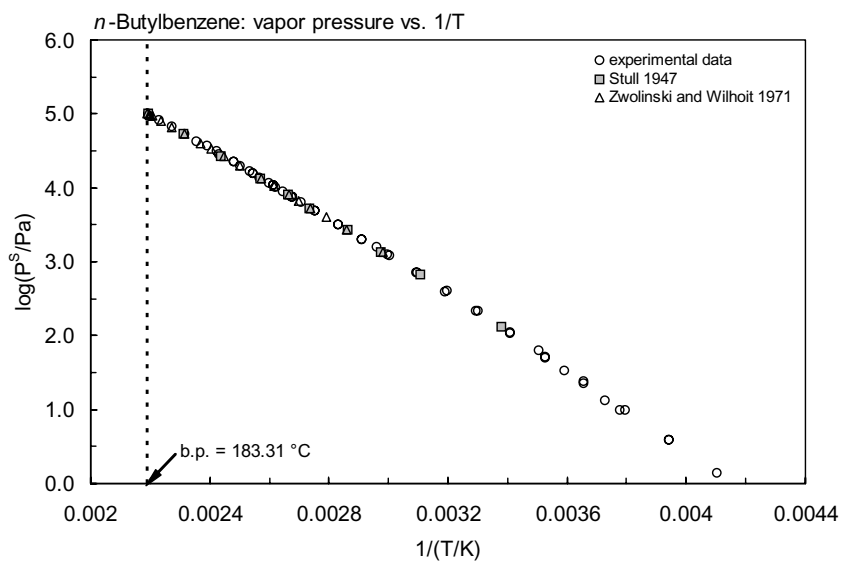
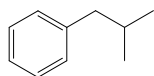


FIGURE 3.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-butylbenzene.

3.1.1.17 Isobutylbenzene



Common Name: Isobutylbenzene

Synonym: i-butylbenzene, 2-methylpropylbenzene, methyl-1-phenylpropane

Chemical Name: isobutylbenzene

CAS Registry No: 538-93-2

Molecular Formula: $C_{10}H_{14}$, $C_6H_5CH_2CH(CH_3)_2$

Molecular Weight: 134.218

Melting Point ($^{\circ}C$):

−51.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

170.5 (Stephenson & Malanowski 1987)

Density (g/cm^3 at $20^{\circ}C$):

0.8532 (Weast 1982–83)

Molar Volume (cm^3/mol):

157.3 ($20^{\circ}C$, calculated-density)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

12.51 (Dreisbach 1955)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

10.1 (shake flask-GC, Price 1976)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

667* ($21.1^{\circ}C$, summary of literature data, Stull 1947)

6415* ($86.637^{\circ}C$, ebulliometry, measured range 86.637 – $173.814^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 6.93033 - 1526.384/(204.171 + t/^{\circ}C)$; temp range 86.6 – $173.8^{\circ}C$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

257 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 6.93033 - 1526.384/(204.171 + t/^{\circ}C)$; temp range 75 – $210^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

248* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.92804 - 1525.446/(204.122 + t/^{\circ}C)$; temp range 53.21 – $202.45^{\circ}C$ (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 8567.8/(T/K)] + 7.048112$; temp range: -9.8 to $170.5^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 445.940/T) \times 10^{(0.870338 - 6.75481 \times 10^{-4} \cdot T + 5.59009 \times 10^{-7} \cdot T^2)}$; T in K, temp range 285.0 – 645.0 K (Cox vapor pressure eq., Chao et al. 1983)

249 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.06156 - 1530.811/(204.675 + t/^{\circ}C)$; temp range 86.64 – $173.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.06898 - 1536.514/(-67.788 + T/K)$; temp range 373 – 447 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -7.0438 - 2.6892 \times 10^3/(T/K) + 8.7843 \cdot \log(T/K) - 2.1426 \times 10^{-2} \cdot (T/K) + 1.1248 \times 10^{-5} \cdot (T/K)^2$; temp range 222 – 650 K (Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

1160, 1714 (calculated- C_w/C_A , calculated-bond contribution, Hine & Mookerjee 1975)

3300 (calculated-P/C, Mackay & Shiu 1981)

1393 (calculated-QSAR, Nirmalakhandan & Speece 1988b)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 4.01 (headspace GC, Hutchinson et al. 1980)
 4.54, 4.82 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
 4.68 (average lit. value, Sangster 1993)
 4.54 (Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants or Half-Lives:

Volatilization: estimated $t_{1/2} \sim 3.2$ h, evaporation from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s at 20°C (Lyman et al. 1982).

Half-Lives in the Environment:

TABLE 3.1.1.17.1

Reported vapor pressures of isobutylbenzene at various temperatures and the coefficients for vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−9.8	133.3	86.637	6415	53.21	1333
21.1	666.6	91.118	7697	66.97	2666
37.3	1333	95.026	8991	75.73	4000
54.7	2666	98.62	10328	82.29	5333
73.2	5333	101.946	11722	87.602	6666
84.1	7999	106.45	13840	92.087	7999
99	13332	111.582	16640	99.452	10666
120.7	26664	116.808	19945	105.422	13332
145.2	53329	121.659	23474	116.893	19998
170.2	101325	128.149	28979	125.561	26664
mp/°C		134.112	34918	132.614	33331
		141.301	43352	138.694	39997
		148.724	53693	149.502	53329
		156.632	66793	156.583	66661
		165.217	83754	163.465	79993
		171.27	97647	169.492	93326
		171.92	99247	170.615	95992
		172.526	100737	171.714	98659
		173.209	102457	172.789	101325
		173.814	103990		
				eq. 2	P/mmHg
		eq. 2	P/mmHg	A	6.92804
		A	6.93033	B	1525.446
		B	1526.384	C	204.122
		C	204.171	bp/°C	172.789
				$\Delta H_v/(kJ\ mol^{-1}) =$	
		bp/°C	172.759	at 25°C	49.45
				at bp	37.82

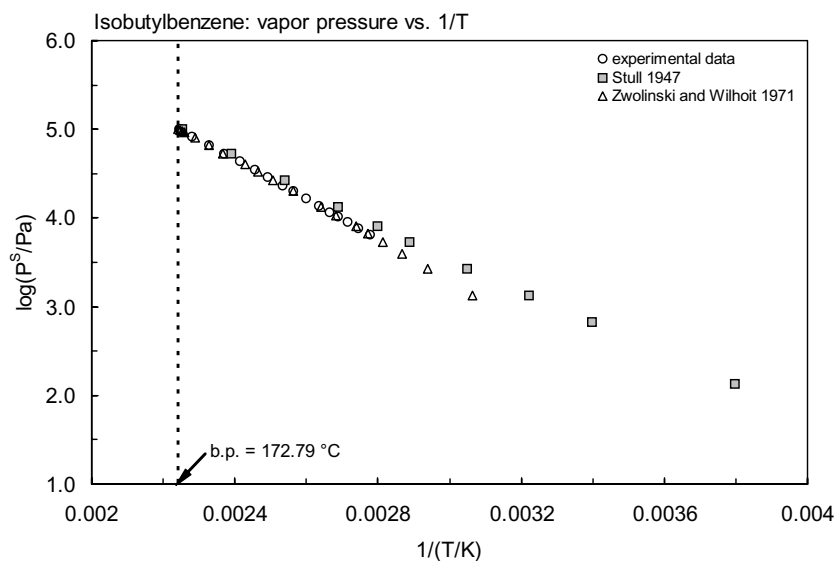
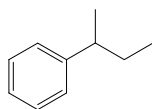


FIGURE 3.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for isobutylbenzene.

3.1.1.18 *sec*-Butylbenzene

Common Name: *sec*-Butylbenzene

Synonym: 2-phenylbutane, (1-methylpropyl)benzene, *s*-butylbenzene

Chemical Name: *sec*-butylbenzene

CAS Registry No: 135-98-8

Molecular Formula: $C_{10}H_{14}$, $C_6H_5CH(CH_3)C_2H_5$

Molecular Weight: 134.218

Melting Point ($^{\circ}C$):

−82.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

173.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8621 (Weast 1982–83)

Molar Volume (cm^3/mol):

155.7 ($20^{\circ}C$, calculated from density)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

9.83 (Dreisbach 1955)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

30.9 (shake flask-UV, Andrews & Keefer 1950)

17.6 (shake flask-GC, Sutton & Calder 1975)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

70.7* ($9.8^{\circ}C$, mercury manometer, measured range -8.6 to $9.8^{\circ}C$, Linder 1931)

133.3* ($18.6^{\circ}C$, summary of literature data, temp range 18.6 – $173.5^{\circ}C$, Stull 1947)

6415* ($87.118^{\circ}C$, ebulliometry, measured range 87.118 – $174.358^{\circ}C$, Forziati et al. 1949)

$\log(P/mmHg) = 6.95097 - 1540.174/(205.101 + t/^{\circ}C)$; temp range 87.1 – $174.4^{\circ}C$, (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

250 (extrapolated, Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 6.95097 - 1540.174/(205.101 + t/^{\circ}C)$; temp range 75 – $210^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

241* (extrapolated, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.94866 - 1539.233/(205.052 + t/^{\circ}C)$; temp range 53.7 – $202.95^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 11609.3/(T/K)] + 8.318014$; temp range 18.6 – $173.5^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 446.499/T) \times 10^{(0.870844 - 6.72060 \times 10^{-4}T + 5.52698 \times 10^{-7}T^2)}$; T in K, temp range 285.0 – $645.0\ K$ (Cox vapor pressure eq., Chao et al. 1983)

240 (extrapolated, Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.05072 - 1533.897/(204.382 + t/^{\circ}C)$; temp range 87.12 – $174.4^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.94219 - 1533.95/(204.39 + t/^{\circ}C)$; temp range 87 – $174^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.10298 - 1559.452/(C + T/K)$; temp range 384 – $448\ K$ (Antoine eq., Stephenson & Malanowski 1987)

188* ($20.33^{\circ}C$, static method, measured range 243.92 – $373.39\ K$, Kasehgari et al. 1993)

$\log(P/kPa) = 6.47915 - 1781.723/(208.35 + t/^{\circ}C)$; temp range 243.92 – $373.39\ K$ (static method, Kasehgari et al. 1993)

$$\log (P/\text{mmHg}) = 61.5904 - 4.5093 \times 10^3/(T/K) - 19.522 \cdot \log (T/K) + 6.9865 \times 10^{-3} \cdot (T/K) + 7.8205 \times 10^{-14} \cdot (T/K)^2,$$

temp range 198–665 K (Yaws 1994)

186* (20.23°C, static method, measured range 263.52–393.39 K, Mokbel et al. 1998)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

- 4.44, 4.70 (RP-HPLC-k' correlations, Sherblom & Eganhouse 1988)
- 4.57 (average lit. value, Sangster 1993)
- 4.44 (Hansch et al. 1995)
- 3.90 (computed-expert system SPARC, Kollig 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

- 2.71 (aquifer material with f_{OC} of 0.006 and measured partition coeff. K_p = 3.06 mL/g., Abdul et al. 1990)
- 3.60 (computed-K_{OW}, Kollig 1995)

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 3.1.1.18.1

Reported vapor pressures of sec-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Linder 1931		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-8.6	13.33	18.6	133.3	87.118	6415	53.7	1333
-3.0	24	44.2	666.6	91.684	7695	67.49	2666
2.6	42.66	57	1333	95.62	8990	76.26	4000
9.8	70.66	70.6	2666	99.179	10328	82.84	5333
		86.2	5333	102.523	11722	88.15	6666
		96	7999	107.009	13840	92.614	7999
		109.5	13332	112.151	16641	100.012	10666
		128.8	26664	117.387	19945	105.986	13332
		150.3	53329	122.232	23475	117.462	19998
		173.5	101325	128.715	28979	126.132	26664
				134.683	43352	133.185	33331
		mp/°C	-82.87	141.867	53693	139.175	39997
				149.288	66793	149.069	53329
				157.194	83754	157.133	66661
				165.768	97647	164.021	79993

(Continued)

TABLE 3.1.1.18.1 (Continued)

1.

Linder 1931		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				171.82	99245	170.042	93326
				173.068	100737	171.164	95992
				173.754	102457	172.261	98659
				174.358	103990	173.864	101325
				eq. 2	P/mmHg	eq. 2	P/mmHg
				A	6.95097	A	6.94866
				B	1540.174	B	1539.223
				C	205.101	C	205.052
				bp/°C	173.035	bp/°C	173.335
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	49.5
						at bp	37.95

2.

Kasehgari et al. 1993		Mokbel et al. 1998	
static method		static method	
T/K	P/Pa	T/K	P/Pa
243.92	2.92	263.52	16.31
253.79	7.99	273.42	43.34
263.69	19.3	283.40	92.39
273.55	44.9	293.38	186.0
283.50	93.3	303.42	357.0
293.48	188	313.44	652.0
303.49	358	323.55	1145
313.61	654	333.55	1943
313.61	655	343.57	3088
323.60	1136	353.62	4862
323.60	1139	363.43	7329
328.60	1478	373.39	10789
333.57	1904		
343.57	3088	data fitted to Wagner eq.	
363.43	4862		
373.39	7329		
Antoine eq.			
eq. 2	P/kPa		
A	6.47915		
B	1781.723		
C	226.989		

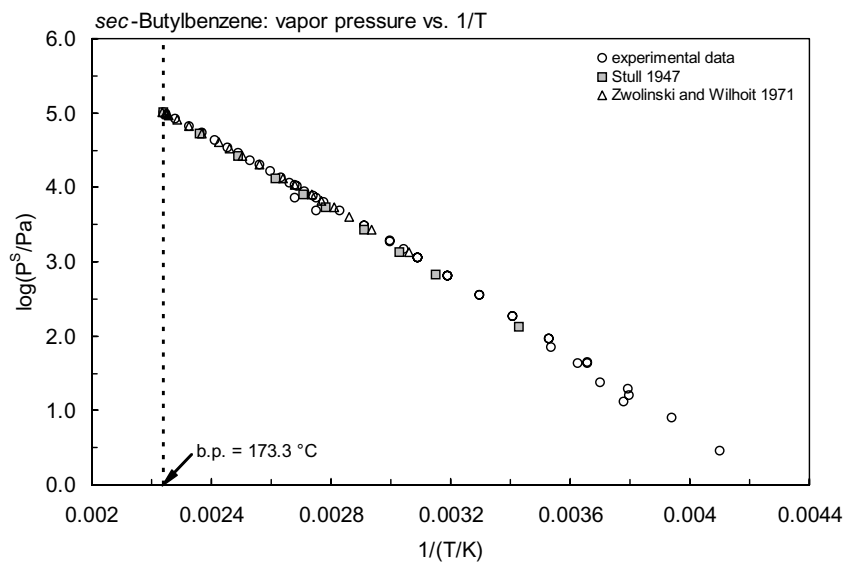
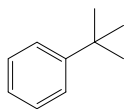


FIGURE 3.1.1.18.1 Logarithm of vapor pressure versus reciprocal temperature for sec-butylbenzene.

3.1.1.19 *tert*-Butylbenzene

Common Name: *tert*-Butylbenzene

Synonym: (1,1-dimethylethyl)benzene, 2-methyl-2-phenylpropane, trimethylphenylmethane, pseudobutylbenzene, *t*-butylbenzene

Chemical Name: *tert*-butylbenzene

CAS Registry No: 98-06-6

Molecular Formula: C₁₀H₁₄, C₆H₅C(CH₃)₃

Molecular Weight: 134.218

Melting Point (°C):

−58 (Stephenson & Malanowski 1987)

Boiling Point (°C):

169.1 (Lide 2003)

Density (g/cm³ at 20°C):

0.8665 (Weast 1982–83)

Molar Volume (cm³/mol):

154.9 (20°C, calculated from density)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

8.38 (Dreisbach 1955)

8.40 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} (J/mol K):

39.1, 45.4 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

34.0 (shake flask-UV, Andrews & Keefer 1950)

29.5 (shake flask-GC, Sutton & Calder 1975)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

144* (13.7°C, mercury manometer, measured range −2 to 13.7°C, Linder 1931)

133.3* (13°C, summary of literature data, temp range 13–168.5°C, Stull 1947)

6426* (83.887°C, ebulliometry, measured range 83.887–170.165°C, Forziati et al. 1949)

log (P/mmHg) = 9.2050 − 1504.572/(203.328 + t/°C); temp range 83.9–170.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

295 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 6.92050 − 1504.572/(203.328 + t/°C); temp range 70–205°C (Antoine eq. for liquid state, Dreisbach 1955)

286* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.91829 − 1503.651/(203.280 + t/°C); temp range 50.79–198.54°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [−0.2185 × 10705.5/(T/K)] + 8.195269; temp range 13–168°C (Antoine eq., Weast 1972–73)

log (P/atm) = (1 − 442.319/T) × 10⁴(0.881530 − 7.21114 × 10⁴·T + 6.01764 × 10⁷·T²); T in K, temp range 285.0–635.0 K (Cox vapor pressure eq., Chao et al. 1983)

285 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.03861 − 1499.886/(202.792 + t/°C); temp range 83.88–170.2°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

286 (extrapolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.92255 − 1505.987/(203.49 + t/°C); temp range 84–170°C (Antoine eq., Dean 1985, 1992)

$\log (P_L/\text{kPa}) = 6.06067 - 1515.51/(-68.551 + T/\text{K})$; temp range 368–444 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 41.4522 - 3.9027 \times 10^3/(T/\text{K}) - 11.410 \cdot \log (T/\text{K}) + 2.4320 \times 10^{-10} \cdot (T/\text{K}) + 2.2517 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 215–660 K (Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1200 (calculated-P/C, Mackay & Shiu 1981)

1300 (calculated- C_A/C_w , Eastcott et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.11 (Leo et al. 1971; Hansch & Leo 1979)

4.07 (shake flask-HPLC, Nahum & Horvath 1980)

4.25, 4.49 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)

4.11 (recommended, Sangster 1989, 1993)

4.11 (recommended, Hansch et al. 1995)

3.73 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation:

Photolysis:

Oxidation: rate constant $k = 4.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas phase reaction with OH radical at room temp. (Ohta & Ohyama 1985; Atkinson 1989);

rate constant $k = 4.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with OH radical at 298 K (Atkinson 1990).

Oxidation:

Hydrolysis:

Biodegradation:

Bioconcentration

Half-Lives in the Environment:

TABLE 3.1.1.19.1

Reported vapor pressures of *tert*-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Linder 1931		Stull 1947		Forziati et al. 1949		Zwolinski & Wilhoit 1971	
mercury manometer		summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−2.0	36	13	133.3	83.887	6426	50.79	1333
2.3	57.3	39	666.6	88.312	7695	64.41	2666
10.8	140	51.7	1333	92.194	8990	73.07	4000
13.7	144	65.6	2666	95.715	10332	79.56	5333
		80.8	5333	99.017	11722	84.816	6666
		90.6	7999	103.471	13840	89.254	7999
		103.8	13332	108.546	16641	96.542	10666
		123.7	26664	113.72	19945	102.449	13332
		145.8	53329	118.524	23475	113.802	19998
		168.5	101325	124.936	28979	122.449	26664
				137.968	43354	129.364	33331
		mp/°C	−58.0	145.315	53692	135.295	39997
				153.149	66781	145.095	53329
				161.649	83754	153.097	66661
				167.646	97647	159.913	79993
				168.287	99247	165.882	93326
				168.886	100737	166.994	95992
				169.565	102458	168.083	98659
				170.165	103991	169.018	101325
				eq. 2	P/mmHg	eq. 2	P/mmHg
				A	6.9205	A	6.91829
				B	1504.572	B	1503.651
				C	203.328	C	203.28
				bp/°C	169.119	bp/°C	169.148
						$\Delta H_v/(\text{kJ mol}^{-1}) =$	
						at 25°C	49.8
						at bp	37.61

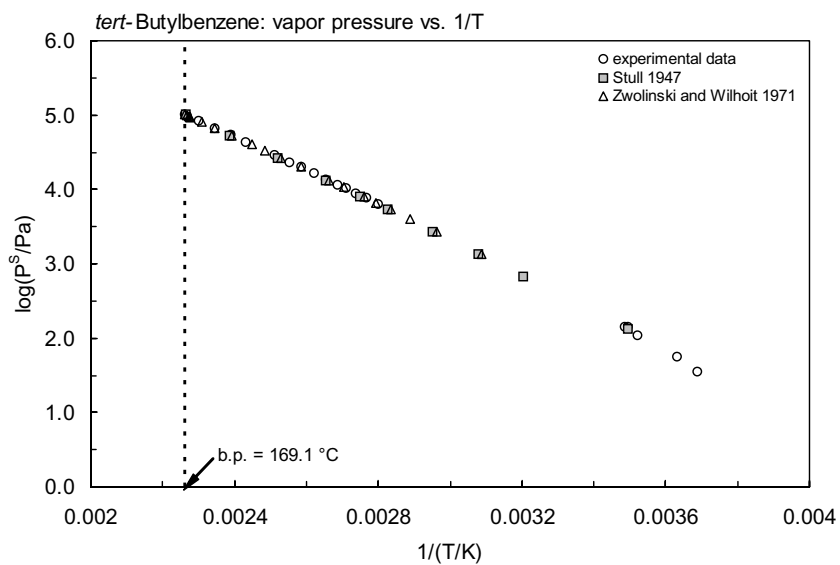
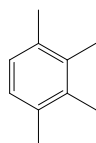


FIGURE 3.1.1.19.1 Logarithm of vapor pressure versus reciprocal temperature for *tert*-butylbenzene.

3.1.1.20 1,2,3,4-Tetramethylbenzene



Common Name: 1,2,3,4-Tetramethylbenzene

Synonym: perhintene, prebnitene

Chemical Name: 1,2,3,4-tetramethylbenzene

CAS Registry No: 488-23-3

Molecular Formula: $C_{10}H_{14}$, $C_6H_2(CH_3)_4$

Molecular Weight: 134.218

Melting Point ($^{\circ}C$):

−6.2 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

205 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9052 (Weast 1982–83)

Molar Volume (cm^3/mol):

148.3 ($20^{\circ}C$, calculated-density)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

11.21 (Dreisbach 1955)

11.23 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

42.31, 45.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($42.6^{\circ}C$, summary of literature data, temp range 42.6 – $204.4^{\circ}C$, Stull 1947)

49.20 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.0584 - 1689.10/(199.28 + t/^{\circ}C)$; temp range 100 – $250^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* ($79.515^{\circ}C$, compiled data, temp range 79.515 – $235.815^{\circ}C$, Bond & Thodos 1960)

45.01* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0594 - 1690.54/(199.48 + t/^{\circ}C)$; temp range 79.5 – $235.9^{\circ}C$ (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 12258.0/(T/K)] + 8.534237$; temp range 42.6 – $204.4^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 478.255/T) \times 10^{(0.889494 - 6.47585 \times 10^4/T + 4.96841 \times 10^7/T^2)}$; T in K, temp range 310.0 – $690.0\ K$ (Cox vapor pressure eq., Chao et al. 1983)

45.01 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.0594 - 1690.54/(199.48 + t/^{\circ}C)$; temp range 80 – $217^{\circ}C$ (Antoine eq., Dean 1985, 1992)

45.02 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.1843 - 1690.54/(-73.67 + T/K)$; temp range 352 – $509\ K$ (liquid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.84 (generator column-HPLC, Wasik et al. 1982)

4.11 (HPLC- k' correlation, Hammers et al. 1982)

- 4.30, 4.53 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
 4.00 (recommended, Sangster 1989, 1993)
 4.09 (normal phase HPLC- k' correlation, Govers & Evers 1992)
 3.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.20.1

Reported vapor pressures of 1,2,3,4-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
$\log P = A - B/(T/K) - C \cdot \log (T/K) + D \cdot P/(T/K)^2$		(5)					
Stull 1947		Bond & Thodos 1960		Zwolinski & Wilhoit 1971			
summary of literature data		compiled data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
42.6	133.3	79.515	1333	79.5	1333	201.6	93326
68.7	666.6	128.415	10666	94.1	2666	202.83	95992
81.8	1333	188.185	66661	103.4	4000	204.54	98659
95.8	2666	216.925	133322	110.3	5333	205.09	101325
111.5	5333	235.815	199984	115.9	6666		
121.8	7999			120.6	7999	eq. 2	P/mmHg
135.7	13332	bp/°C	205.055	128.4	10666	A	7.0594
1155.7	26664			134.7	13332	B	1690.54
180	53329	eq. 5	P/mmHg	146.7	19998	C	199.48
204.4	101325	A	27.4323	155.8	26664	bp/°C	205.9
		B	3713.52	163.2	33331	$\Delta H_v/(kJ\ mol^{-1}) =$	
mp/°C	−4.0	C	6.77416	169.2	39997	at 25°C	57.15
		D	3.81118	179.8	53329	at bp	45.02
				188.22	66661		
				195.99	79993		

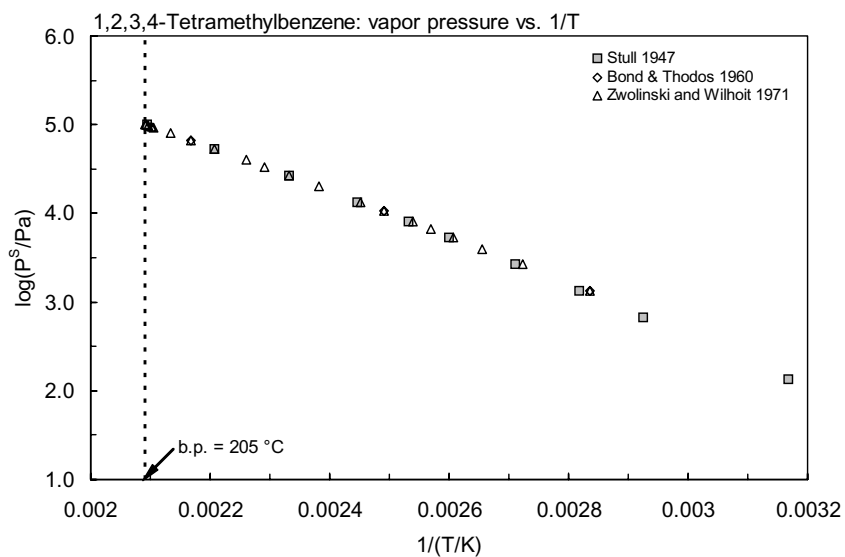
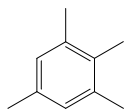


FIGURE 3.1.1.20.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,4-tetramethylbenzene.

3.1.1.21 1,2,3,5-Tetramethylbenzene



Common Name: 1,2,3,5-Tetramethylbenzene

Synonym: isodurene

Chemical Name: 1,2,3,5-tetramethylbenzene

CAS Registry No: 527-53-7

Molecular Formula: $C_{10}H_{14}$, $C_6H_2(CH_3)_4$

Molecular Weight: 134.218

Melting Point ($^{\circ}C$):

−24.1 (Stephenson & Malanowski 1987)

Boiling Point ($^{\circ}C$):

198 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8903 (Weast 1982–83)

Molar Volume (cm^3/mol):

150.8 ($20^{\circ}C$, calculated-density)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

12.93 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

52.01, 46.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

16.2, 16.4, 19.4 (15, 25, $35^{\circ}C$, estimated- RP-HPLC- k' correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($40.6^{\circ}C$, summary of literature data, temp range 40.6 – $197.9^{\circ}C$, Stull 1947)

67.10 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.0769 - 1674.00/(200.94 + t/^{\circ}C)$; temp range 95 – $240^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

62.22* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.70779 - 1675.43/(201.14 + t/^{\circ}C)$; temp range 74.5 – $228.3^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = [-0.2185 \times 12358.4/(T/K)] + 8.680246$; temp range 40.6 – $197.9^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = (1 - 471.208/T) \times 10^{(0.891876 - 6.64575 \times 10^4/T + 5.21861 \times 10^7/T^2)}$; T in K, temp range 305.0 – 675.0 K (Cox vapor pressure eq., Chao et al. 1983)

62.22 (extrapolated, Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.0779 - 1675.43/(201.14 + t/^{\circ}C)$; temp range 75 – $228^{\circ}C$ (Antoine eq., Dean 1985, 1992)

62.23 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.2028 - 1675.43/(-72.01 + T/K)$; temp range 348 – 502 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -3.9778 - 2.960 \times 10^3/(T/K) + 7.3226 \cdot \log(T/K) - 1.7725 \times 10^{-2} \cdot (T/K) + 8.6365 \times 10^{-6} \cdot (T/K)^2$, temp range 249 – 679 K (Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.04 (generator column-HPLC/UV, Wasik et al. 1982)

4.17 (HPLC- k' correlation, Hammers et al. 1982)

- 4.30 (average value, RP-HPLC- k' correlation, Sherblom & Eganhouse 1988)
 4.10 (recommended, Sangster 1989, 1993)
 4.23 (normal phase HPLC- k' correlation, Govers & Evers 1992)
 4.04 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.21.1

Reported vapor pressures of 1,2,3,5-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

Stull 1947

Zwolinski & Wilhoit 1971

summary of literature data		selected values			
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
40.6	133.3	74.5	1333	194.68	93326
65.8	666.6	88.9	2666	195.83	95992
77.8	1333	98	4000	196.95	98659
91	2666	104.8	5333	198.05	101325
105.8	5333	110.3	6666		
115.4	7999	115	7999	eq. 2	P/mmHg
128.3	13332	122.6	10666	A	7.0779
149.9	26664	128.8	13332	B	1675.43
173.7	53329	140.7	19998	C	201.14
197.9	101325	149.6	26664		
		156.9	33331	bp/ $^{\circ}\text{C}$	198.05
mp/ $^{\circ}\text{C}$	-24.0	163	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
		173.2	53329	at 25 $^{\circ}\text{C}$	55.82
		181.5	66661	at bp	43.81
		188.5	79993		

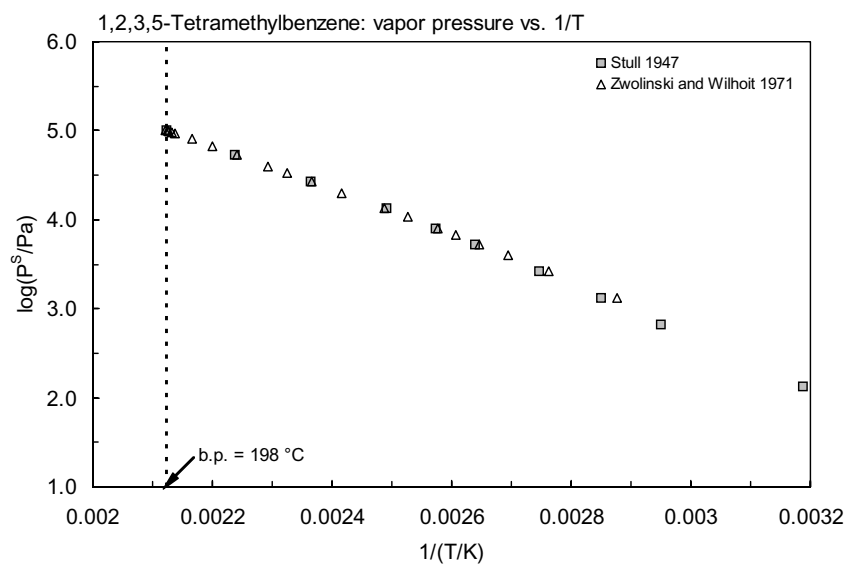
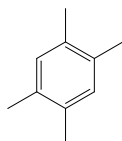


FIGURE 3.1.1.21.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,5-tetramethylbenzene.

3.1.1.22 1,2,4,5-Tetramethylbenzene



Common Name: 1,2,4,5-Tetramethylbenzene

Synonym: durene

Chemical Name: 1,2,4,5-tetramethylbenzene

CAS Registry No: 95-93-2

Molecular Formula: $C_{10}H_{14}$, $C_6H_2(CH_3)_4$

Molecular Weight: 134.218

Melting Point ($^{\circ}C$):

79.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

196.8 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$): 0.838

Molar Volume (cm^3/mol):

160.1 ($20^{\circ}C$, calculated-density)

184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

21.0 (Dreisbach 1955; Tsonopoulos & Prausnitz 1971)

20.88 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

59.83 (Tsonopoulos & Prausnitz 1971)

59.25, 46.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.293 (mp at $79.3^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

19.5 (Deno & Berkheimer 1960)

3.48 (shake flask-GC, Price 1976)

3.48 (shake flask-GC, Krzyzanowska & Szeliga 1978)

13.9 (HPLC- k' correlation, converted from reported activity coeff γ_w , Hafkenscheid & Tomlinson 1983)

17.2, 18.6, 28.2 (15, 25, $35^{\circ}C$, RP-HPLC- k' correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4.4* ($1.75^{\circ}C$, mercury manometer, measured range -1.7 – $1.75^{\circ}C$, Linder 1931)

133.3* ($45^{\circ}C$, summary of literature data, temp range 45 – $195.9^{\circ}C$, Stull 1947)

70.9 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.0790 - 1671.0/(201.23 + t/^{\circ}C)$; temp range 95 – $240^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

65.9* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 7.0800 - 1672.43/(201.43 + t/^{\circ}C)$; temp range 73.6 – $227^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = [-0.2185 \times 12582.6/(T/K)] + 8.822113$; temp range 45 – $195.9^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log (P/atm) = (1 - 470.032/T) \times 10^{(0.884259 - 6.36677 \times 10^{-4} \cdot T + 4.97646 \times 10^{-7} \cdot T^2)}$; T in K, temp range 346.75 – $675.0 K$ (Cox vapor pressure eq., Chao et al. 1983)

65.9 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 7.0800 - 1672.43/(201.43 + t/^{\circ}C)$; temp range 74 – $277^{\circ}C$ (Antoine eq., Dean 1985, 1992)

65.9 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.2049 - 1672.43/(-71.72 + T/K)$; temp range 353 – $500 K$ (Antoine eq., Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = -51.3593 - 1.6523 \times 10^3/(T/K) + 26.656 \cdot \log (T/K) - 3.5721 \times 10^{-2} \cdot (T/K) + 1.5018 \times 10^{-5} \cdot (T/K)^2,$$

temp range 352–Y675K (Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

2541 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow}:

4.00 (Hansch & Leo 1979)
4.24 (HPLC-RV correlation, Garst 1984)
4.13, 4.34 (RP-HPLC-k' correlations, Sherblom & Eganhouse 1988)
4.10 (recommended, Sangster 1989, 1993)
4.27 (normal phase HPLC-k' correlation, Govers & Evers 1992)
4.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

3.12 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981)
2.99 (soil, calculated-MCI χ , Sabljic 1987a,b)
2.76 (aquifer material with f_{OC} of 0.006 and measured K_p = 3.42 mL/g., Abdul et al. 1990)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: rate constant k = 1.1 × 10⁴ cm³ mol⁻¹ s⁻¹ for reaction with ozone at 300 K (estimated, Lyman 1982).

Hydrolysis:

Biodegradation:

Bioconcentration:

Half-Lives in the Environment:

TABLE 3.1.1.22.1

Reported vapor pressures of 1,2,4,5-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Linder 1931		Stull 1947		Zwolinski & Wilhoit 1971			
Hg manometer		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-1.7	1.733	45	133.3	73.6	1333	193.49	93326
-1.3	21.33	63	666.6	88	2666	194.63	95992
1.3	4.4	74.6	1333	97.1	4000	195.75	98659
1.75	4.4	88	2666	103.9	5333	196.84	101325
		104.2	5333	109.4	6666		
		114.8	7999	114	7999	eq. 2	P/mmHg
		128.1	13332	121.6	10666	A	7.08
		149.5	26664	127.8	13332	B	1672.43
		172.1	53329	139.6	19998	C	201.43
		195.9	101325	148.5	26664		
				155.8	33331	bp/°C	196.84
		mp/°C	79.5	161.9	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				172.1	53329	at 25°C	75
				180.3	66661	at bp	44.52
				187.3	79993		

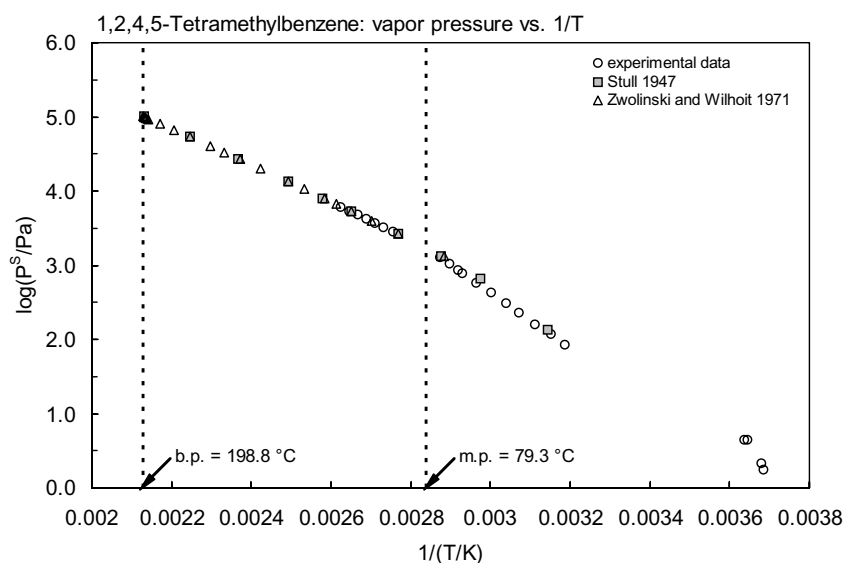
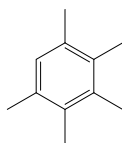


FIGURE 3.1.1.22.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4,5-tetramethylbenzene.

3.1.1.23 Pentamethylbenzene



Common Name: Pentamethylbenzene

Synonym:

Chemical Name: pentamethylbenzene

CAS Registry No: 700-12-9

Molecular Formula: $C_{11}H_{16}$, $C_6H(CH_3)_5$

Molecular Weight: 148.245

Melting Point ($^{\circ}C$):

54.5 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

232 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.917, 0.913 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

0.917 (Weast 1982–83)

Molar Volume (cm^3/mol):

161.7 ($20^{\circ}C$, calculated from density)

207.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

12.34 (Tsonopoulos & Prausnitz 1971)

1.98, 10.67; 12.65 (23.65, $55.05^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

37.70 (Tsonopoulos & Prausnitz 1971)

39.33, 47.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.514 (mp at $54.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

15.6 (Deno & Berkheimer 1960)

15.52 (calculated- K_{ow} , Yalkowsky et al. 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

13.84 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.13756 - 1833.8/(199.0 + t/^{\circ}C)$; temp range 125 – $280^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

9.52 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.3509 - 1867/(-75.15 + T/K)$; temp range 338 – $503\ K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.56 (HPLC- k' correlation, Hammers et al. 1982)

4.57 (HPLC-RV correlation, Garst 1984)

4.56 (recommended, Sangster 1989, 1993)

4.59 (normal phase HPLC- k' correlation, Govers & Evers 1992)

4.56 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

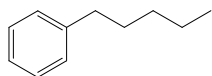
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

3.1.1.24 Pentylbenzene



Common Name: *n*-Pentylbenzene

Synonym: phenylpentane

Chemical Name: pentylbenzene

CAS Registry No: 538-68-1

Molecular Formula: $C_{11}H_{16}$, $C_6H_5(CH_2)_4CH_3$

Molecular Weight: 148.245

Melting Point ($^{\circ}C$):

−75 (Dreisbach 1955; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

205.4 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8585 (Weast 1982–83)

Molar Volume (cm^3/mol):

172.7 ($20^{\circ}C$, calculated from density)

207.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

10.5 (shake flask-UV, Andrews & Keefer 1950)

3.84 (generator column-HPLC/UV, Tewari et al. 1982c)

3.37* (generator column-HPLC/UV, measured range 7 – $45^{\circ}C$, Owens et al. 1986)

$\ln x = -387.920 + 16274.64/(T/K) + 55.9266 \cdot \ln (T/K)$; temp range 290 – $400\ K$ (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

43.7 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.04709 - 1670.68/(195.6 + t/^{\circ}C)$; temp range 105 – $270^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

43.7* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.97833 - 1639.91/(194.76 + t/^{\circ}C)$; temp range 80 – $237^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 34.2755 - 3.6829 \times 10^3/(T/K) - 9.3387 \cdot \log (T/K) + 2.7727 \times 10^{-3} \cdot (T/K) - 8.8315 \times 10^{-15} \cdot (T/K)^2$, temp range 198 – $680\ K$ (Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

600 (calculated-P/C, Mackay & Shiu 1981)

617 (calculated- C_A/C_w , Eastcott et al. 1988)

1689 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

1628.2 (modified EPICS method-GC, Ryu & Park 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.56 (HPLC- k' correlation, Hammers et al. 1982)

4.90 (generator column-HPLC/UV, Tewari et al. 1982c)

4.90 (recommended, Sangster 1989, 1993)

4.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environment Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 5.0 \times 10^4 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with ozone at 300 K (Lyman 1982).

Hydrolysis:

Biodegradation:

Bioconcentration:

Half-Lives in the Environment:

TABLE 3.1.1.24.1

Reported aqueous solubilities and vapor pressures of *n*-pentylbenzene at various temperatures

Aqueous solubility		Vapor pressure			
Owens et al. 1986		Zwolinski & Wilhoit 1971			
generator column-HPLC		selected values			
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
7	3.48	80	1333	283.18	95992
10	3.18	94	2666	203.16	97325
12.5	3.44	103.3	4000	204.33	98659
15	3.19	110.3	5333	204.9	99992
17.5	3.43	115.87	6666	205.46	101325
20	3.18	120.6	7999		
25	3.37	128.36	10666	$\log P = A - B/(C + t/^{\circ}\text{C})$	
30	3.61	134.65	13332	Antoine eq.	P/mmHg
35	3.92	146.73	19998	A	6.97833
40	4.25	155.85	26664	B	1639.91
45	4.69	163.27	33331	C	194.76
		169.57	39997		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 6.50$		179.97	53329	bp/ $^{\circ}\text{C}$	205.46
at 25°C		188.45	66661	$\Delta H_v/(\text{kJ mol}^{-1})$	
		196.68	79993	at 25°C	55.06
		202	93326	at 25°C	41.21
		202.59	94659		

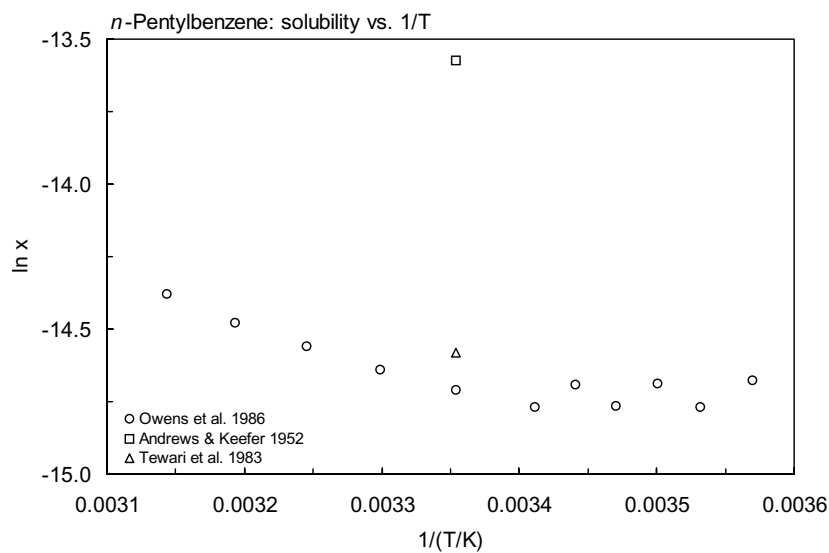


FIGURE 3.1.1.24.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *n*-pentylbenzene.

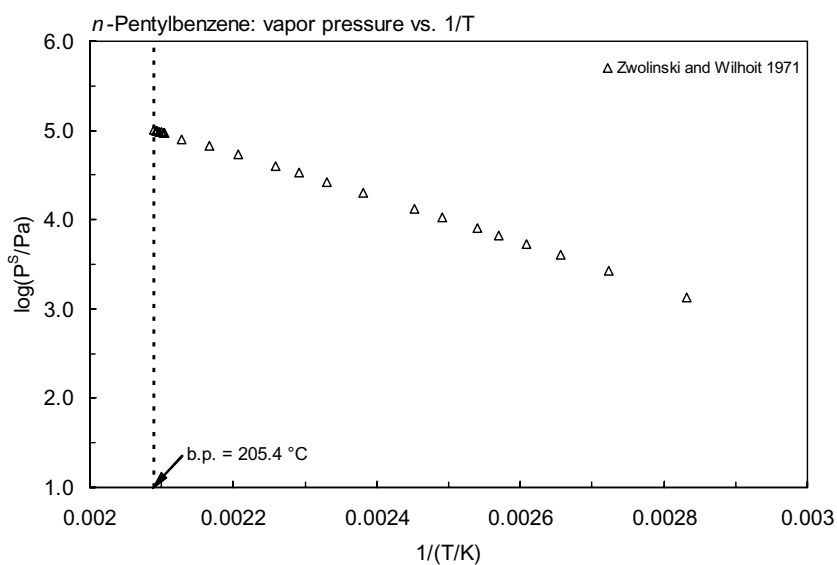
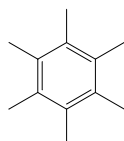


FIGURE 3.1.1.24.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-pentylbenzene.

3.1.1.25 Hexamethylbenzene



Common Name: *n*-Hexamethylbenzene

Synonym: mellitene

Chemical Name: *n*-hexamethylbenzene

CAS Registry No: 87-95-4

Molecular Formula: $C_{12}H_{18}$, $C_6(CH_3)_6$

Molecular Weight: 162.271

Melting Point ($^{\circ}C$):

165.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

263.4 (Weast 1982–83)

Density (g/cm^3 at $25^{\circ}C$):

1.063 (Weast 1982–83)

Molar Volume (cm^3/mol):

152.6 ($25^{\circ}C$, calculated-density)

229.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

20.46 (Tsonopoulos & Prausnitz 1971)

1.76, 20.63; 22.38 (110.5, $165.55^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} (J/mol K):

46.44 (Tsonopoulos & Prausnitz 1971)

51.6, 47.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio (assuming $\Delta S_{fus} = 56$ J/mol K, F: 0.042 (mp = $166.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.235 (generator column-GC, Doucette & Andren 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.004* ($41.07^{\circ}C$, transpiration method, measured range 41 – $90.5^{\circ}C$, Overberger et al. 1969)

0.28* ($30^{\circ}C$, diaphragm pressure gauge, measured range 30 – $70^{\circ}C$, Ambrose et al. 1976)

0.160 (calculated-vapor pressure eq., Ambrose et al. 1976)

$\log(P/Pa) = 13.134 - 3855/[(T/K) - 21]$; temp range 202 – 343 K (diaphragm pressure gauge measurements, Antoine eq., Ambrose et al. 1976)

$\log(P/atm) = (1 - 571.163/T) \times 10^{(1.00973 - 5.04725 \times 10^4/T - 6.310130 \times 10^7/T^2)}$; T in K, temp range 303.1 – 343.02 K (Cox vapor pressure eq., Chao et al. 1983)

0.155 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.6223 - 2965.633/(-59.583 + T/K)$; temp range 303 – 343 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.89588 - 1629.9/(-118.46 + T/K)$; temp range 443 – 537 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.61 (generator column-HPLC, Wasik et al. 1982)

5.11 (HPLC- k' correlation, Hammers et al. 1982)

4.31 (HPLC-RV correlation, Garst & Wilson 1984)

4.60 (shake flask/slow stirring-GC, Brooke et al. 1986)

- 4.60, 4.88 (reversed phase HPLC- k' correlations, Sherblom & Eganhouse 1988)
 4.75 (recommended, Sangster 1989)
 4.95 (normal phase HPLC- k' correlation, Govers & Evers 1992)
 5.11 (recommended, Sangster 1993)
 4.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 6.31 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 2.4 \times 10^5 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with ozone at 300K (Lyman et al. 1982)

Hydrolysis:

Biodegradation:

Bioconcentration

Half-Lives in the Environment:

TABLE 3.1.1.25.1

Reported vapor pressures of hexamethylbenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Overberger et al. 1969		Ambrose et al. 1976	
transpiration method		diaphragm gauge	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
41.07	1.004	29.95	0.28
49.11	2.306	35.07	0.49
54.68	3.912	40.02	0.85
62.62	8.015	44.96	1.41
68.71	13.62	49.95	2.34
68.72	13.58	55.04	3.81
75.21	23.71	59.95	6.05
75.33	23.79	64.91	9.39
79.75	33.69	69.87	14.4
79.75	33.5		
84.2	48.3	mp/ $^{\circ}\text{C}$	165.55
89.46	72		
89.48	72.16	eq. 3	P/Pa
90.54	77.91	A	13.134
		B	3855
		C	-21.0

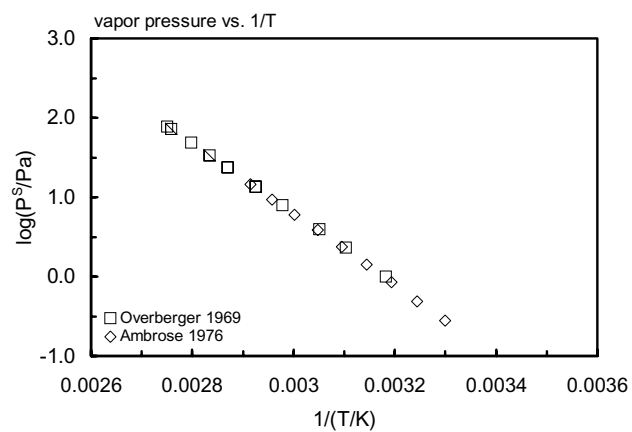
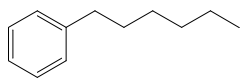


FIGURE 3.1.1.25.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-hexamethylbenzene.

3.1.1.26 *n*-Hexylbenzene

Common Name: *n*-Hexylbenzene

Synonym: 1-phenylhexane, hexylbenzene

Chemical Name: *n*-hexylbenzene

CAS Registry No: 1077-16-3

Molecular Formula: $C_{12}H_{18}$, $C_6H_5(CH_2)_5CH_3$

Molecular Weight: 162.271

Melting Point ($^{\circ}C$):

−61.0 (Dreisbach 1955; Lide 2003)

Boiling Point ($^{\circ}C$):

226.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8613 (Weast 1982–83)

Molar Volume (cm^3/mol):

188.4 ($20^{\circ}C$, calculated from density)

229.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.02 (generator column-HPLC/UV, Tewari et al. 1982c)

0.995* (generator column-HPLC, measured range 5 – $29^{\circ}C$, May et al. 1983)

0.902* (generator column-HPLC/UV, measured range 7 – $45^{\circ}C$, Owens et al. 1986)

$\ln x = -429.463 + 18024.83/(T/K) + 61.9402 \cdot \ln (T/K)$; temp range 290 – $400\ K$ (eq. derived from literature calorimetric and solubility data, Tsionopoulos 1999)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

14.01 (extrapolated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.18284 - 1813.74/(195.5 + t/^{\circ}C)$; temp range 120 – $290^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

13.61* (extrapolated, Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.9853 - 1700.5/(188.2 + t/^{\circ}C)$; temp range 96 – $258^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

10.52* ($20.51^{\circ}C$, static method, measured range 273.73 – $462.97\ K$, Kasehgari et al. 1993)

$\log (P/kPa) = 6.50020 - 1946.435/(208.935 + t/^{\circ}C)$; temp range 273.73 – $462.97\ K$ (static method, Kasehgari et al. 1993)

$\log (P/mmHg) = 6.7694 - 3.6050 \times 10^3/(T/K) + 3.3416 \cdot \log (T/K) - 1.5306 \times 10^{-2} \cdot (T/K) + 7.8479 \times 10^{-6} \cdot (T/K)^2$, temp range 212 – $698\ K$ (Yaws 1994)

10.52* ($20.51^{\circ}C$, measured range 263.88 – $462.97\ K$, Mokbel et al. 1998)

Henry's Law Constant ($Pa\ m^3/mol$):

1977 (calculated- C_A/C_W , Eastcott et al. 1988)

2172 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.25 (calculated-fragment const., Rekker 1977)

5.52 (generator column-HPLC/UV, Tewari et al. 1982c)

5.24 (TLC-RT correlation, Bruggeman et al. 1982)

- 5.45, 5.25 (quoted of HPLC methods, Harnisch et al. 1983)
 5.26, 5.62 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)
 5.52 (recommended, Sangster 1989, 1993)
 5.52 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.26.1

Reported aqueous solubilities of *n*-hexylbenzene at various temperatures

May et al. 1983				Owens et al. 1986	
generator column-HPLC				generator column-HPLC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
5	0.921	20	0.043	7	0.834
6	0.921	21	0.949	10	0.836
8	0.92	22	0.956	15	0.826
9	0.996	23	0.953	20	0.951
11	0.904	24	0.983	25	0.902
12	0.928	25	0.995	30	0.996
13	0.93	26	0.999	35	1.069
14	0.92	27	0.999	40	1.069
15	0.925	29	1.012	45	1.298
16.01	0.908	29	1.016		
17	0.919				
18	0.91	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 7.60$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 8.0$	
19	0.921	at 25°C		at 25°C	

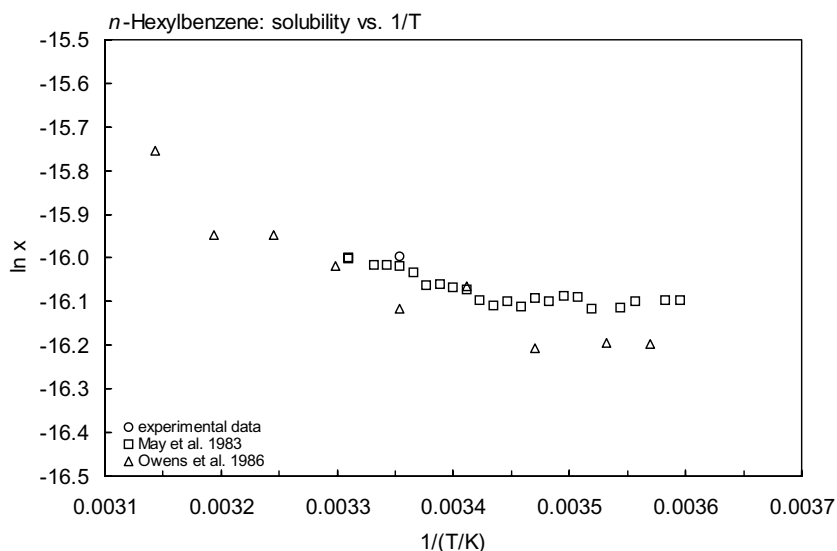


FIGURE 3.1.1.26.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *n*-hexylbenzene.

TABLE 3.1.1.26.2

Reported vapor pressures of *n*-hexylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Zwolinski & Wilhoit 1971		Kasehgari et al. 1993		Mokbel et al. 1998			
selected values		static method		static method			
t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa		
96	1333	273.73	1.653	263.88	0.609		
111	2666	283.63	4.239	273.73	1.648		
121	4000	293.66	10.52	283.63	4.236		
128	5333	303.64	23.20	293.66	10.52		
133.5	6666	313.62	48.66	303.64	23.20		
138.4	7999	323.59	97.32	313.62	48.72		
146.4	10666	333.58	184.9	323.59	97.36		
152.9	13332	343.57	336.63	333.58	185.0		
165.4	19998	353.58	589.1	343.57	336.0		
174.8	26664	363.58	997.8	353.58	589.0		
182.5	33331	372.84	1606	363.58	998.0		
189.0	39997	382.77	2519	372.84	1606		
199.8	53329	392.70	3841	382.77	2520		
208.5	66661	402.74	5722	392.70	3841		
216.0	79993	412.76	8320	402.74	5722		
222.5	93326	422.76	11828	412.76	8321		
223.1	94659	432.75	16516	422.76	11829		
223.7	95992	442.89	22640	432.75	16517		
224.3	97325	452.83	30575	442.80	22641		
224.9	98659	462.97	40693	452.83	30576		
225.5	99992			462.79	40694		
226.1	101325	eq. 2	P/kPa	data fitted to Wagner eq.			
		A	6.50020				
Antoine eq.	P/mmHg	B	1946.435				
A	6.9853	C	208.935				
B	1700.5						
C	1882.2						
bp/°C	226.1						
$\Delta H_v/(\text{kJ mol}^{-1}) =$							
at 25°C	60						
at bp	43.1						

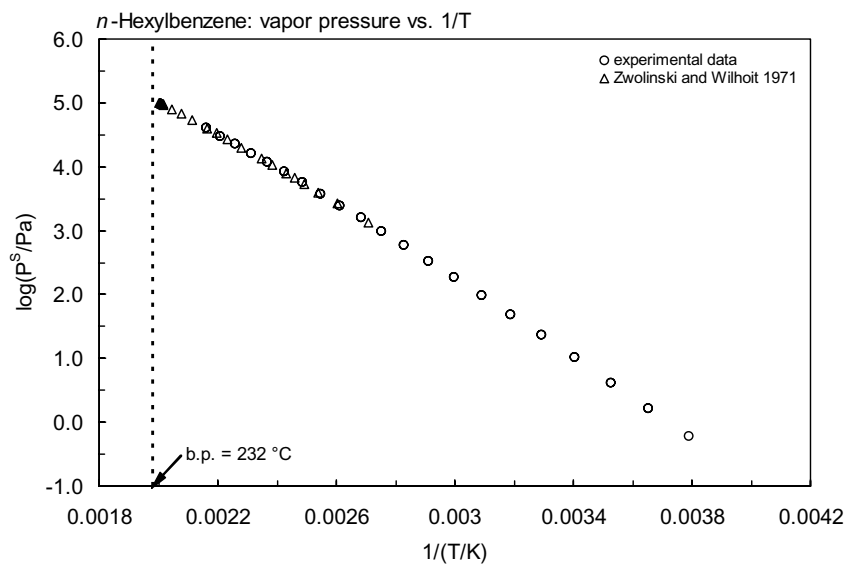
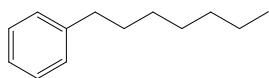


FIGURE 3.1.1.26.2 Logarithm of vapor pressure versus reciprocal temperature for *n*-hexylbenzene.

3.1.1.27 Heptylbenzene



Common Name: Heptylbenzene

Synonym: 1-phenylheptane

Chemical Name: *n*-heptylbenzene

CAS Registry No: 1078-71-3

Molecular Formula: $C_{13}H_{20}$, $C_6H_5(CH_2)_6CH_3$

Molecular Weight: 176.298

Melting Point ($^{\circ}C$):

−48 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

240 (Lide 2003)

Density (g/cm^3):

0.8567 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

205.8 ($20^{\circ}C$, calculated-density)

251.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.686; 0.925 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($66.2^{\circ}C$, summary of literature data, temp range 66.2 – $233^{\circ}C$, Stull 1947)

1333* ($112^{\circ}C$, derived from compiled data, temp range 112 – $246^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0006 - 1761.2/(181.5 + t/^{\circ}C)$; temp range 112 – $279^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.1255 - [1761.2/(T - 91.65)]$; temp range 423 – 527 K (liquid, Antoine equation, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 89.2811 - 6.4093 \times 10^3/(T/K) - 29.248 \cdot \log(T/K) + 1.0328 \times 10^{-2} \cdot (T/K) + 6.2451 \times 10^{-14} \cdot (T/K)^2$, temp range 225 – 714 K (Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.768 (HPLC- k' correlation, Hanai & Hubert 1981)

5.37 (HPLC- k' correlation, Ritter et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.27.1

Reported vapor pressures of heptylbenzene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Zwolinski & Wilhoit 1971			
summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
66.2	133.3	112	1333	243	94659
94.8	666.6	128	2666	243.6	95992
109	1333	137	4000	244.2	97325
124.2	2666	145	5333	244.8	98659
141.6	5333	150.7	6666	245.4	99992
151.5	7999	155.7	7999	246	101325
165.7	13332	164	10666		
186.6	26664	170.7	13332	eq. 2	P/mmHg
210	53329	183.6	19998	A	6.97833
233	101325	193.3	26664	B	1639.91
		201.1	33331	C	194.76
mp/°C	-	207.8	39997		
		218.9	53329	bp/°C	205.46
		227.9	66661	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
		235.6	79993	at 25°C	55.06
		242.3	93326	at bp	41.21

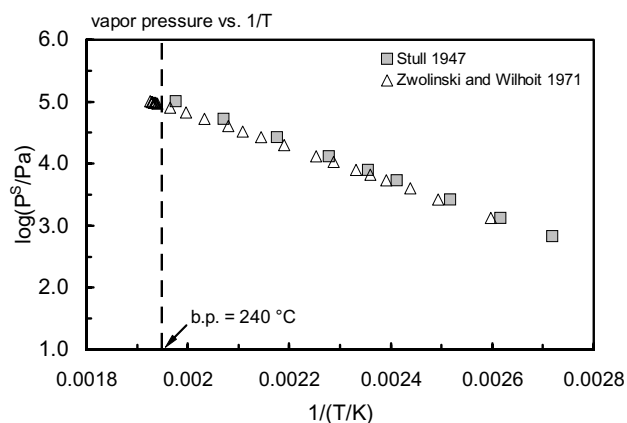
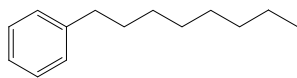


FIGURE 3.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for heptylbenzene.

3.1.1.28 *n*-Octylbenzene

Common Name: *n*-Octylbenzene

Synonym: 1-phenyloctane, octylbenzene

Chemical Name: *n*-octylbenzene

CAS Registry No: 2189-60-8

Molecular Formula: $C_{14}H_{22}$, $C_6H_5(CH_2)_7CH_3$

Molecular Weight: 190.325

Melting Point ($^{\circ}C$):

−36 (Lide 2003)

Boiling Point ($^{\circ}C$):

264 (Lide 2003)

Density (g/cm^3):

0.8582 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

222.2 ($20^{\circ}C$, calculated-density)

273.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

29.96 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

127.91, 110.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.219; 0.204 (calculated-regression eq.; calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1333* ($127^{\circ}C$, derived from compiled data, temp range 127 – $264.4^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0086 - 1812.2/(174.6 + t/^{\circ}C)$; temp range 127 – $298^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

7.666* ($43^{\circ}C$, gas saturation, measured range 43 – $125.6^{\circ}C$, Allemand et al. 1986)

$\log(P/kPa) = 8.35571 - 3293.744/(T/K)$; temp range 368 – $400\ K$ (liquid, Antoine equation, Stephenson & Malanowski 1987)

1.15* ($20.01^{\circ}C$, static method, measured range 293.16 – $462.87\ K$, Kasehgari et al. 1993)

$\log(P/kPa) = 6.50210 - 2183.874/(207.887 + t/^{\circ}C)$; temp range 293.16 – $462.87\ K$ (static method, Kasehgari et al. 1993)

$\log(P/mmHg) = 1.8919 - 4.1324 \times 10^3/(T/K) + 6.1473 \cdot \log(T/K) - 2.0294 \times 10^{-2} \cdot (T/K) + 9.6879 \times 10^{-6} \cdot (T/K)^2$, temp range 237 – $729\ K$ (Yaws 1994)

1.105* ($20.34^{\circ}C$, static method, measured range 293.49 – $462.87\ K$, Mokbel et al. 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.30 (RP-TLC-RT correlation, Bruggeman et al. 1982)

6.52, 6.29 (RP-HPLC- k' correlation, Harnisch et al. 1982)

6.297 (HPLC- k' correlation, Hanai & Hubert 1984)

6.35, 6.85 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)

6.30 (recommended, Sangster 1993)

5.89 (HPLC- k' correlation, Ritter et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.28.1

Reported vapor pressures of octylbenzene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Zwolinski & Wilhoit 1971		Allemand et al. 1986		Kasehgari et al. 1993		Mokbel et al. 1998	
selected values		gas saturation		static method		static method	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
127	1333	43.0	7.666	293.16	1.15	293.49	1.105
143	2666	52.43	14.8	303.13	3.01	313.49	2.690
153	4000	72.75	66.8	313.01	6.87	303.48	6.316
161	5333	84.2	134.7	323.01	15.3	23.47	13.92
166.7	6666	95.39	262.7	333.15	31.5	333.48	28.76
171.9	7999	106.0	437.3	343.15	60.8	343.45	57.64
180.4	10666	125.64	1205	353.13	114	353.45	109.0
187.2	13332			363.14	207	363.42	198.0
200.3	19998			373.22	362	373.45	350.0
210.4	26664			383.25	609	403.00	1513
218.4	33331			393.32	994	412.96	2329
225.3	39997			403.33	1574	422.92	3504
236.7	53329			412.96	2329	432.94	5143
235.9	66661			422.92	3504	442.96	7395
253.8	79993			432.94	5143	452.90	10366
260.7	93326			442.96	7395	462.87	14266
261.9	95992			452.90	10370		
263.2	98659			462.87	14270	data fitted to Wagner eq.	
264.4	101325						
				Antoine eq.			
eq. 2	P/mmHg			eq. 2	P/kPa		
A	7.0086			A	6.50210		
B	1812.2			B	2183.874		
C	174.6			C	207.887		
bp/°C	264.4						
ΔH _v /(kJ mol ⁻¹) =							
at 25°C	69.96						
at bp	46.9						

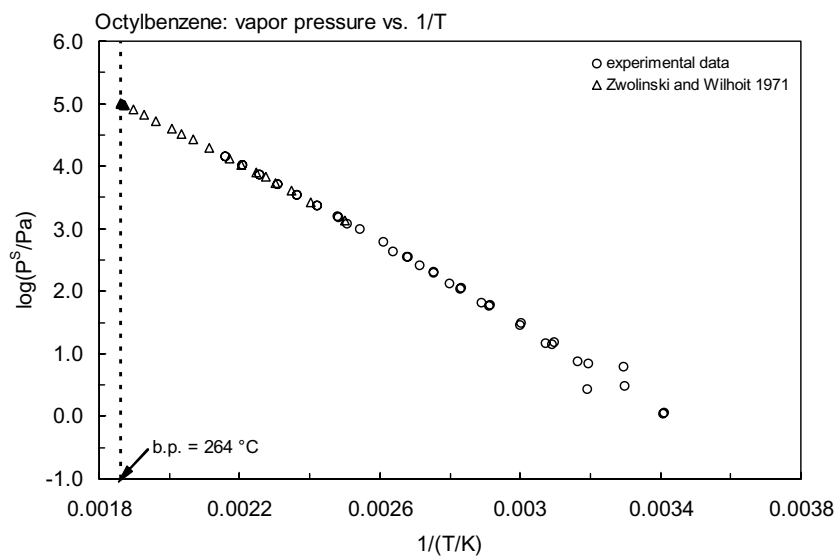
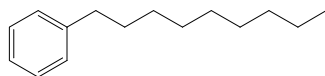


FIGURE 3.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for octylbenzene.

3.1.1.29 Nonylbenzene



Common Name: Nonylbenzene

Synonym: 1-phenylnonane

Chemical Name: *n*-nonylbenzene

CAS Registry No: 1081-77-2

Molecular Formula: $C_{15}H_{24}$, $C_6H_5(CH_2)_8CH_3$

Molecular Weight: 204.352

Melting Point ($^{\circ}C$):

−24 (Dreisbach 1955; Lide 2003)

Boiling Point ($^{\circ}C$):

280.5 (Lide 2003)

Density (g/cm^3):

0.8558, 0.8522 (20 $^{\circ}C$, 25 $^{\circ}C$, Dreisbach 1955)

0.8584 (20 $^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

238.1 (20 $^{\circ}C$, calculated-density)

295.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

0.0725; 0.112 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.573 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.19041 - 1991.0/(180.0 + t/^{\circ}C)$; temp range 165–330 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* (142 $^{\circ}C$, derived from compiled data, temp range 142–282 $^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0245 - 1862.6/(167.5 + t/^{\circ}C)$; temp range 142–316 $^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

2.906* (43 $^{\circ}C$, gas saturation, measured range 43–142 $^{\circ}C$, Allemand et al. 1986)

0.338 (GC-RT correlation, Sherblom et al. 1992)

$\log(P/mmHg) = -0.9235 - 4.2232 \times 10^3/(T/K) + 7.3073 \cdot \log(T/K) - 2.0964 \times 10^{-2} \cdot (T/K) + 9.7152 \times 10^{-6} \cdot (T/K)^2$, temp range 249–741 K (Yaws 1994)

0.8747* (30.52 $^{\circ}C$, static method, measured range 313.67–466.46 K, Mokbel et al. 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25 $^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.828 (HPLC- k' correlation, Hanai & Hubert 1981)

6.83, 7.40 (RP-HPLC- k' correlations, Sherblom & Eganhouse 1988)

7.11 (recommended, Sangster 1993)

6.41 (HPLC- k' correlation, Ritter et al. 1995)

6.83 (quoted from Sherblom & Eganhouse 1988, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.29.1

Reported vapor pressures of nonylbenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & \end{aligned}$$

Zwolinski & Wilhoit 1971				Allemand et al. 1986		Mokbel et al. 1998	
selected values				gas saturation		static method	
t/°C	P/Pa			t/°C	P/Pa	T/K	P/Pa
142	1333	eq. 2	P/mmHg	43	2.906	303.67	0.8474
158	2666	A	7.0245	50	5.186	313.65	2.271
168	4000	B	1862.6	59	10.36	323.67	5.369
176	5333	C	167.5	64	15.07	333.61	12.07
182.3	6666			74.32	31.73	343.53	25.20
187.5	7999	bp/°C	282.0	85.0	64.26	351.83	44.97
196.2	10666	ΔH_v /(kJ mol ⁻¹)		91.3	95.33	361.84	85.44
203.2	13332	at 25°C	74.81	98.28	146.7	371.75	155
216.7	19998	at bp	49.0	108.57	260.0	381.65	270
226.8	26664			120.0	480.0	391.62	459
235.1	33331			130.73	780.0	401.56	752
247.1	39997			142.0	1352	411.48	1207
253.7	53329					411.60	1203
263.1	66661					421.45	1881
271.1	79993					431.44	2835
278.2	93326					441.49	4201
279.5	95992					451.48	6053
280.7	98659					461.48	8591
282	101325					466.46	10099

data fitted to Wagner eq.

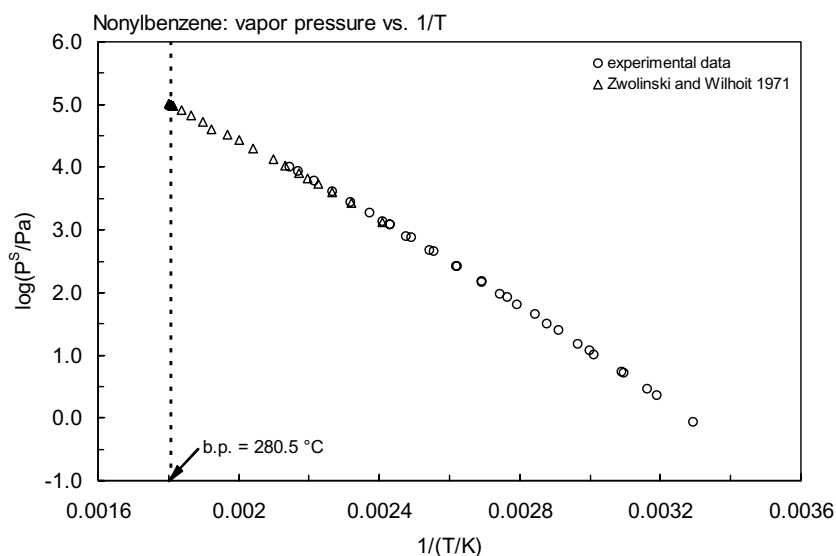
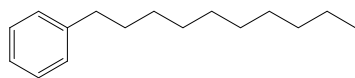


FIGURE 3.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for nonylbenzene.

3.1.1.30 Decylbenzene



Common Name: Decylbenzene

Synonym: 1-phenyldecane

Chemical Name: *n*-decylbenzene

CAS Registry No: 104-72-3

Molecular Formula: $C_{16}H_{26}$, $C_6H_5(CH_2)_9CH_3$

Molecular Weight: 218.337

Melting Point ($^{\circ}C$):

-14.4 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

293 (Lide 2003)

Density (g/cm^3):

0.85553, 0.85189 ($20^{\circ}C$, $25^{\circ}C$, Camin et al. 1954; Dreisbach 1955)

Molar Volume (cm^3/mol):

255.3 ($20^{\circ}C$, calculated-density)

318.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.50 (vapor-phase saturation, shake flask-GC, Sherblom et al. 1992)

5.59, 8.47, 10.55 (calculated- V_M , K_{ow} , TSA, Sherblom et al. 1992)

0.023; 0.0188 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

8329* ($202.987^{\circ}C$, ebulliometry, measured range 202.987 – $297.799^{\circ}C$, Camin et al. 1954)

$\log(P/mmHg) = 7.03642 - 1904.132/(160.318 + t/^{\circ}C)$; temp range 202.9 – $297.9^{\circ}C$ (Antoine eq., manometer measurements, Camin et al. 1954)

0.20 (extrapolated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.27177 - 2107.7/(180.0 + t/^{\circ}C)$; temp range 185 – $345^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* ($155.1^{\circ}C$, derived from compiled data, temp range 155.1 – $297.89^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.03642 - 1904.132/(160.318 + t/^{\circ}C)$; temp range 155.1 – $322.9^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.16274 - 1905.56/(160.503 + t/^{\circ}C)$; temp range 203 – $297.8^{\circ}C$ (Antoine eq. from reported exptl. data of Camin et al. 1954, Boublik et al. 1984)

$\log(P/kPa) = 4.03653 - 876.208/(T/K - 203.15)$; temp range 317 – 427 K (liquid, Antoine equation, Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.15658 - [1900.916/(T/K - 113.16)]$; temp range 475 – 571 K (liquid, Antoine equation, Stephenson & Malanowski 1987)

0.133, 0.127 (P_L , GC-RT correlation, Sherblom et al. 1992)

0.707* ($39.85^{\circ}C$, static method, measured range 313.0 – 433.23 K, Kasehgari et al. 1993)

$\log(P/kPa) = 6.37655 - 2098.329/(180.620 + t/^{\circ}C)$; temp range 313.0 – 433.23 K (static method, Kasehgari et al. 1993)

$\log(P/mmHg) = -4.4754 - 4.4669 \times 10^3/(T/K) + 9.1965 \cdot \log(T/K) - 2.4010 \times 10^{-2} \cdot (T/K) + 1.0848 \times 10^{-5} \cdot (T/K)^2$, temp range 259 – 753 K (Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

- 7.35 (RP-TLC retention time correlation, Bruggeman et al. 1982)
- 7.60, 7.33 (RP-HPLC-k' correlations, Harnisch et al. 1982)
- 7.358 (HPLC-k' correlation, Hanai & Hubert 1984)
- 7.37, 8.01 (RP-HPLC-k' correlation, Sherblom & Eganhouse 1988)
- 7.38 (HPLC-k' correlation, Sherblom et al. 1992)
- 7.35 (recommended, Sangster 1993)
- 6.94 (HPLC-k' correlation, Ritter et al. 1995)
- 7.37 (quoted from Sherblom & Eganhouse 1988, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

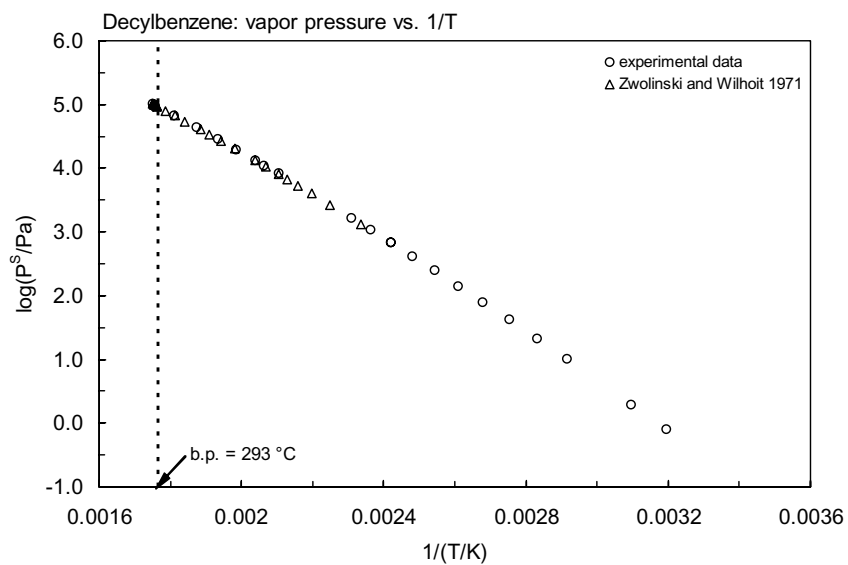
Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

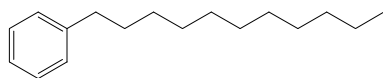
TABLE 3.1.1.30.1

Reported vapor pressures of decylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Camin et al. 1954		Zwolinski & Wilhoit 1971				Kasehgari et al. 1993	
ebulliometry		selected values				static method	
t/°C	P/Pa	t/°C	P/Pa			T/K	P/Pa
202.987	8329	155.1	1333	eq. 2	P/mmHg	313.0	0.797
211.392	10938	171.7	2666	A	7.03642	323.13	1.92
217.156	13088	182.19	4000	B	1904.132	343.15	10.3
230.476	19442	190.07	5333	C	160.318	353.11	21.6
244.331	28555	196.431	6666			363.12	41.9
260.372	43172	201.803	7999	bp/°C	297.89	373.25	78.5
278.950	67077	210.617	10666	$\Delta H_v/(kJ\ mol^{-1}) =$		383.28	142
296.370	98146	217.755	13332	at 25°C	79.75	393.34	248
297.799	101113	231.452	19998	at bp	50.6	403.37	417
		241.789	26664			413.33	683
bp/°C	297.083	250.19	33331			413.33	684
		257.18	39997			423.21	1081
		269.86	53329			433.23	1687
		278.68	66661				
		286.843	79993				
		293.986	93326			Antoine eq	
		295.969	95992			eq. 2	P/kPa
		296.616	98659			A	6.37655
		297.89	101325			B	2098.329
						C	180.620



3.1.1.31 Undecylbenzene



Common Name: Undecylbenzene

Synonym: 1-phenylundecane

Chemical Name: *n*-undecylbenzene

CAS Registry No: 6742-54-7

Molecular formula: $C_{17}H_{28}$, $C_6H_5(CH_2)_{10}CH_3$

Molecular Weight: 232.404

Melting Point ($^{\circ}C$):

−5.0 (Dreisbach 1955; Lide 2003)

Boiling Point ($^{\circ}C$):

316 (Dreisbach 1955; Lide 2003)

Density (g/cm^3):

0.8553, 0.8517 (20 $^{\circ}C$, 25 $^{\circ}C$, Dreisbach 1961)

Molar Volume (cm^3/mol):

271.7 (20 $^{\circ}C$, calculated-density)

340.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

0.00702; 0.00377 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.080 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.34672 - 2215.1/(180.0 + t/^{\circ}C)$; temp range 195–375 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* (168 $^{\circ}C$, derived from compiled data, temp range 168–313.2 $^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0509 - 1944.1/(153.0 + t/^{\circ}C)$; temp range 168–349 $^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

0.050, 0.047 (P_L , GC-RT correlation, Sherblom et al. 1992)

$\log(P/mmHg) = 124.1549 - 8.8970 \times 10^3/(T/K) - 41.223 \cdot \log(T/K) + 1.3662 \times 10^{-2} \cdot (T/K) - 8.1321 \times 10^{-14} \cdot (T/K)^2$, temp range 268–764 K (Yaws 1994)

0.7156* (50.42 $^{\circ}C$, static method, measured range 323.57–467.33 $^{\circ}C$, data fitted to Wagner eq., Mokbel et al. 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25 $^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.14 (RP-HPLC-RT correlation, Sherblom et al. 1992, quoted, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.31.1

Reported vapor pressures of undecylbenzene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1)$$

$$\ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2)$$

$$\ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log(T/K)$$

Zwolinski & Wilhoit 1971

Mokbel et al. 1998

selected values				static method			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
168	1333	309.2	93326	323.57	0.7156	462.28	3088
185	2666	310.6	95992	333.59	1.820	467.33	37726
196	4000	311.9	98659	343.71	4.304		
204	5333	313.2	101325	352.69	9.405	data fitted to Wagner eq.	
210.3	6666			363.78	19.39		
215.7	7999	eq. 2	P/mmHg	372.07	34.36		
224.7	10666	A	7.0590	382.06	64.41		
231.9	13332	B	1944.1	392.06	117		
245.8	19998	C	153.0	402.11	204		
256.3	26664			412.11	344		
264.8	33331	bp/°C	313.2	422.09	564		
272.1	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$		422.19	568		
284	53329	at 25°C	84.68	432.25	908		
293.7	66661	at bp	52.3	442.27	1369		
302	79993			452.29	2080		

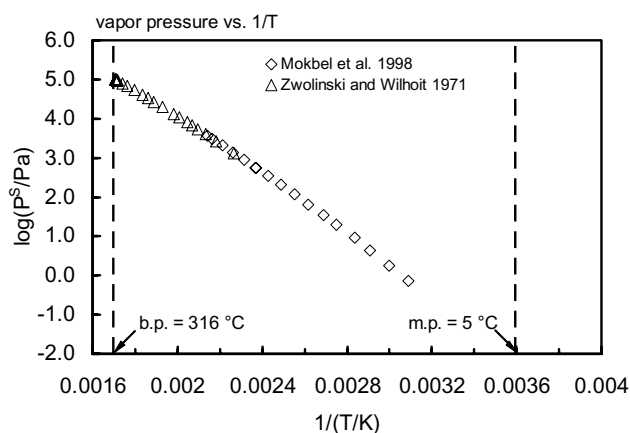
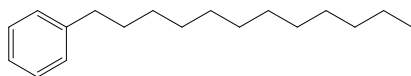


FIGURE 3.1.1.31.1 Logarithm of vapor pressure versus reciprocal temperature for undecylbenzene.

3.1.1.32 Dodecylbenzene



Common Name: Dodecylbenzene

Synonym: 1-phenyldodecane

Chemical Name: *n*-dodecylbenzene

CAS Registry No: 123-01-3

Molecular Formula: $C_{18}H_{30}$, $C_6H_5(CH_2)_{11}CH_3$

Molecular Weight: 246.431

Melting Point ($^{\circ}C$):

3.0 (Dreisbach 1955; Lide 2003)

Boiling Point ($^{\circ}C$):

328 (Lide 2003)

Density (g/cm^3):

0.8551, 0.8516 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

Molar Volume (cm^3/mol):

288.2 ($20^{\circ}C$, calculated-density)

362.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

26.66* ($78.4^{\circ}C$, ebulliometry-McLeod gauge, measured range 78.4 – $288.6^{\circ}C$, Myers & Fenske 1955)

0.032 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.41934 - 2319.2/(180.0 + t/^{\circ}C)$; temp range 210 – $385^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* ($181^{\circ}C$, derived from compiled data, temp range 181 – $327.6^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0693 - 1981.6/(145.5 + t/^{\circ}C)$; temp range 181 – $363^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

1.08* ($53.7^{\circ}C$, gas saturation, measured range 53.7 – $192.7^{\circ}C$, Allemand et al. 1986)

0.019, 0.017 (P_L , GC-RT correlation, Sherblom et al. 1992)

0.727* ($69.771^{\circ}C$, static method, measured range 332.92 – $453.26 K$, Kasehgari et al. 1993)

$\log(P/kPa) = 6.66087 - 2371.902/(182.311 + t/^{\circ}C)$; temp range 332.92 – $453.26 K$ (static method, Kasehgari et al. 1993)

$\log(P/mmHg) = 145.6916 - 1.0165 \times 10^3/(T/K) - 48.761 \cdot \log(T/K) + 1.5985 \times 10^{-2} \cdot (T/K) + 4.881 \times 10^{-13} \cdot (T/K)^2$, temp range 276 – $774 K$ (Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.65 (RP-HPLC- k' correlation, Sherblom et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.32.1

Reported vapor pressures of dodecylbenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Myers & Fenske 1955		Zwolinski & Wilhoit 1971		Allemand et al. 1986		Kasehgari et al. 1993	
ebulliometry-McLeod gauge		selected values		gas saturation		static method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
78.4	26.66	181	1333	53.7	1.080	343.21	0.640
91.2	66.66	198	2666	86.19	6.733	353.26	1.61
102.3	133.3	209	4000	93.0	11.15	363.23	3.72
114.2	266.6	217	5333	103.0	21.60	363.23	3.73
122.4	400.0	223.5	6666	111.0	36.40	373.21	8.11
128.2	533.3	229.0	7999	124.02	79.86	383.22	16.9
133.4	666.6	238.1	10666	136.47	158.7	393.22	32.8
137.0	800	245.4	13332	160.44	540	403.27	59.5
143.5	1067	259.5	19998	192.71	1464	413.28	106
148.8	1333	270.1	26664			423.29	182
158.5	2000	278.7	33331			433.37	306
165.6	2666	286	39997			443.39	493
176.4	4000	298.1	53329			453.33	760
184.2	5333	307.9	66661			463.38	1167
191.0	6666	316.3	79993				
196.0	7999	323.6	93326				
205.5	10666	325	95992			Antoine eq	
212.0	13332	326.3	98659			eq. 2	P/kPa
225.4	19998	327.6	101325			A	6.66087
235.8	26664					B	2371.902
250.3	39997					C	182.311
262.0	53329	eq. 2	P/mmHg				
270.4	66661	A	7.0693				
278.2	79992	B	1981.6				
285.5	93326	C	145.5				
288.6	101325						
		bp/°C	327.6				
		$\Delta H_v/(\text{kJ mol}^{-1})$					
		at 25°C	89.62				
		at bp	54.4				

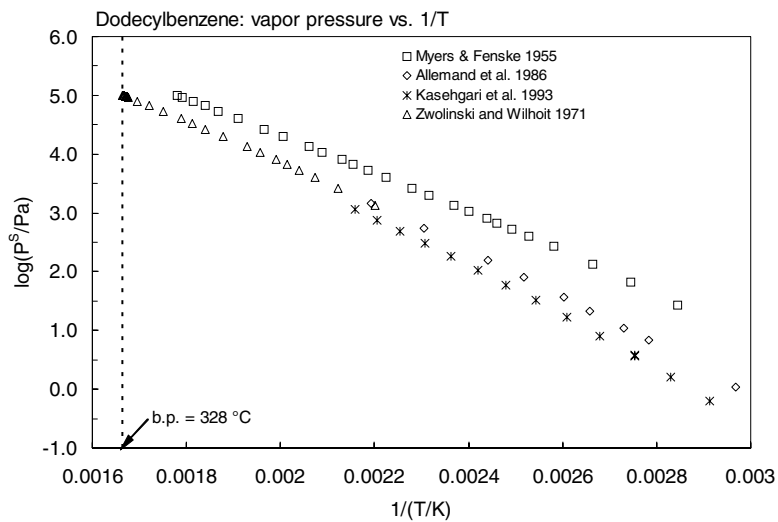
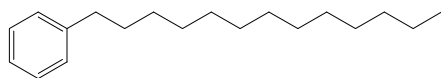


FIGURE 3.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for dodecylbenzene.

3.1.1.33 Tridecylbenzene



Common Name: Tridecylbenzene

Synonym: 1-phenyltridecane

Chemical Name: *n*-tridecylbenzene

CAS Registry No: 123-02-4

Molecular Formula: $C_{19}H_{32}$, $C_6H_5(CH_2)_{12}CH_3$

Molecular Weight: 260.457

Melting Point ($^{\circ}C$):

10 (Dreisbach 1955; Lide 2003)

Boiling Point ($^{\circ}C$):

346 (Dreisbach 1955; Lide 2003)

Density (g/cm^3):

0.8550, 0.8515 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

Molar Volume (cm^3/mol):

304.6 ($20^{\circ}C$, calculated-density)

384.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.233 (vapor saturation-shake flask-GC, Sherblom et al. 1992)

0.233, 0.0885, 0.181 (calculated- V_m , K_{OW} , TSA, Sherblom et al. 1992)

0.00067; 0.00137 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0125 (extrapolated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.49437 - 2626.7/(180.0 + t/^{\circ}C)$; temp range $226-405^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* ($193^{\circ}C$, derived from compiled data, temp range $193-341.2^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.0843 - 2013.9/(137.9 + t/^{\circ}C)$; temp range $193-376^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

0.008, 0.07 (P_L , GC-RT correlation, Sherblom et al. 1992)

0.64* ($70.06^{\circ}C$, static method, measured range $343.21-463.38$ K, Kasehgari et al. 1993)

$\log(P/kPa) = 6.13410 - 2087.968/(153.790 + t/^{\circ}C)$; temp range $343.21-463.38$ K (static method, Kasehgari et al. 1993)

$\log(P/mmHg) = 160.3924 - 1.1093 \times 10^4/(T/K) - 53.875 \cdot \log(T/K) + 1.7532 \times 10^{-2} \cdot (T/K) + 3.727 \times 10^{-13} \cdot (T/K)^2$, temp range $283-783$ K (Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

9.36 (RP-HPLC- k' correlation, Sherblom et al. 1992)

8.97; 8.54 (calculated-fragment const., calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

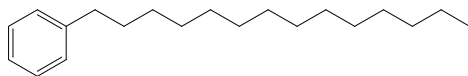
Half-Lives in the Environment:

TABLE 3.1.1.33.1

Reported vapor pressures of tridecylbenzene at various temperatures

Zwolinski & Wilhoit 1971				Kasehgari et al. 1993	
selected values				static method	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	T/K	P/Pa
193	1333	338.5	95992	343.20	6.40×10^{-4}
210	2666	339.9	98659	353.26	1.61×10^{-3}
221	4000	341.2	101325	363.23	3.73×10^{-3}
229	5333			373.21	8.11×10^{-3}
236	6666	$\log P = A - B/(C + t/^{\circ}\text{C})$		383.22	0.0169
242	7999		P/mmHg	393.22	0.0328
251	10666	A	7.0843	403.27	0.0595
258.2	13332	B	2013.9	413.28	0.106
271.6	19998	C	137.9	423.29	0.182
283.1	26664			433.37	0.306
291.8	33331	bp/ $^{\circ}\text{C}$	341.2	443.39	0.493
299.2	39997	$\Delta H_v/(\text{kJ mol}^{-1})$		453.33	0.760
311.4	53329	at 25°C	94.6	463.38	1.167
321.3	66661	at bp	56.1		
329.8	79993				
337.2	93326				

3.1.1.34 Tetradecylbenzene



Common Name: Tetradecylbenzene

Synonym: 1-phenyltetradecane

Chemical Name: *n*-tetradecylbenzene

CAS Registry No: 1459-10-5

Molecular Formula: $C_{20}H_{34}$, $C_6H_5(CH_2)_{13}CH_3$

Molecular Weight: 274.484

Melting Point ($^{\circ}C$):

16 (Dreisbach 1955; Lide 2003)

Boiling Point ($^{\circ}C$):

359 (Dreisbach 1955; Lide 2003)

Density (g/cm^3):

0.8549, 0.8514 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

Molar Volume (cm^3/mol):

321.7 ($20^{\circ}C$, calculated-density)

406.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1333* ($205^{\circ}C$, derived from compiled data, temp range 205 – $354^{\circ}C$, Zwolinski & Wilhoit 1971)

0.0055 (extrapolated-Antoine eq., Dreisbach 1955; quoted, Sherblom et al. 1992)

$\log(P/mmHg) = 7.56143 - 2522.8/(180.0 + t/^{\circ}C)$; temp range 235 – $410^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = 7.101 - 2042/(130 + t/^{\circ}C)$; temp range 205 – $300^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

0.002 (P_L , GC-RT correlation, Sherblom et al. 1992)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

9.95 (RP-HPLC- k' correlation, Sherblom et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

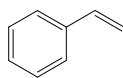
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.34.1**Reported vapor pressures of tetradecylbenzene at various temperatures****Zwolinski & Wilhoit 1971**

selected values			
t/°C	P/Pa	t/°C	P/Pa
205	1333	351	95992
222	2666	353	98659
233	4000	354	101325
241	5333		
248	6666		
254	7999	log P = A - B/(C + t/°C)	
263	10666	eq. 2	P/mmHg
270	13332	A	7.010
285	19998	B	2042.0
295	26664	C	130.0
304	33331	bp/°C	354.0
312	39997	ΔH_v /(kJ mol ⁻¹)	
324	53329	at 25°C	99.6
334	66661	at bp	57.7
342	79993		
350	93326		

3.1.1.35 Styrene



Common Name: Styrene

Synonym: phenylethene, styrol, styrolene cinnamene, cinnamol, phenylethylene, vinylbenzene, ethenylbenzene

Chemical Name: styrene

CAS Registry No: 100-42-5

Molecular Formula: C_8H_8 , $C_6H_5CH=CH_2$

Molecular Weight: 104.150

Melting Point ($^{\circ}C$):

-30.65 (Lide 2003)

Boiling Point ($^{\circ}C$):

145 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9060, 0.9012 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949; Dreisbach 1955; Riddick et al. 1986)

0.906 (Weast 1982-83)

Molar Volume (cm^3/mol):

115.0 ($20^{\circ}C$, calculated-density)

133.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

43.932, 38.7 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.95 (Riddick et al. 1986; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

45.15, 52.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

330* ($24^{\circ}C$, shake flask-Karl Fischer titration, measured range $7-51^{\circ}C$, Lane 1946)

310* (cloud point method, measured range $10-60^{\circ}C$, Lane 1946)

220 (shake flask-method not specified, Friette & Hohenstein 1948)

300 (shake flask-UV, Andrews & Keefer 1950)

160 (shake flask-HPLC/UV, Banerjee et al. 1980)

250* (recommended best value, temp range $10-60^{\circ}C$, Shaw 1989b)

$\ln x = -19.471 - 1655.9/(T/K) - 4.6244 \times 10^{-5} \cdot (T/K)^2$; temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

288* ($8.2^{\circ}C$, mercury manometer, measured range -7.7 to $8.2^{\circ}C$, Linder 1931)

$\log (P/mmHg) = 7.929 - 2103/(T/K)$; temp range $33.5-116.3^{\circ}C$ (isoteniscope method, Burchfield 1942)

841.3* (static-Hg manometer, measured range $12.5-60^{\circ}C$, Pitzer et al. 1946)

969.4* (calculated-Antoine eq. regression, Stull 1947)

$\log (P/mmHg) = 7.22302 - 1629.2/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

6799* ($66.7^{\circ}C$, mercury manometer, Buck et al. 1949)

$\log (P/mmHg) = -3151/(T/K) - 6.294 \cdot \log (T/K) + 26.92$; temp range $80-120^{\circ}C$ (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)

807 (extrapolated by formula, Dreisbach 1955)

$\log (P/mmHg) = 6.92409 - 1430.0/(206.0 + t/^{\circ}C)$; temp range $55-205^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1093* ($29.92^{\circ}C$, measured range $29.92-110.06^{\circ}C$, Dreyer et al. 1955)

1333* ($32.24^{\circ}C$, measured range $32.4-82.9^{\circ}C$, Chaiyavech & van Winkle 1959)

- $\log (P/\text{mmHg}) = 8.2696 - 2221.21/(T/K)$; temp range 32.4–82.9°C (Chaiyavech & van Winkle 1959)
 $\log (P/\text{mmHg}) = [-0.2185 \times 9634.7/(T/K)] + 7.922049$; temp range –7.0 to 145.2°C (Antoine eq., Weast 1972–73)
 879, 812 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.14016 - 1574.511/(224.087 + t/^{\circ}\text{C})$; temp range 32.4–62.19°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.06623 - 1507.434/(214.985 + t/^{\circ}\text{C})$; temp range 29.92–144.77°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 $\log (P/\text{atm}) = (1 - 418.675/T) \times 10^{(0.886470 - 8.14267 \times 10^4 \cdot T + 7.57896 \times 10^7 \cdot T^2)}$; T in K, temp range 281.35–417.92 K (Cox vapor pressure eq., Chao et al. 1983)
 878, 811 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P_L/\text{kPa}) = 6.235 - 1557.406/(222.538 + T/K)$; temp range 32.4–62.19°C (Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.18301 - 1501.162/(214.42 + t/^{\circ}\text{C})$; temp range 29.92–144.77°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 879 (extrapolated, Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 7.14016 - 1774.51/(224.09 + t/^{\circ}\text{C})$; temp range 32–82°C (Antoine eq., Dean, 1985, 1992)
 841 (lit. average, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.34792 - 1629.20/(230.0 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 880 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.3945 - 2221.3/(T/K)$; temp range 245–334 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.08201 - 1445.58/(-63.72 + T/K)$; temp range 334–419 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 55.8621 - 4.024 \times 10^3/(T/K) - 17.609 \cdot \log (T/K) + 6.6842 \times 10^{-3} \cdot (T/K) + 1.9438 \times 10^{-13} \cdot (T/K)^2$, temp range 243–648 K (Yaws 1994)
 $\log (P/\text{kPa}) = 7.3945 - 2221.3/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 233 (calculated-P/C, Mackay & Shiu 1990)
 285, 527 (quoted, Howard et al. 1989)
 267 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 297 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 261 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 5.628 - 1935/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.14 (calculated-fragment const., Rekker 1977)
 2.95 (shake flask, Hansch & Leo 1979)
 3.16 (shake flask-HPLC, Banerjee et al. 1980)
 2.76 (HPLC-RT correlation Fujisawa & Masuhara 1981)
 2.90 (HPLC-RT correlation, Wang et al. 1986)
 3.05 (recommended, Sangster 1989, 1993)
 2.95 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

- 1.13 (goldfish, Ogata et al. 1984)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.42–2.74 (Swann et al. 1983)
 2.96, 2.71 (quoted exptl., calculated-MCI χ , Meylan et al. 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: Volatilization and biodegradation may be dominant transport and transformation processes for styrene in water; calculated volatilization $t_{1/2} = 3$ h from a river 1-m deep with a current speed of 1.0 m/s and wind velocity of 3 m/s (Howard 1989);

volatilized rapidly from shallow layers of lake water with $t_{1/2} = 1$ to 3 h, but much slower from soil (Fu & Alexander 1992).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = 1.8 \times 10^4 \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with ozone at 30°C (Bufalini & Altshuller 1965)

$k_{O_3} = (22.6 \pm 4.6) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1982)

$k_{OH} = 5.25 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1985)

$k_{O_3} = 22 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = (5.87 \pm 0.15) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = (1.51 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson & Aschmann 1988)

$k_{OH} = 5.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{O_3} = 1.71 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Tuazon et al. 1993)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: $t_{1/2}(\text{aerobic}) = 336\text{--}672 \text{ h}$, based on unacclimated grab samples of aerobic soil and a subsurface sample; $t_{1/2}(\text{anaerobic}) = 1344\text{--}2688 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

styrene will be rapidly destroyed by biodegradation in most aerobic environments, and the rate may be slow at low concentrations in aquifers and lake waters and in environments at low pH (Fu & Alexander 1992)

$t_{1/2}(\text{aerobic}) = 14 \text{ d}$, $t_{1/2} = 56 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4\text{--}24 \text{ h}$, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976); will react rapidly with both hydroxyl radical and ozone in air with a combined $t_{1/2}(\text{calc}) = 2.5 \text{ h}$, the reaction $t_{1/2} = 3.5 \text{ h}$ with OH radicals and $t_{1/2} = 9 \text{ h}$ with ozone (Howard 1989);

photooxidation $t_{1/2} = 0.9$ to 7.3 h , based on measured rate data for the reaction with OH radical and O_3 in air (Howard et al. 1991);

calculated lifetimes of styrene due to reaction with OH radicals, NO_3 radicals and O_3 are $\sim 3 \text{ h}$, $\sim 4 \text{ h}$ and 1 d , respectively, for ambient atmospheric conditions (Tuazon et al. 1993);

calculated lifetimes of 1.4 h , 3.7 h and 1.0 d for reactions with OH radical, NO_3 radical and O_3 respectively (Atkinson 2000).

Surface water: $t_{1/2} = 0.6 \text{ d}$ in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 336\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2}(\text{calc}) = 0.75\text{--}51 \text{ d}$ for styrene loss from surface waters (Fu & Alexander 1992).

Ground water: $t_{1/2} = 672\text{--}5040 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life and acclimated aqueous screening test data (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 336\text{--}672 \text{ h}$, based on unacclimated grab samples of aerobic soil and acclimated aqueous screening test data (Howard et al. 1991).

Biota:

TABLE 3.1.1.35.1

Reported aqueous solubilities of styrene at various temperatures

Lane 1946				Shaw 1989b (IUPAC)	
shake flask-titration		shake flask-cloud pt.		recommended values	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
7	290	15	250	10	290
24	330	25	310	20	300
32	360	44	400	25	340
40	400	49	450	30	340
51	450	65	500	40	400
				50	460
				60	530

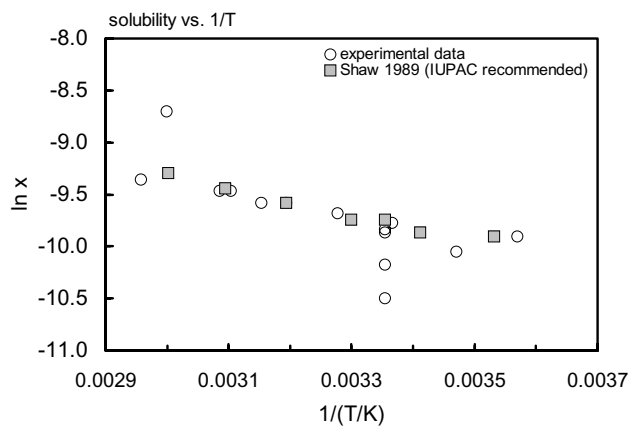
FIGURE 3.1.1.35.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for styrene.

TABLE 3.1.1.35.2

Reported vapor pressures of styrene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log(T/K) \quad (4)$$

1.

Linder 1931		Pitzer et al. 1946		Stull 1947		Buck et al. 1949	
Hg manometer		static-Hg manometer		summary of literature data		Hg manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-7.7	86.66	12.5	384	-7.0	133.3	66.7	6799
-0.5	105.7	25	841.3	18	666.6	75.4	9866
8.2	288	37.5	1692	30.8	1333	82.4	13332
		50	3230	44.6	2666	88	16665
		60	5177	59.8	5333	91.7	18932
				69.5	7999	95.1	21732
Burchfield 1942				82	13332	98.2	24665
isoteniscope method		mp/°C	-30.68	101.3	26664	119.1	48129
t/°C	P/Pa			122.5	53329	132.6	71461
data presented by		eq. 4	P/mmHg	145.2	101325	145	100658
Clausius-Clapeyron eq.		A	28.8631				
		B	3203				
		C	7	mp/°C	-30.6		
eq. 1	P/mmHg					eq. 4	P/mmHg
A	7.929	$\Delta H_{\text{fus}}(\text{kJ mol}^{-1}) = 10.95$				A	26.92
B	2103					B	3151
measured temp range:		$\Delta H_{\text{v}}(\text{kJ mol}^{-1}) = 43.93$				C	6.294
	33.5–116.3°C		at 25°C				

2.

Dreyer et al. 1955		Chaiyavech & Van Winkle 1959	
t/°C	P/Pa	t/°C	P/Pa
29.92	1093	32.4	1333
39.21	1827	35.6	2666
60.04	5106	53.86	4000
74.42	9639	60.05	5333
85.53	14999	65.45	6666
99.51	25105	76.6	10666
110.06	56877	82.9	13332
		eq. 1	P/mmHg
		A	8.2696
		B	2221.3

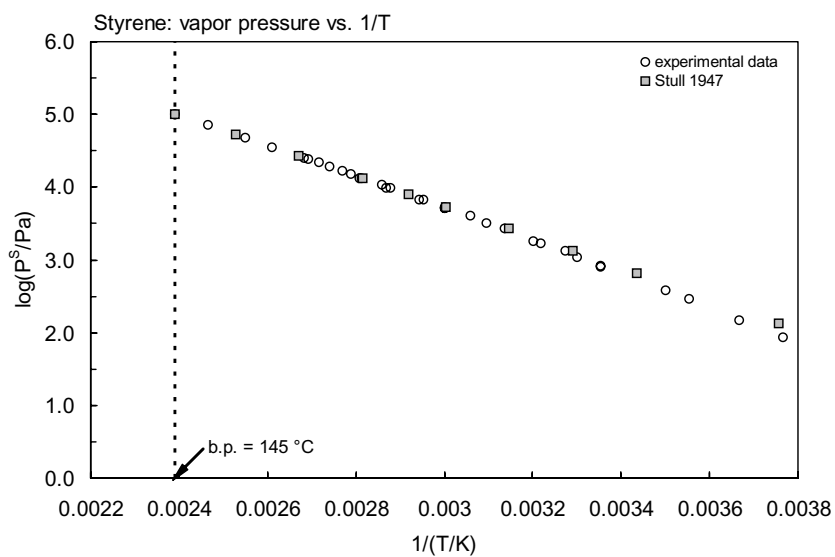
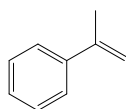


FIGURE 3.1.135.2 Logarithm of vapor pressure versus reciprocal temperature for styrene.

3.1.1.36 α -Methylstyrene

Common Name: α -Methylstyrene

Synonym: isopropenylbenzene

Chemical Name: α -Methylstyrene

CAS Registry No: 98-83-9

Molecular Formula: C_9H_{10} , $C_6H_5C(CH_3)=CH_2$

Molecular Weight: 118.175

Melting Point ($^{\circ}C$):

-23.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

165.4 (Lide 2003)

Density (g/cm^3):

0.9106, 0.9062 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

0.9082 ($20^{\circ}C$, Weast 1982-83)

Molar Volume (cm^3/mol):

129.8 ($20^{\circ}C$, calculated-density)

155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.92 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

47.55, 53.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($7.4^{\circ}C$, summary of literature data, temp range 7.4 – $165.4^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.28240 - 1740.3/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

333 (extrapolated by formula., Dreisbach 1855)

$\log(P/mmHg) = 6.92366 - 1486.88/(202.4 + t/^{\circ}C)$; temp range 70 – $220^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 10214.6/(T/K)] + 7.959753$; temp range 7.4 – $165.4^{\circ}C$ (Antoine eq., Weast 1972-73)

$\log(P/mmHg) = 6.92366 - 1486.88/(202.4 + t/^{\circ}C)$; temp range not specified (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.04856 - 1486.88/(-70.75 + T/K)$; temp range 343 – $493 K$ (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.294 - 1599.88/(-63.72 + T/K)$; temp range 353 – $413 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -0.8626 - 2.5638 \times 10^3/(T/K) + 5.3807 \cdot \log(T/K) - 1.3516 \times 10^{-2} \cdot (T/K) + 6.7181 \times 10^{-6} \cdot (T/K)^2$, temp range 250 – $654 K$ (Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.48 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation: $k = (52 \pm 6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at $298 \pm 2 \text{ K}$ (Atkinson 1989).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 3.1.1.36.1

Reported vapor pressures of α -methylstyrene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947

summary of literature data

$t/^{\circ}\text{C}$	P/Pa
7.4	133.3
34.0	666.6
47.1	1333
61.8	2666
77.8	5333
88.3	7999
102.2	13332
121.8	26664
143	53329
165.4	101325
mp/ $^{\circ}\text{C}$	-23.2

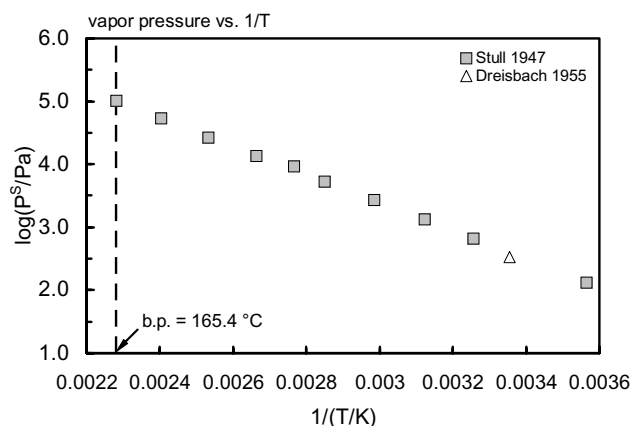
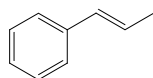


FIGURE 3.1.1.36.1 Logarithm of vapor pressure versus reciprocal temperature for α -methylstyrene.

3.1.1.37 β -MethylstyreneCommon Name: β -Methylstyrene

Synonym: propenylbenzene

Chemical Name: β -MethylstyreneCAS Registry No: 766-90-5 (*cis*-); 873-66-5 (*trans*-)Molecular Formula: C_9H_{10} , $C_6H_5CH=CHCH_3$

Molecular Weight: 118.175

Melting Point ($^{\circ}C$):-61.6 (*cis*-, Stephenson & Malanowski 1987; Lide 2003)-29.3 (*trans*-, Stephenson & Malanowski 1987; Lide 2003)Boiling Point ($^{\circ}C$):174 (*cis*-, Stephenson & Malanowski 1987)175–176 (*trans*-, Stephenson & Malanowski 1987)167.5 (*cis*-, Lide 2003)178.3 (*trans*-, Lide 2003)Density (g/cm^3):0.9088 ($20^{\circ}C$, *cis*-, Lide 2003)0.9023 ($25^{\circ}C$, *trans*-, Lide 2003)Molar Volume (cm^3/mol):129.7 (*cis*-, Stephenson & Malanowski 1987)131.0 (*trans*-, Stephenson & Malanowski 1987)

155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):133.3* ($17.5^{\circ}C$, summary of literature data, measured range 32.1 – $112^{\circ}C$, temp range 17.5 – $179^{\circ}C$, Stull 1947)

267 (calculated by formula, Dreisbach 1955)

 $\log(P/mmHg) = 6.92339 - 1499.80/(201.0 + t/^{\circ}C)$; temp range 75 – $200^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955) $\log(P/mmHg) = [-0.2185 \times 10701.3/(T/K)] + 8.071487$; temp range 17.5 – $179^{\circ}C$ (Antoine eq., Weast 1972–73) $\log(P/mmHg) = 6.92339 - 1499.80/(201.0 + t/^{\circ}C)$; temp range not specified (Antoine eq., Dean 1985, 1992) $\log(P_L/kPa) = 6.04829 - 1499.8/(-72.15 + T/K)$; temp range 348 – 498 K (*cis*-, liquid, Antoine eq., Stephenson & Malanowski 1987) $\log(P_L/kPa) = 6.58873 - 1915.94/(-33.996 + T/K)$; temp range 291 – 452 K (*trans*-, liquid, Antoine eq., Stephenson & Malanowski 1987)Henry's Law Constant ($Pa \cdot m^3/mol$):Octanol/Water Partition Coefficient, $\log K_{OW}$:Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$ or $\log K_B$:Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Photooxidation: rate constant $k = (59 \pm 6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at $298 \pm 2 \text{ K}$ (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

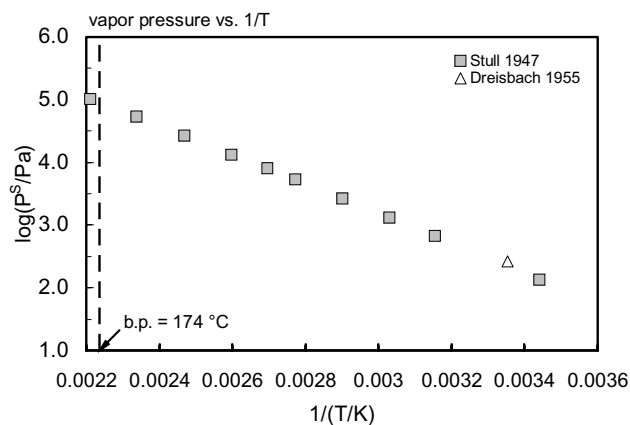
TABLE 3.1.1.37.1

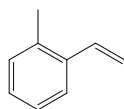
Reported vapor pressures of β -methylstyrene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947**summary of literature data**

$t/^{\circ}\text{C}$	P/Pa
17.5	133.3
43.8	666.6
57	1333
71.5	2666
87.7	5333
97.8	7999
111.7	13332
132	26664
154.7	53329
179.0	101325
mp/ $^{\circ}\text{C}$	-30.1

**FIGURE 3.1.1.37.1** Logarithm of vapor pressure versus reciprocal temperature for β -methylstyrene.

3.1.1.38 *o*-Methylstyrene

Common Name: *o*-Methylstyrene

Synonym: 2-methylstyrene, 2-vinyl toluene, *o*-methylvinylbenzene

Chemical Name: 2-methylstyrene

CAS Registry No: 611-15-4

Molecular Formula: C₉H₁₀, 2-CH₃C₆H₄CH=CH₂

Molecular Weight: 118.175

Melting Point (°C):

−68.5 (Lide 2003)

Boiling Point (°C):

169.8 (Lide 2003)

Density (g/cm³):

0.9106 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):

129.8 (20°C, calculated-density)

155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

387* (32.1°C, differential manometer, measured range 32.1–112°C, Clements et al. 1953)

log (P/mmHg) = 7.15212 – 1628.405/(211.386 + t/°C); temp range 32.1–112°C (Antoine eq. from differential manometer measurements, Clements et al. 1953)

240.8 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 7.09235 – 1582.7/(206.0 + t/°C); temp range 75–200°C (Antoine eq. for liquid state, Dreisbach 1955)

298.9 (extrapolated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 7.21287 – 1644.083/(214.585 + t/°C); temp range 32–112.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

log (P/atm) = (1 – 443.504/(T/K) × 10⁴[0.890379 – 7.17666 × 10⁴·(T/K) + 5.97058 × 10⁷·(T/K)²]; temp range 305.16–385.5 K (Cox vapor pressure eq., Chao et al. 1983)

246.4 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.33107 – 1660.041/(214.219 + t/°C); temp range 32–112.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 7.2129 – 1644.08/(214.59 + t/°C); temp range 32–112°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.88461 – 1485.41/(200.0 + t/°C); temp range 75–255°C (Antoine eq., Dean 1985, 1992)

log (P_L/kPa) = 6.27762 – 1628.405/(−61.764 + T/K); temp range 305–385 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 36.8413 – 3.7269 × 10³/(T/K) – 9.7997·log (T/K) + 1.4115 × 10^{−10}·(T/K) + 1.9658 × 10^{−6}·(T/K)², temp range 205–659 K (Yaws 1994)

Henry's Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.38.1
Reported vapor pressures of *o*-methylstyrene at various temperatures

Clements et al. 1953	
differential manometer	
$t/^{\circ}\text{C}$	P/Pa
32.01	387
40.85	663
58.51	1753
58.54	1765
70.2	3113
82.8	5529
82.83	5534
100.35	11310
112.35	17698
mp/ $^{\circ}\text{C}$	-68.57
bp/ $^{\circ}\text{C}$	169.8
$\Delta H_v = 35.54 \text{ kJ/mol}$	
$\log P = A - B/(C + t/^{\circ}\text{C})$	
eq. 2	mmHg
A	7.15272
B	1628.405
C	211.386

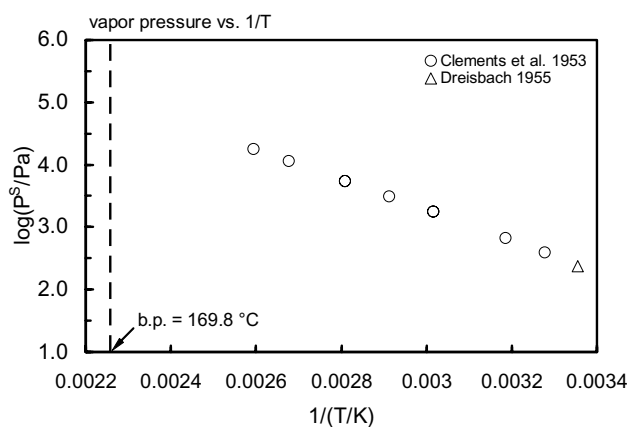
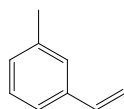


FIGURE 3.1.1.38.1 Logarithm of vapor pressure versus reciprocal temperature for *o*-methylstyrene.

3.1.1.39 *m*-Methylstyrene

Common Name: *m*-Methylstyrene

Synonym: methylvinylbenzene, 3-vinyl toluene, *m*-methylvinylbenzene

Chemical Name: 3-methylstyrene

CAS Registry No: 100-42-1

Molecular Formula: C₉H₁₀, 3-CH₃C₆H₄CH=CH₂

Molecular Weight: 118.175

Melting Point (°C):

−86.3 (Lide 2003)

Boiling Point (°C):

164 (Lide 2003)

Density (g/cm³ at 20°C):

0.9028 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):

130.9 ((20°C, calculated-density)

155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

89.0 (*m*- and *p*-methylstyrene commercial product, Dreisbach 1955)

89.0, 100 (quoted, *m*- and *p*-methylstyrene, calculated-group contribution, Irmann 1965)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2693* (67.6°C, mercury manometer, measured range 67.6–169.1°C, Buck et al. 1949)

log (P/mmHg) = −3563/(T/K) − 7.553·log (T/K) + 30.90; temp range 80–120°C (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)

687* (41.48°C, differential manometer, Clements et al. 1953)

log (P/mmHg) = 6.95079 − 1520.412/(210.967 + t/°C); temp range 41.48–111.8°C (Antoine eq. from differential manometer measurements, measured range 41.48–111.8°C, Clements et al. 1953)

257 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.99468 − 1553.4/(206.0 + t/°C); temp range 75–225°C (Antoine eq. for liquid state, Dreisbach 1955)

228, 244 (extrapolated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 7.06423 − 1564.74/(204.083 + t/°C); temp range 67.6–169°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

log (P/mmHg) = 7.11224 − 1615.091/(210.809 + t/°C); temp range 41.7–111.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

log (P/atm) = (1 − 442.985/T) × 10⁴/(0.885861 − 7.19653 × 10⁴·T + 6.75359 × 10⁷·T²); T in K, temp range 314.93–442.15 K (Cox vapor pressure eq., Chao et al. 1983)

227, 244 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.17253 − 1553.744/(202.922 + t/°C); temp range 67.6–169.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.22823 − 1609.825/(210.331 + t/°C); temp range 41.7–111.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 7.27534 − 1695.4/(220.0 + t/°C); temp range 10–72°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.87928 − 1471.28/(200.0 + t/°C); temp range 72–250°C (Antoine eq., Dean 1985, 1992)

245 (Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.07569 - 1520.412/(-71.183 + T/\text{K})$; temp range 314–385 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 11.6959 - 2.9912 \times 10^3/(T/\text{K}) + 0.33334 \cdot \log (T/\text{K}) - 8.8935 \times 10^{-3} \cdot (T/\text{K}) + 4.9793 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 187–657 K (Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

387 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.35 (Leo et al. 1971)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.50 (gold fish, flow-through method, Ogata et al. 1984)

1.50, 1.63 (gold fish, quoted, calculated-MCI χ , Ogata et al. 1984)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 3.1.1.39.1

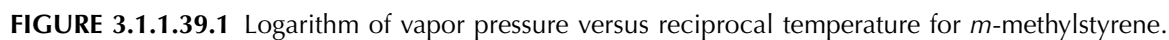
Reported vapor pressures of *m*-methylstyrene at various temperatures and the coefficients for the vapor pressure equations

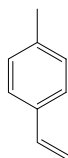
$\log P = A - B/(T/\text{K})$	(1)	$\ln P = A - B/(T/\text{K})$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/\text{K})$	(3)		
$\log P = A - B/(T/\text{K}) - C \cdot \log (T/\text{K})$	(4)		

Buck et al. 1949

Clements et al. 1953

Hg manometer				differential manometer			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
67.6	2693	eq. 4 t/°C	P/mmHg	41.48	687	99.33	10696
72.3	3440	A	30.9	43.22	744	111.8	17020
80.7	4933	B	3563	49.49	1104		
87	6533	C	7.553	52.12	1261	mp/°C	−86.34
93.8	8373			55.73	1499	bp/°C	171.6
96.6	9733			57.8	1673		
106.9	14399			65.2	2445	$\Delta H_v = 38.79 \text{ kJ/mol}$	
121	12998			70.95	3192		
128.3	30398			71.01	3202	eq. 2	mmHg
138.5	41597			71.02	3204	A	6.95079
147.6	54795			71.1	3248	B	1520.412
159.2	75727			77.12	4234	C	201.967
169.1	98392						



3.1.1.40 *p*-Methylstyrene

Common Name: *p*-Methylstyrene

Synonym: methylvinylbenzene, 4-vinyl toluene, *p*-methylvinylbenzene

Chemical Name: 4-methylstyrene

CAS Registry No: 622-97-9

Molecular Formula: C_9H_{10} , $4-CH_3C_6H_4CH=CH_2$

Molecular Weight: 118.17

Melting Point ($^{\circ}C$):

−34.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

172.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9016, 0.9060 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

0.8760 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

129.8 ($20^{\circ}C$, calculated-density)

155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

89.0 (quoted, *m*- and *p*-methylstyrene commercial product, Dreisbach 1955)

89.0, 100 (quoted, *m*- and *p*-methylstyrene, calculated-group contribution, Irrmann 1965)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($16^{\circ}C$, summary of literature data, temp range 16 – $175^{\circ}C$, Stull 1947)

2773* ($68.6^{\circ}C$, mercury manometer, measured range 68.6 – $170^{\circ}C$, Buck et al. 1949)

$\log(P/mmHg) = -3476/(T/K) - 6.923 \cdot \log(T/K) + 29.03$; temp range 80 – $120^{\circ}C$ (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)

$\log(P/mmHg) = 7.34046 - 1791.0/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

4954* ($90.98^{\circ}C$, ebulliometry, measured range 90.98 – $171.06^{\circ}C$, Dreisbach & Shrader 1949)

376* ($31.82^{\circ}C$, differential manometer, measured range 31.8 – $96.9^{\circ}C$, Clements et al. 1953)

$\log(P/mmHg) = 7.0483 - 1594.747/(209.889 + t/^{\circ}C)$; temp range 31.8 – $96.9^{\circ}C$ (Antoine eq. from differential manometer measurements, Clements et al. 1953)

241.5 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.35420 - 1765.6/(223.8 + t/^{\circ}C)$; temp range 75 – $205^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 10724.2/(T/K)] + 8.130903$; temp range 16.0 – $175^{\circ}C$ (Antoine eq., Weast 1972–73)

216.6, 241 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log(P/mmHg) = 7.01119 - 1535.073/(200.732 + t/^{\circ}C)$; temp range 68.6 – $170^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log(P/mmHg) = 6.11531 - 1591.082/(209.441 + t/^{\circ}C)$; temp range 31.8 – $96.93^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log(P/atm) = (1 - 443.748/(T/K)) \times 10^4 [0.875061 - 7.08160 \times 10^{-4} \cdot (T/K) + 7.33467 \times 10^{-7} \cdot (T/K)^2]$; temp range: 289.15 – $443.15\ K$, (Cox vapor pressure eq., Chao et al. 1983)

215, 241 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.11531 - 1521.514/(199.299 + t/^{\circ}\text{C})$; temp range 68.6–170°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.16144 - 1586.596/(209.046 + t/^{\circ}\text{C})$; temp range 31.8–96.93°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.0112 - 1535.1/(200.7 + t/^{\circ}\text{C})$; temp range 68–170°C (Antoine eq., Dean 1985, 1992)
242 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.1732 - 1594.147/(-63.261 + T/\text{K})$; temp range 304–370 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 50.6506 - 4.0628 \times 10^3/(T/\text{K}) - 15.524 \cdot \log (T/\text{K}) + 5.5381 \times 10^{-3} \cdot (T/\text{K}) - 1.1313 \times 10^{-13} \cdot (T/\text{K})^2$,
temp range 239–665 K (Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

287 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.35 (Leo et al. 1971; quoted, Ogata et al. 1984)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.55 (gold fish, flow-through method, Ogata et al. 1984)

1.55, 1.62 (gold fish, quoted, calculated-MCI χ , Ogata et al. 1984)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

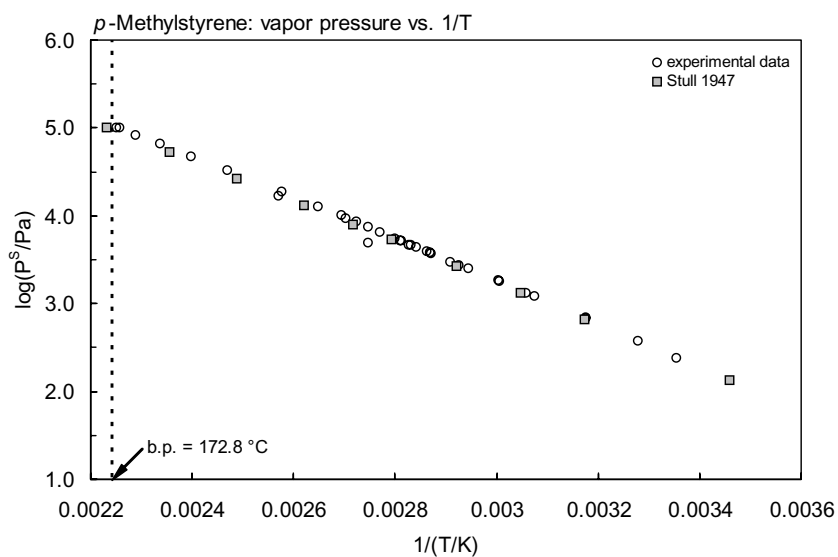
TABLE 3.1.1.40.1

Reported vapor pressures of *p*-methylstyrene at various temperatures and the coefficients for the vapor pressure equations

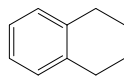
$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}C)$		(2)		$\ln P = A - B/(C + t/^{\circ}C)$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Buck et al. 1949		Dreisbach & Shrader 1949		Clements et al. 1953	
summary of literature data		Hg manometer		ebulliometry		differential manometer	
t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa
16	133.3	68.6	2773	90.98	4954	31.82	376
42	666.6	70.6	2986	98.13	10351	41.76	689
55.1	1333	75.1	3733	116.06	16959	41.83	693
6.2	2666	78.8	4400	171.06	101325	52.17	1207
85	5333	80.6	4720			53.94	1331
95	7999	82.7	5200	mp/^{\circ}C	-70.3	59.56	1797
108.6	13332	84.2	5573	bp/^{\circ}C	171.06	59.91	1855
128.7	26664	87	6559			66.62	2538
151.2	53329	94.1	8559			75.4	3858
175	101325	104.4	12826			76.19	3974
		115.1	18958			80.2	4718

TABLE 3.1.1.40.1 (Continued)

Stull 1947		Buck et al. 1949		Dreisbach & Shrader 1949		Clements et al. 1953	
summary of literature data		Hg manometer		ebulliometry		differential manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
mp/°C	—	131.9	33197			82.44	5208
		144	47996			90.9	7439
		154.7	65728			96.93	9466
		163.7	83193				
		170	99725			mp/°C	−34.15
						bp/°C	172.78
		mp/°C	−37.8			$\Delta H_v = 38.95$ kJ/mol	
		eq. 4	P/mmHg			eq. 2	P/mmHg
		A	29.03			A	7.0483
		B	3476			B	1594.747
		C	6.923			C	209.889

FIGURE 3.1.1.40.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-methylstyrene.

3.1.1.41 Tetralin



Common Name: Tetralin

Synonym: naphthalene-1,2,3,4-tetrahydride

Chemical Name: 1,2,3,4-tetrahydronaphthalene

CAS Registry No: 119-64-2

Molecular Formula: $C_{10}H_{12}$

Molecular Weight: 132.202

Melting Point ($^{\circ}C$):

−35.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

207.6 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9702 ($20^{\circ}C$, Weast 1982–83; Dean 1985)

0.9695, 0.9660 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

136.4 ($20^{\circ}C$, calculated- density)

177.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.477 (Riddick et al. 1986)

12.45 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

52.44, 49.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

14.94 (calculated-QSAR Data base, Passino & Smith 1987)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2666* ($93.8^{\circ}C$, temp range 93.8 – $171.06^{\circ}C$, Herz & Schuftan 1922)

53.3* (mercury manometer, measured range -2.4 – $65^{\circ}C$, Linder 1931)

66.66* ($39.3^{\circ}C$, ebulliometry, measured range 39.3 – $148.6^{\circ}C$, Gardner & Brewer 1937)

133.3* ($38^{\circ}C$, summary of literature data, temp range 38 – $207^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11613.0/(T/K)] + 8.194951$; temp range 38 – $207.2^{\circ}C$ (Antoine eq., Weast 1972–73)

1737* ($82.3^{\circ}C$, diaphragm gauge, measured range 82.3 – $276.21^{\circ}C$, Nasir et al. 1980)

$\log(P/mmHg) = [1 - 480.364/(T/K)] \times 10^{0.85916 - 5.75417 \times 10^{-4} \cdot (T/K) + 4.41971 \times 10^{-7} \cdot (T/K)^2}$; temp range 311.15 – $710.93 K$, (Cox eq., Chao et al. 1983)

53.75 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.07055 - 1741.30/(208.26 + t/^{\circ}C)$; temp range 94 – $206^{\circ}C$ (Antoine eq., Dean 1985, 1992)

53.0 (selected lit. average, Riddick et al. 1986)

$\log(P/kPa) = 11.079 - 2797.90/(T/K) + 1.187 \cdot \log(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

56.7 (Antoine eq., extrapolated, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.35719 - 1854.82/(-54.237 + T/K)$; temp range 311 – $481 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 39.9174 - 4.132 \times 10^3/(T/K) - 10.78 \cdot \log(T/K) + 1.9691 \times 10^{-10} \cdot (T/K) + 2.0405 \times 10^{-6} \cdot (T/K)^2$, temp range 237 – $720 K$ (Yaws 1994)

38.35* ($20.26^{\circ}C$, static method, measured range 253.8 – $442.8 K$, Mokbel et al. 1998)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

76.0, 106.4, 137.8, 189.5, 271.6 (0, 15, 20, 25, 30°C , EPICS-GC, Ashworth et al. 1988)

$\ln [H/(\text{atm m}^3 \text{mol}^{-1})] = 11.83 - 5392/(T/K)$; temp range $10\text{--}30^\circ\text{C}$ (EPICS-GC, Ashworth et al. 1988)

142.8 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 6.332 - 2215/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.83 (calculated-fragment const., Rekker 1977)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (3.43 \pm 0.06) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = (8.6 \pm 1.3) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate method, Atkinson & Aschmann 1988)

$k_{\text{OH}} = 3.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1990)

$k_{\text{OH}}(\text{calc}) = 11.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{exptl}) = 34.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 3.1.1.41.1

Reported vapor pressures of tetralin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}C)$		(2)		$\ln P = A - B/(C + t/^{\circ}C)$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Herz & Schuftan 1922		Stull 1947		Gardner & Brewer 1937		Mokbel et al. 1998	
		summary of literature data		ebulliometry		static method	
t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	T/K	P/Pa
93.8	2666	38	133	39.3	66.66	253.8	1.279
103	4000	65.3	666.6	40.1	79.99	264.01	3.349
140	15732	79	1333	40.8	93.33	273.65	7.984
150	21598	93.8	2666	41.8	93.33	283.54	17.94
167.5	36397	110	5333	46.6	226.7	293.51	38.35
206.2	98658	121.3	7999	48.9	253.3	303.52	78.52
		135.3	13332	49.4	253.3	313.51	153.0
		157.2	26664	54	293.3	323.55	284.0
Linder 1931		181.8	53329	74.4	946.6	333.57	506.0
mercury manometer		207.2	101325	75.1	959.9	343.62	868.0
t/^{\circ}C	P/Pa			101.1	3040	353.66	1443
		mp/^{\circ}C	-31.0	126.6	9040	358.64	1801
-2.4	2			148.6	19625	363.62	2254
-1.2	3.133					373.66	3508
25	53.33			bp/^{\circ}C	210.5	383.00	5179
65	110.7					392.95	7617
						402.89	10948
				Nasir et al. 1980		412.86	15444
				diaphragm gauge		422.82	21388
				t/^{\circ}C	P/Pa	432.84	29254
						442.80	39128
				82.3	1737		
				125.81	10500		
				150.15	22419		
				200.11	84002		
				250.66	257307		
				276.21	348091		
						data fitted to Wagner eq.	

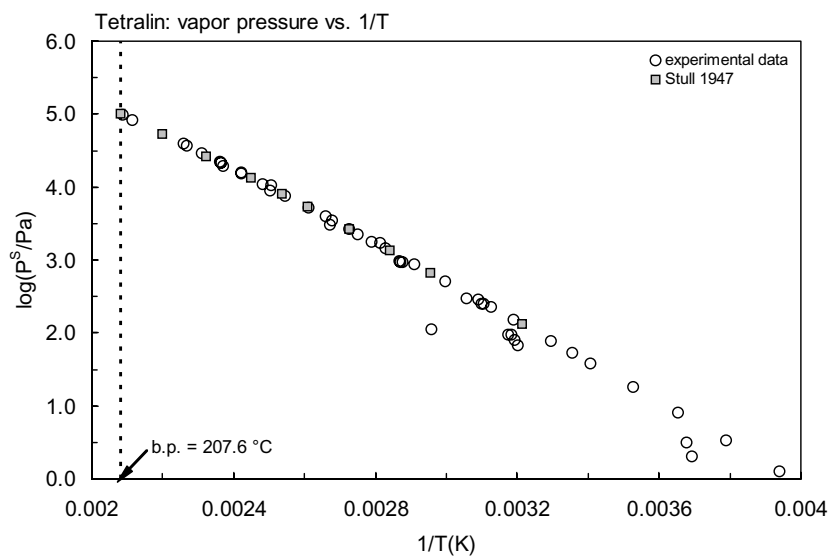


FIGURE 3.1.1.41.1 Logarithm of vapor pressure versus reciprocal temperature for tetralin.

3.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 3.2.1
Summary of the physical properties of mononuclear aromatic hydrocarbons

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	mp °C	bp °C	Fugacity ratio, F at 25 °C*	Density, ρ g/cm ³ at 20°C	Molar volume, V_M cm ³ /mol	
								MW/p at 20°C	Le Bas
Benzene	71-43-2	C ₆ H ₆	78.112	5.49	80.09	1	0.8765	89.12	96.0
Toluene	108-88-3	C ₇ H ₈	92.139	-94.95	110.63	1	0.8668	106.30	118.2
Ethylbenzene	100-41-4	C ₈ H ₁₀	106.165	-94.96	136.19	1	0.867	122.45	140.4
<i>o</i> -Xylene	95-47-6	C ₈ H ₁₀	106.165	-25.2	144.5	1	0.8802	120.61	140.4
<i>m</i> -Xylene	108-38-3	C ₈ H ₁₀	106.165	-47.8	139.12	1	0.8842	120.07	140.4
<i>p</i> -Xylene	106-42-3	C ₈ H ₁₀	106.165	13.25	138.37	1	0.8611	123.29	140.4
1,2,3-Trimethylbenzene	526-73-8	C ₉ H ₁₂	120.191	-25.4	176.12	1	0.8944	134.38	162.6
1,2,4-Trimethylbenzene	95-63-6	C ₉ H ₁₂	120.191	-43.77	169.38	1	0.8758	137.24	162.6
1,3,5-Trimethylbenzene	108-67-8	C ₉ H ₁₂	120.191	-44.72	164.74	1	0.8800	136.58	162.6
<i>n</i> -Propylbenzene	103-65-1	C ₉ H ₁₂	120.191	-99.6	159.24	1	0.862	139.43	162.6
Isopropylbenzene	98-82-8	C ₉ H ₁₂	120.191	-96.02	152.41	1	0.8618	139.47	162.6
1-Ethyl-2-methylbenzene (<i>o</i> -Ethyltoluene)	611-14-3	C ₉ H ₁₂	120.191	-79.83	165.2	1	0.8807	136.47	162.6
1-Ethyl-3-methylbenzene (<i>m</i> -Ethyltoluene)	620-14-4	C ₉ H ₁₂	120.191	-95.6	161.3	1	0.8645	139.03	162.6
1-Ethyl-4-methylbenzene (<i>p</i> -Ethyltoluene)	622-96-8	C ₉ H ₁₂	120.191	-62.35	162	1	0.8614	139.53	162.6
Isopropyl-4-methylbenzene (<i>p</i> -Cymene)	99-87-6	C ₁₀ H ₁₄	134.218	-67.94	177.1	1	0.8573	156.56	184.8
<i>n</i> -Butylbenzene	104-51-8	C ₁₀ H ₁₄	134.218	-87.85	183.31	1	0.8601	156.05	184.8
Isobutylbenzene	538-93-2	C ₁₀ H ₁₄	134.218	-51.4	172.79	1	0.8532	157.31	184.8
<i>sec</i> -Butylbenzene	135-98-8	C ₁₀ H ₁₄	134.218	-82.7	173.3	1	0.8621	155.69	184.4
<i>tert</i> -Butylbenzene	98-06-6	C ₁₀ H ₁₄	134.218	-57.8	169.1	1	0.8665	154.90	184.8
1,2,3,4-Tetramethylbenzene	488-23-3	C ₁₀ H ₁₄	134.218	-6.2	205	1	0.9052	148.27	184.8
1,2,3,5-Tetramethylbenzene	527-53-7	C ₁₀ H ₁₄	134.218	-23.7	198	1	0.8903	150.76	184.8
1,2,4,5-Tetramethylbenzene	95-93-2	C ₁₀ H ₁₄	134.218	79.3	196.8	0.293	0.8380	160.16	184.8
<i>n</i> -Pentylbenzene	538-68-1	C ₁₁ H ₁₆	148.245	-75	205.4	1	0.8585	172.68	207.0

Pentamethylbenzene	700-12-9	C ₁₁ H ₁₆	148.245	54.5	232	0.514	0.917	161.66	207.0
<i>n</i> -Hexylbenzene	1077-16-3	C ₁₂ H ₁₈	162.271	-61	226.1	1	0.8613	188.40	229.2
Hexamethylbenzene	87-85-4	C ₁₂ H ₁₈	162.271	165.5	263.4	0.0418	1.063	152.65#	229.2
Heptylbenzene	1078-71-3	C ₁₃ H ₂₀	176.298	-48	240	1	0.8567	205.79	251.4
Octylbenzene	2189-60-8	C ₁₄ H ₂₂	190.325	-36	264	1	0.8562	222.29	273.6
Nonylbenzene	1081-77-2	C ₁₅ H ₂₄	204.352	-24	280.5	1	0.8584	238.06	295.8
Decylbenzene	104-72-3	C ₁₆ H ₂₆	218.377	-14.4	293	1	0.8555	255.26	318.0
Undecylbenzene	6742-54-7	C ₁₇ H ₂₈	232.404	-5	316	1	0.8553	271.72	340.2
Dodecylbenzene	123-01-3	C ₁₈ H ₃₀	246.431	3	328	1	0.8551	288.19	362.4
Tridecylbenzene	123-02-4	C ₁₉ H ₃₂	260.457	10	346	1	0.8550	304.63	384.6
Tetradecylbenzene	1459-10-5	C ₂₀ H ₃₄	274.484	16	359	1	0.8549	321.07	406.8
Styrene	100-42-5	C ₈ H ₈	104.150	-30.65	145	1	0.9060	114.96	133.0
<i>o</i> -Methylstyrene	611-15-4	C ₉ H ₁₀	118.175	-68.5	169.8	1	0.9106	129.78	155.2
<i>m</i> -Methylstyrene	100-80-1	C ₉ H ₁₀	118.175	-86.3	164	1	0.9028	130.90	155.2
<i>p</i> -Methylstyrene	622-97-9	C ₉ H ₁₀	118.175	-34.1	172.8	1	0.9016	131.07	155.2
α -Methylstyrene	98-83-9	C ₉ H ₁₀	118.175	-23.2	165.4	1	0.9106	129.78	155.2
β -Methylstyrene, <i>cis</i> -	766-90-5	C ₉ H ₁₀	118.175	-61.6	167.5	1	0.9088	130.03	155.2
β -Methylstyrene, <i>trans</i> -	873-66-5	C ₉ H ₁₀	118.175	-29.3	178.3	1	0.9023	130.97#	155.2
Tetralin	119-64-2	C ₁₀ H ₁₂	132.202	-35.7	207.6	1	0.9695	136.36	177.4

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

at 25°C.

TABLE 3.2.2
Summary of selected physical-chemical properties of mononuclear aromatic hydrocarbons at 25°C

Compound	Selected properties:						Henry's law constant
	Vapor pressure		Aqueous solubility			log K _{OW}	H/(Pa·m ³ /mol) calculated P/C
	P ^s /Pa	P _L /Pa	S/(g/m ³)	C ^s /(mol/m ³)	C _L /(mol/m ³)		
Benzene	12700	12700	1780	22.788	22.788	2.13	557
Toluene	3800	3800	515	5.590	5.590	2.69	680
Ethylbenzene	1270	1270	152	1.431	1.431	3.13	887
<i>o</i> -Xylene	1170	1170	220	2.072	2.072	3.15	565
<i>m</i> -Xylene	1100	1100	160	1.507	1.507	3.20	730
<i>p</i> -Xylene	1170	1170	215	2.024	2.024	3.18	578
1,2,3-Trimethylbenzene	200	200	70	0.582	0.582	3.55	343
1,2,4-Trimethylbenzene	270	270	57	0.474	0.474	3.60	569
1,3,5-Trimethylbenzene	325	325	50	0.416	0.416	3.58	781
<i>n</i> -Propylbenzene	450	450	52	0.433	0.433	3.69	1040
Isopropylbenzene	610	610	50	0.416	0.416	3.63	1466
1-Ethyl-2-methylbenzene	330	330	75	0.624	0.624	3.63	529
1-Ethyl-3-methylbenzene	391	391					
1-Ethyl-4-methylbenzene	395	395	95	0.790	0.790	3.63	500
Isopropyl-4-methylbenzene	204	204	34	0.253	0.253	4.10	805
<i>n</i> -Butylbenzene	137	137	13.8	0.103	0.103	4.26	1332
Isobutylbenzene	250	250	10.1	0.075	0.075	4.01	3322
<i>sec</i> -Butylbenzene	240	240	17	0.127	0.127		1890
<i>tert</i> -Butylbenzene	286	286	30	0.224	0.224	4.11	1280
1,2,3,4-Tetramethylbenzene	45	45				3.90	
1,2,3,5-Tetramethylbenzene	62	62				4.04	
1,2,4,5-Tetramethylbenzene	66	66	3.48	0.026	0.026	4.10	2546
<i>n</i> -Pentylbenzene	44	44	3.85	0.026	0.026	4.90	1694
Pentamethylbenzene	9.52	18.63	15.5	0.105	0.205		
<i>n</i> -Hexylbenzene	13.61	13.61	1.02	0.006	0.006	5.52	2165
Hexamethylbenzene	0.155	3.90	0.235	0.001	0.036	4.61	
Heptylbenzene	3.95	3.95				5.37	
Octylbenzene	2.03	2.03				6.30	
Nonylbenzene	0.30	0.30				6.82	
Decylbenzene	0.077	0.077				7.37	

Undecylbenzene	0.045	0.045				8.14
Dodecylbenzene	0.017	0.017				8.65
Tridecylbenzene	0.00070	0.0007				9.36
Tetradecylbenzene	0.000113	0.000113				9.95
Styrene	880	880	250	2.40	2.40	2.95
<i>o</i> -Methylstyrene	245	245				
<i>m</i> -Methylstyrene	250	250				3.35
<i>p</i> -Methylstyrene	242	242				3.35
α -Methylstyrene	324	324				3.48
β -Methylstyrene, <i>cis</i> -	258	258				3.35
β -Methylstyrene, <i>trans</i> -	216.6	216.6				
Tetralin	54	54				3.83

TABLE 3.2.3

Suggested half-life classes of mononuclear aromatic hydrocarbons in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Benzene	3	4	5	6
Toluene	2	5	6	7
Ethyl benzene	2	5	6	7
<i>o</i> -Xylene	2	5	6	7
<i>m</i> -Xylene	2	5	6	7
<i>p</i> -Xylene	2	5	6	7
1,2,3-Trimethylbenzene	2	5	6	7
1,2,4-Trimethylbenzene	2	5	6	7
1,3,5-Trimethylbenzene	2	5	6	7
<i>n</i> -Propylbenzene	2	5	6	7
Isopropylbenzene	2	5	6	7
1-Isopropyl-4-methylbenzene (<i>p</i> -Cymene)	2	5	6	7
1,2,4,5-Tetramethylbenzene	2	5	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

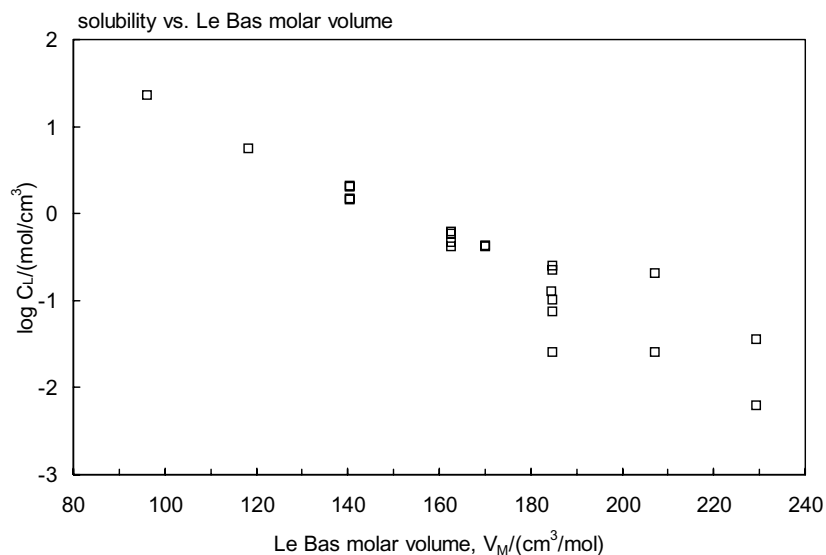


FIGURE 3.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.

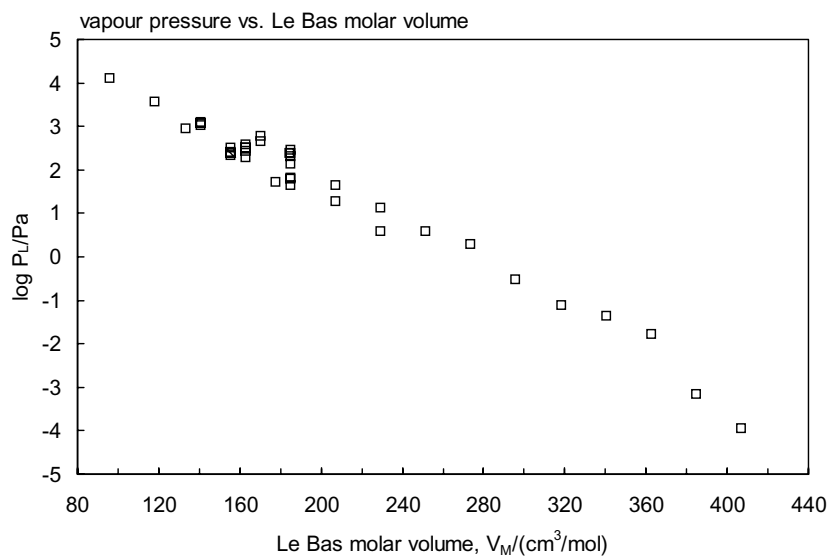


FIGURE 3.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.

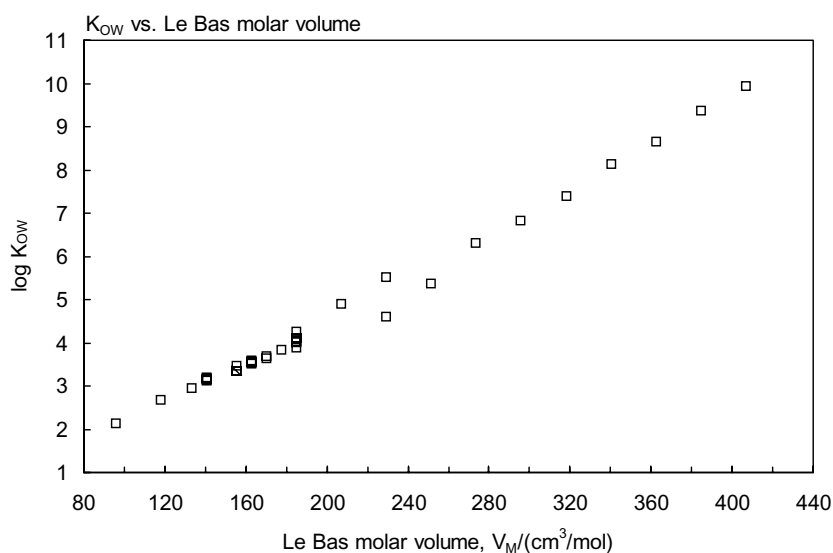


FIGURE 3.2.3 Octanol-water partition coefficient versus Le Bas molar volume for mononuclear aromatic hydrocarbons.

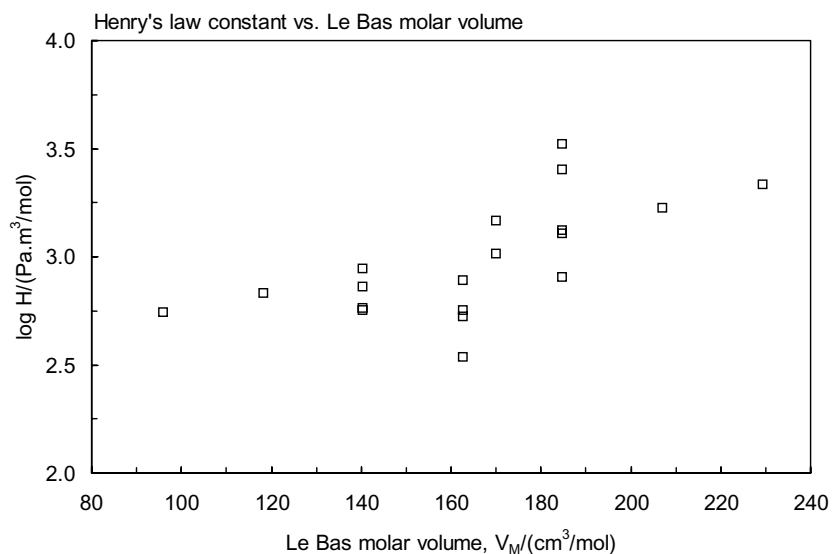


FIGURE 3.2.4 Henry's law constant versus Le Bas molar volume for mononuclear aromatic hydrocarbons.

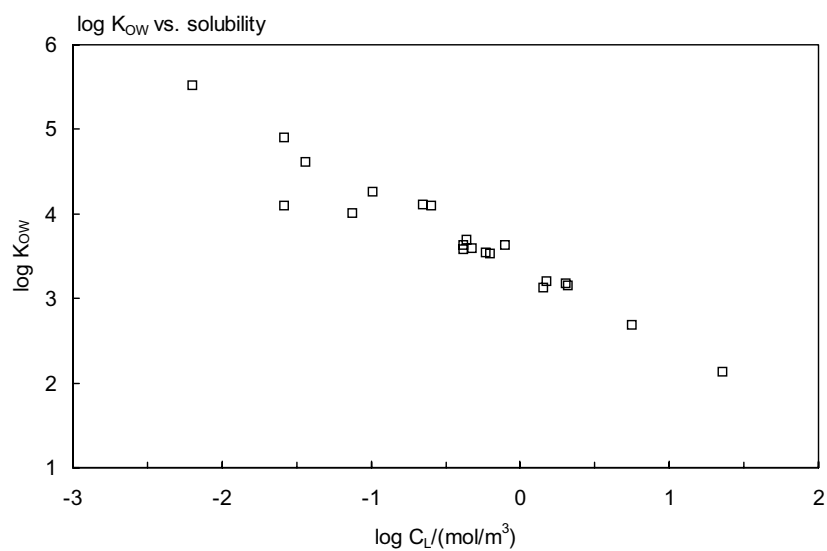


FIGURE 3.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for mononuclear aromatic hydrocarbons.

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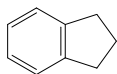
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4.1. LIST OF CHEMICALS AND DATA COMPILATIONS

4.1.1 POLYNUCLEAR AROMATIC HYDROCARBONS (PAHs)

4.1.1.1 Indan



Common Name: Indan

Synonym: hydroindene, 2,3-dihydroindene, 2,3-dihydro-1H-indene, indane

Chemical Name: indan

CAS Registry No: 496-11-7

Molecular Formula: C₉H₁₀

Molecular Weight: 118.175

Melting Point (°C):

−51.38 (Lide 2003)

Boiling Point (°C):

177.97 (Lide 2003)

Density (g/cm³ at 20°C):

0.9639 (Weast 1982–83; Dean 1985; Lide 2003)

Molar Volume (cm³/mol):

123.0 (20°C, calculated-density)

143.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, ΔH_v (kJ/mol):

49 ± 1.5 (Ambrose & Sprake 1976)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.60 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

38.77, 45.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

88.9 (shake flask-GC, Price 1976)

109.1 (shake flask-fluorescence, Mackay & Shiu 1977)

100 (recommended-IUPAC, Shaw 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

5523* (91.68°C, ebulliometry, measured range 91.68–129.05°C, Stull et al. 1961)

204.0* (comparative ebulliometry, extrapolated from vapor pressure equation derived from exptl data, Ambrose & Sprake 1976)

$\log (P/\text{kPa}) = 6.10462 - 1574.160/[(T/\text{K}) - 67.079]$; temp range 355.006–482.437 K (vapor pressure eq., ebulliometry, Ambrose & Sprake 1976)

9585* (101.124°C, comparative ebulliometry, measured range 101.124–192.408°C, Osborn & Scott 1978)

$\log (P/\text{atm}) = [1 - 451.051/(T/\text{K})] \times 10^4 \{0.859420 - 6.08324 \times 10^{-4} \cdot (T/\text{K}) + 4.77502 \times 10^{-7} \cdot (T/\text{K})^2\}$; temp range 355.01–452.24 K (Cox eq., Chao et al. 1983)

195.6 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.1012 - 1571.723/(205.798 + t/^\circ\text{C})$; temp range 81.86–209.3°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1976, Boublik et al. 1984)

196.9 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.11622 - 1580.315/(-66.49 + T/\text{K})$; temp range 374–466 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.33	(Hansch & Leo 1979)
3.30	(calculated-TSA, Yalkowsky & Valvani 1976)
3.57	(calculated-fragment const., Valvani & Yalkowsky 1980)
3.29	(calculated-solubility, Mackay et al. 1980)
3.31	(calculated-fragment const., Yalkowsky et al. 1983)
3.33	(shake flask, Log P Database, Hansch & Leo 1987)
3.36	(calculated-molar volume, Wang et al. 1991)
3.33	(recommended, Sangster 1993)
3.18	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolysis rate $k < 3 \times 10^{-5} \text{ s}^{-1}$ with $t_{1/2} > 1 \text{ d}$ (Kwok et al. 1997)

Oxidation: rate constant k for gas-phase second-order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated; *data at other temperatures see reference:

$k_{OH} = 9.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1989)

$k_{OH}(\text{exptl}) = (19 \pm 5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 8 h; $k_{NO_3}(\text{exptl}) = (6.6 \pm 2.0) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 7 d; and $k_{O_3}(\text{exptl}) < 3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of $> 55 \text{ d}$ at $297 \pm 2 \text{ K}$ (relative rate method; calculated-SAR structure-activity relationship, Kwok et al. 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photolysis $t_{1/2} > 1 \text{ d}$; calculated tropospheric lifetimes of 8 h, 7 d and $> 55 \text{ d}$ due to reactions with OH radical, NO_3 radical and O_3 , respectively, at room temp. (Kwok et al. 1997)

TABLE 4.1.1.1.1

Reported vapor pressures of indan at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log(T/K)$	(4)		

Stull et al. 1961		Ambrose & Sprake 1976		Osborn & Scott 1978	
ebulliometry		comparative ebulliometry		comparative ebulliometry	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
91.68	5523	81.856	4343	101.124	9585
107.38	12086	88.012	5650	104.381	10887
128.56	25246	93.482	7069	107.849	12339
152.36	51766	98.033	6471	111.229	13955
176.03	96999	101.96	9860	114.621	15748

(Continued)

TABLE 4.1.1.1.1 (Continued)

Stull et al. 1961		Ambrose & Sprake 1976		Osborn & Scott 1978	
ebulliometry		comparative ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
178.04	101729	109.194	12920	118.027	17735
129.05	104442	116.391	16722	121.442	19933
		120.345	19150	128.315	25023
mp/K	221.77	123.556	21300	135.235	31177
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 8.60$		128.597	25174	142.204	38565
Antoine eq.		134.718	30586	149.224	47375
eq. 2	P/mmHg	139.494	35453	156.300	57817
A	7.05483	146.528	43667	263.418	70120
B	1625.70	152.479	51799	170.590	84432
C	211.645	158.969	61998	177.812	101325
		164.763	72392	177.812	101325
		171.453	86085	177.811	101325
		176.521	97757	185.085	120790
		177.075	99114	192.408	143240
		177.531	100222		
		25.0	204.0	$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 39.67$	
				at bp	
		bp/K	451.12 K	$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 49.03$	
				at 298.15 K	
		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 39.8$ at bp			
		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 49.0$			
		at 298.15 K			
		eq. 3	P/kPa		
		A	6.10462		
		B	1574.160		
		C	-67.079		

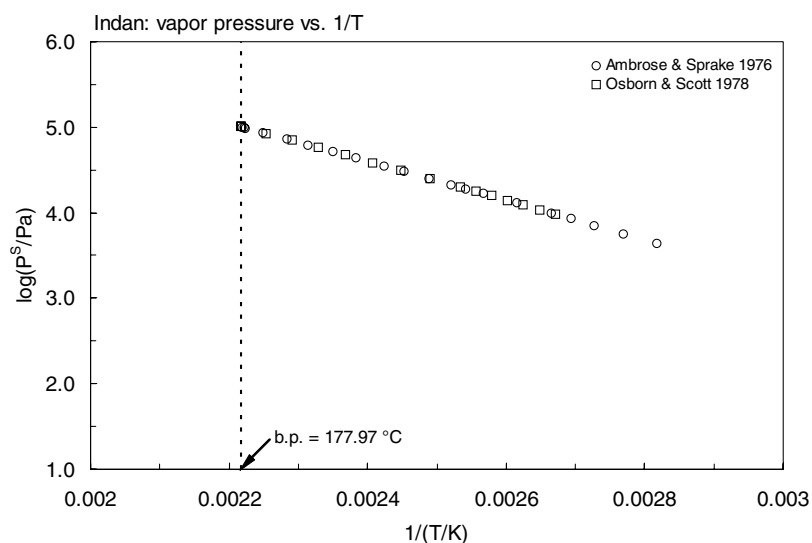
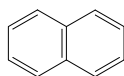


FIGURE 4.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for indan.

4.1.1.2 Naphthalene



Common Name: Naphthalene

Synonym: naphthene, tar camphor, moth balls

Chemical Name: naphthalene

CAS Registry No: 91-20-3

Molecular Formula: $C_{10}H_8$

Molecular Weight: 128.171

Melting Point ($^{\circ}C$):

80.26 (Lide 2003)

Boiling Point ($^{\circ}C$):

217.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0253 (Weast 1983–84)

Molar Volume (cm^3/mol):

125.0 ($20^{\circ}C$, calculated-from density)

133.2 (from density, Bohon & Claussen 1951)

147.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

73.93 (Colomina et al. 1982)

72.92 (Van Ekeren et al. 1983)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.29 (Parks & Huffman 1931)

19.08 (Wauchope & Getzen 1972; Podoll et al. 1989)

19.10 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

54.39 (Casellato et al. 1973)

54.81 (Ubbelohde 1978)

53.75, 44.4 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.287 (mp at $80.26^{\circ}C$)

0.310 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

30.0* (shake flask-gravimetric, measured range 0 – $25^{\circ}C$, Hilpert 1916)

31.5 (shake flask-UV, Andrews & Keefer 1949)

12.5 (shake flask-UV, Klevens 1950)

34.4* (shake flask-UV, measured range 2 – $42^{\circ}C$, Bohon & Claussen 1951)

30.6 (Stephen & Stephen 1963)

20.4 (shake flask, Sahyun 1966)

33.47 (shake flask-GC, Gordon & Thorne 1967)

38.4 ($20^{\circ}C$, shake flask-UV, Eisenbrand & Baumann 1970)

31.2* (shake flask-UV, measured range 29 – $73.4^{\circ}C$, Wauchope & Getzen 1972)

$R \cdot \ln x = -8690/(T/K) + (0.000408)[(T/K) - 291.15]^2 - 13.4 + 0.0139 \cdot (T/K)$; temp range 29.2 – $73.4^{\circ}C$ (shake flask-UV, Wauchope & Getzen 1972)

32.17 (shake flask-UV, Vesala 1974)

31.3 (shake flask-GC, Eganhouse & Calder, 1976)

22.0 (fluorescence, Schwarz & Wasik 1976)

31.7 (shake flask-fluorescence, Mackay & Shiu, 1977)

30.0* ($25^{\circ}C$, shake flask-fluorescence, measured range 8 – $31^{\circ}C$, Schwarz & Wasik 1977)

30.25* ($25^{\circ}C$, shake flask-fluorescence, measured range 8.4 – $31.8^{\circ}C$, Schwarz 1977)

- 31.69 (generator column-HPLC/UV, measured temp range 5–30°C, May et al. 1978)
 $S/(\text{mg/kg}) = 13.66 + 0.2499 \cdot (t/^\circ\text{C}) + 0.0189 \cdot (t/^\circ\text{C})^2$; temp range 5–30°C (generator column-HPLC/UV, May et al. 1978)
- 30.64 (generator column-HPLC/UV, Wasik et al. 1983)
- 31.94* (25°C, generator column-HPLC/UV, measured range 8.2–27°C, May et al. 1983)
 $R \cdot \ln x = -80.55/(\theta/K) + 28.7/[1/(\theta/K) - 1/(T/K)] + 0.31 \cdot \{(\theta/K)/(T/K) - 1 - \ln [(\theta/K)/(T/K)]\}$, $\theta = 298.15 \text{ K}$, temp range 8.2–27°C (generator column-HPLC/UV, May et al. 1983)
- 32.2 (average lit. value, Pearlman et al. 1984)
- 32.90 (generator column-HPLC/fluorescence, Walters & Luthy 1984)
- 30.75* (25.2°C, shake flask-UV, Bennet & Canady 1984)
 $\ln x = -1767.4601/R \cdot (T/K) + (17.95209/R) \cdot \ln (T/K) + 1$; temp range 2–45°C (shake flask-UV, Bennet & Canady 1984)
- 30.6 (shake flask-HPLC/UV, Fu & Luthy 1985)
- 31.12 (vapor saturation-GC, Akiyoshi et al. 1987)
- 31.3, 31.9 (generator column-HPLC/UV, Billington et al. 1988)
- 31* (recommended, IUPAC Solubility Data Series, Shaw 1989)
- 33.71* (shake flask-UV, measured range 5–40°C, Perez-Tejeda et al. 1990)
 $\log [S/(\text{mol/dm}^3)] = -31.24 - 143.5/(T/K) + 4.772 \cdot \ln (T/K)$; temp range 5–40°C (shake flask-UV, Perez-Tejeda et al. 1990)
- 30.6 (generator column-HPLC, Vadas et al. 1991)
- 29.9 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
- 34.8 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
 $\log [S_L/(\text{mol/L})] = 2.992 - 1001/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\ln x = -1.54117 - 3191.9/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- $\log (P/\text{mmHg}) = 7.091 - 3465/(T/K)$; temp range 87–224 (static isotenoscope method, Mortimer & Murphy 1923)
- 8.64* (20°C, effusion, measured range 10–30°C Swan & Mack 1925)
 $\log (P/\text{mmHg}) = 29.820/(T/K) - 200.682 \cdot \log (T/K) + 595.642$; measured temp range 10–30°C (effusion, Swan & Mack 1925)
- $\log (P/\text{mmHg}) = 10.40 - 3429/(T/K)$; temp range 15–33°C (effusion, Zil'berman-Granovskaya 1940)
- 133.3* (52.6°C, summary of literature data, temp range 52.6–217.9°C, Stull 1947)
- 14.26* (manometry-Rodebush gauge, Sears & Hopke 1949)
 $\log (P/\text{mmHg}) = -[108.30/(t/^\circ\text{C} + 27)] + 1.115$; temp range 19–35°C (manometry-Rodebush gauge, Sears & Hopke 1949)
- 10.8* (effusion method, measured range 6.7–20.7°C, Bradley & Cleasby 1953)
 $\log (P/\text{cmHg}) = 10.597 - 3783/(T/K)$; temp range 6.7–20.7°C, (Antoine eq., effusion, Bradley & Cleasby 1953)
- 6815* (126.325°C, manometry, measured range 126.325–218.638°C, Camin & Rossini 1955)
 $\log (P/\text{mmHg}) = 6.84577 - 1606.529/(187.227 + t/^\circ\text{C})$; temp range 126.3–218.6°C (Antoine eq. Camin & Rossini 1955)
- $\log (P/\text{mmHg}) = 10.75 - 3616/(T/K)$; temp range –20 to 10°C (Knudsen effusion method, Hoyer & Peperle 1958)
- 0.1188* (–13°C, Knudsen effusion, measured range –43 to –13°C, Miller 1963)
- 46.66* (40.33°C, Hg manometer, measured range 40.33–80.34°C, Fowler et al. 1968)
- 10.98, 32.95 (manometry, extrapolated solid, supercooled liquid P_L , Fowler et al. 1968)
 $\log (P_S/\text{mmHg}) = 9.58102 - 2692.92/(t/^\circ\text{C} + 220.651)$; temp range 40–80°C (Antoine eq., mercury manometer, Fowler et al. 1968)
- $\log (P_L/\text{mmHg}) = 7.03382 - 1756.91/(t/^\circ\text{C} + 204.931)$; temp range 81–180°C (Antoine eq., mercury manometer, Fowler et al. 1968)
- 30.66* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
 $\log (P/\text{mmHg}) = 7.01065 - 1733.71/(201.859 + t/^\circ\text{C})$; temp range 86.581–250.27°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 11.60 (interpolated-Antoine eq., Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 17065.2/(T/K)] + 11.450$; temp range 0–80.0°C (Antoine eq., Weast 1972–73)
- $\log (P/\text{mmHg}) = [-0.2185 \times 12311.6/(T/K)] + 8.413089$; temp range 52.6–217.9°C (Antoine eq., Weast 1972–73)
- 12.26* (Knudsen effusion method, extrapolated from measured data, Radchenko & Kitiagorodskii 1974)

- log (P/mmHg) = 11.7041 – 3796.574/(T/K); temp range 9.0–23.91°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)
- 10.93* (gas saturation, Sinke 1974)
- 11.21* (Baratron model diaphragm pressure gauge, Ambrose et al. 1975)
- T·log (P/Pa) = $\frac{1}{2}a_0 + \sum a_i E_i(x)$; $a_0 = 310.6247$, $a_1 = 791.4937$, $a_2 = -82536$, $a_3 = 0.4043$; temp range: 230–344 K, (Chebyshev polynomial, diaphragm pressure gauge, Ambrose et al. 1975)
- log (P/Pa) 13.70 – 3773/(T/K) (Antoine eq. derived from exptl data of Ambrose et al. 1975, Wania et al. 1994)
- 13.5 (effusion method-pressure gauge, DePablo 1976)
- 10.64* (gas saturation, interpolated-Clapeyron eq., Macknick & Prausnitz 1979)
- log (P/mmHg) = 26.250 – 8575/(T/K); temp range 7.15–31.85°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
- 11.30* (effusion method, de Kruif 1980)
- log (P/Pa) = 14.187 – 3907/(T/K); temp range 253–273 K (torsion effusion, regression, de Kruif 1980)
- log (P/Pa) = 14.053 – 3860/(T/K); temp range 253–273 K (weighing effusion, regression, de Kruif 1980)
- log (P/Pa) = 14.107 – 3886/(T/K); temp range 253–273 K (effusion, mean regression, de Kruif 1980)
- 10.42* (effusion method, de Kruif et al. 1981)
- 11.41* (Knudsen effusion, extrapolated-Antoine eq. from exptl data, Colomina et al. 1982)
- log (P/Pa) = 14.01 – 3861.8/(T/K); temp range 271.46–284.63 K (Antoine eq., Knudsen effusion, Colomina et al. 1982)
- 11.33* (gas saturation-GC, Grayson & Fosbraey 1982)
- ln (P/Pa) = 31.8 – 8753/(T/K); temp range 302–352 K, (Antoine eq., gas saturation, Grayson & Fosbraey 1982)
- log (P/atm) = $[1 - 490.988/(T/K)] \times 10^{\{0.832267 - 4.41855 \times 10^{-4} \cdot (T/K) + 2.89627 \times 10^{-7} \cdot (T/K)^2\}}$; (Cox eq., temp range 340.15–751.65 K, Chao et al. 1983)
- 6.53 (20°C, Mackay et al. 1983)
- 10.4* (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
- log (P/Pa) = 14.299 – 3960.03/(T/K); temp range 10–50°C (Antoine eq., gas saturation, Sonnefeld et al. 1983)
- 1.63* (244.19°C, spinning-rotor gauge, measured range 244.19–255.86 K, Van Ekeren et al. 1983)
- 10.4 (generator column-HPLC, Wasik et al. 1983)
- log (P_L/kPa) = 5.93404 – 1579.278/(184.062 + t/°C); temp range 126.3–218.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- log (P_L/kPa) = 6.1638 – 1760.018/(215.204 + t/°C), temp range 80.3–179.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 22.64, 28.24 (P_{GC} by GC-RT correlation with BP-1 column, Apolane-87 column, Bidleman 1984)
- log (P_L/mmHg) = 7.01065 – 1733.71/(201.86 + t/°C); temp range 86–250°C (Antoine eq., Dean 1985, 1992)
- log (P_L/mmHg) = 6.8181 – 1585.86/(184.82 + t/°C); temp range 125–218°C (Antoine eq., Dean 1985, 1992)
- 10.7* (25.35°C, gas saturation, temp range 24.85–57.75°C, Sato et al. 1986)
- ln (P_S/Pa) = 22.8929 – 4025.35/(T/K – 102.243); temp range 298.5–330.9 K (Antoine eq., gas saturation, Sato et al. 1986)
- 11.27 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
- log (P_S/kPa) = 8.70592 – 2619.91/(–52.499 + T/K); temp range 310–353 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- log (P_S/kPa) = 9.45562 – 3069.145/(–29.892 + T/K); temp range 263–353 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P_S/kPa) = 11.9681 – 4577.47/(30.394 + T/K); temp range not specified (Antoine eq.-III, Stephenson & Malanowski 1987)
- log (P_L/kPa) = 6.19487 – 1782.509/(–65.637 + T/K); temp range 352–500 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- log (P_L/kPa) = 6.14835 – 1751.644/(–68.319 + T/K); temp range 491–565 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- log (P_L/kPa) = 6.53231 – 2162.182/(–12.108 + T/K); temp range 563–665 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
- log (P_L/kPa) = 7.74783 – 4042.567/(227.985 + T/K); temp range 661–750 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
- 11.37* (pressure gauge, interpolated-Antoine eq., measured range –12.15 to 70.16°C, Sasse et al. 1988)
- log (P_S/mmHg) = 10.05263 – 2907.918/(236.459 + t/°C); temp range –12.15 to 70.16°C (Antoine eq., pressure gauge, Sasse et al. 1988)

$\log (P_L/\text{mmHg}) = 2.25180 - 76.496/(-25.09 + t/^\circ\text{C})$; temp range 80.16–90.15°C (Antoine eq., pressure gauge, Sasse et al. 1988)

22.65 (PGC, GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)

41.88, 38.02 (supercooled liquid P_L values converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)

0.7634* (0°C, gas saturation-GC, measured range –30.6 to 0°C, Wania et al. 1994)

$\log (P/\text{Pa}) = 13.93 - 3851/(T/\text{K})$; temp range –30 to 0°C, (Antoine eq., gas saturation, Wania et al. 1994)

24.0 (supercooled liquid P_L , GC-RT correlation, Donovan 1996)

5.58–12.30; 10.4–14.0; 11.2–14.4; 7.71–17.2; 6.45–8.40 (quoted lit. ranges: effusion method; gas saturation; manometry; calculated; from GC-RT correlation, Delle Site 1997)

11.16 (solid P_S , van der Linde et al. 1998)

40.0; 12.4 (quoted P_L from Hinckley et al. 1990; converted to P_S with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/\text{Pa}) = 10.90 - 2927/(T/\text{K})$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 8.06 - 1923/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)

$\log (P/\text{Pa}) = 13.59 - 3742/(T/\text{K})$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

37.0 (supercooled liquid P_L , GC-RT correlation, Lei et al. 2002)

$\log (P_L/\text{Pa}) = -2930/(T/\text{K}) + 11.39$; $\Delta H_{\text{vap.}} = -56.1 \text{ kJ}\cdot\text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

56.0 (gas stripping, Southworth, 1979)

48.9 (gas stripping, Mackay et al. 1979; Mackay & Shiu 1981)

44.6 (gas stripping, Mackay et al. 1982)

36.5 (20°C, EPICS method, Yurteri et al. 1987)

74.3 (wetted-wall column-GC, Fendinger & Glotfelty 1990)

124 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

47.1 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)

42.6* (gas stripping-GC, measured range 3.7–35.5°C, Alaee et al. 1996)

$\ln K_{\text{AW}} = 13.95 - 5364.45/(T/\text{K})$, temp range: 3.7–35.5°C (gas stripping-GC, Alaee et al. 1996)

26.2, 35.5, 48.1, 62.5, 77.7, 108.1 (9.2, 14.5, 20.1, 24.6, 30.5, 34.8°C, seawater with salinity of 35‰ (0.660M NaCl), gas stripping-GC, Alaee et al. 1996)

44.6 (gas stripping-GC; calculated-P/C, Shiu & Mackay 1997)

45.0 (gas stripping-HPLC/fluor., De Maagd et al. 1998)

57.0 (gas stripping-GC, Altschuh et al. 1999)

$\log K_{\text{AW}} = 6.058 - 2332/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C or as indicated:

3.37 (shake flask, Fujita et al. 1964; Hansch et al. 1973)

3.37, 3.01, 3.45 (Leo et al. 1971)

3.37 (calculated-fragment const., Rekker 1977)

3.395 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

3.30, 3.01, 3.37, 3.45, 3.59 (quoted, Hansch & Leo 1979)

3.17 (HPLC-RT correlation, Veith et al. 1979a,b)

3.36 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)

3.21 (HPLC- k' correlation, Hanai et al. 1981)

3.18 (HPLC- k' correlation, D'Amboise & Hanai 1981)

3.35 (generator column-HPLC/UV, Wasik et al. 1981 1983)

3.35 (RP-TLC- k' correlation, Bruggeman et al. 1982)

3.45 (HPLC-RT correlation, Hammers et al. 1982)

3.31; 3.35 (shake flask; HPLC correlation, Eadsforth & Moser 1983)

3.36 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)

3.35; 3.42 (shake flask; ALPM, Garst & Wilson 1984)

3.57 (HPLC-RV correlation, Garst & Wilson 1984)

3.38 (RP-HPLC correlation, Chin et al. 1986)

3.43 (HPLC-RT correlation, Eadsforth 1986)

3.29	(HPLC-RT correlation, Wang et al. 1986)
3.29	(HPLC-RT correlation, de Kock & Lord 1987)
3.30	(average, HPLC-RT correlation, Ge et al. 1987)
3.35	(shake flask-GC, Opperhuizen et al. 1987)
3.23	(HPLC-RT correlation, Minick et al. 1988)
3.29	(RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
3.35	(recommended, Sangster 1989, 1993)
3.49	(centrifugal partition chromatography, Menges et al. 1990)
3.36	(shake flask-HPLC/UV, Menges & Armstrong 1991)
3.30	(TLC-RT correlation, De Voogt et al. 1990)
3.70	(centrifugal partition chromatography, Berthod et al. 1992)
3.37	(shake flask-UV, pH 7.4, Alcorn et al. 1993)
3.30	(recommended, Hansch et al. 1995)
3.44; 3.68	(26°C; 4°C, quoted, Piatt et al. 1996)
3.47, 3.58; 3.40	(HPLC- k' correlation: ODS column; Diol column; quoted lit. average, Helweg et al. 1997)
3.33	(range 3.24–3.40) (slow stirring method-HPLC/fluor., De Maagd et al. 1998)
3.40	(shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
3.77	(RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

5.10	(calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
5.19	(calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, log BCF at 25°C:

1.64	(mussel <i>Mytilus edulis</i> , Lee et al. 1972)
4.11	(bile of rainbow trout, Melancon & Lech 1978)
2.12	(<i>Daphnia pulex</i> , Southworth et al. 1978)
2.07	(<i>Daphnia pulex</i> , by kinetic estimation, Southworth et al. 1978)
2.63	(fathead minnow, Veith et al. 1979b, 1980)
2.62	(microorganisms-water, calculated from K_{OW} , Mabey et al. 1982)
4.10, 3.84, 4.25	(average, <i>Selenastrum capricornutum</i> -dosed singly, dosed simultaneously, Casserly et al. 1983)
2.11; 2.43	(<i>Chlorella fusca</i> ; calculated- K_{OW} , Geyer et al. 1984)
1.48, 2.10, 3.0	(fish, algae, activated sludge, Freitag et al. 1985)
2.50	(bluegill sunfish, McCarthy & Jimenez 1985)
2.48	(bluegill sunfish with dissolved humic material, McCarthy & Jimenez 1985)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

3.11	(natural sediment, average sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)
2.38	(22°C, suspended particulates, Herbes et al. 1980)
2.94	(sediment/soil, sorption isotherm by batch equilibrium, Karickhoff 1981)
3.62, 3.87, 4.23	(soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
3.50; 4.43; 3.21	(Speyer soils: pH 7.0, 0.69% OC; pH 5.8, 2.24% OC; pH 7.1, 1.12% OC at 0.15–0.5 mm, batch equilibrium-sorption isotherm, Rippen et al. 1982)
3.11; 3.16	(soils: Alfisol 0.76% OC at pH 7.5, Entisol 1.11% OC at pH 7.9, batch equilibrium-sorption isotherm, Rippen et al. 1982)
3.30	(Offshore Grand Haven sediment, batch equilibrium-sorption isotherm, Voice & Weber 1985)
2.67, 2.77	(Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
2.95	(sediment, calculated, Pavlou 1987)
2.93	(sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
3.27	(calculated-MCI χ , Bahnick & Doucette 1988)
3.02; 2.89	(Aldrich and Fluka humic acid, observed; predicted, Chin et al. 1989)

- 2.73–3.91 (aquifer materials, Stauffer et al. 1989)
 5.00 (sediments average, Kayal & Connell 1990)
 3.15, 2.76 (Menlo Park soil, Eustis sand, batch equilibrium-sorption isotherm, Podoll et al. 1989)
 3.21, 3.16, 3.10, 3.00 (15, 25, 35, 50°C, Menlo Park soil 1.6% OC, flow sorption equilibrium, Podoll et al. 1989)
 2.97, 2.67 (modified, unmodified EPA-6 sediments, batch equilibrium-sorption isotherm, Podoll et al. 1989)
 3.11 (soil, RP-HPLC- k' correlation, Szabo et al. 1990a)
 3.29 (sandy surface soil, Wood et al. 1990)
 2.97 (dissolved organic matter, Kan & Tomson 1990)
 2.98; 2.965, 2.98 (sediment: concn ratio $C_{\text{sed}}/C_{\text{w}}$; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
 3.11 (calculated-MCI $^1\chi$, Sabljic et al. 1995)
 3.16, 3.05, 3.06 (RP-HPLC- k' correlation on different stationary phases, Szabo et al. 1995)
 2.75 (HPLC-screening method; Müller & Kördel 1996)
 4.06 (range 3.95–4.15); 2.08 (range 2.08–2.11) (4°C, low organic carbon sediment $f_{\text{OC}} = 0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
 3.90 (range 3.81–4.00); 2.11 (range 2.11–2.13) (26°C, low organic carbon sediment $f_{\text{OC}} = 0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
 3.74 (humic acid, HPLC- k' correlation; Nielsen et al. 1997)
 2.42–2.56 (5 soils, 20°C, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
 2.61, 2.63, 2.68, 2.77, 2.76, mean 2.69 ± 0.073 (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)
 2.91, 2.86, 2.88, 2.87, 2.89, 2.95, 3.07; mean 2.88 ± 0.22 (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)
 3.11 (3.00–3.19), 2.80 (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
 3.60; 3.10 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
 3.09–5.51; 2.60–5.0 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
 3.91; 4.12, 4.06, 4.94 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
 2.91, 3.02, 2.71 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, $0.1 \leq \text{OC} < 0.5\%$, average, Delle Site 2001)
 3.06 (average values for sediments $\text{OC} \geq 0.5\%$, Delle Site 2001)
 4.43 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: rate of evaporation estimated to be $1.675 \times 10^{-9} \text{ mol cm}^{-2} \text{ h}^{-1}$ at 20°C and air flow rate of 50 L h^{-1} (Gückel et al. 1973);
 calculated $t_{1/2} = 7.15 \text{ h}$ from 1 m depth of water (Mackay & Leinonen 1975; quoted, Haque et al. 1980);
 $t_{1/2} = 16 \text{ h}$ for surface waters for a river 1-m deep, water velocity 0.5 m/s, wind velocity 1m/s (Southworth 1979; Herbes et al. 1980);
 evaporation $t_{1/2} = 50 \text{ h}$ in a river and $t_{1/2} = 200 \text{ h}$ in a lake when considering current velocity and wind speed in combined with typical reaeration rates for natural bodies of water (Howard 1989);
 $t_{1/2}(\text{exptl}) = 28 \text{ min}$ and $t_{1/2}(\text{calc}) = 32 \text{ min}$ from solution (Mackay et al. 1983).

Photolysis:

$t_{1/2} = 71 \text{ h}$ calculated for direct photochemical transformation near-surface water and $t_{1/2} = 550 \text{ d}$ in 5-m deep inland water body at 40°N at midday of midsummer (Zepp & Schlotzhauer 1979)
 $k = 0.0392 \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988)
 $k = 0.028 \text{ h}^{-1}$ in distilled water with $t_{1/2} = 25 \text{ h}$ (Fukuda et al. 1988)
 $k = 6.0 \times 10^{-4} \text{ min}^{-1}$ and $t_{1/2} = 19.18 \text{ h}$, photodegradation in methanol-water (3:7, v/v) solution with initial concentration of 50.0 ppm by high-pressure mercury lamp or sunlight (Wang et al. 1991);

$k(\text{exptl}) = 0.000511 \text{ min}^{-1}$ with $t_{1/2}(\text{calc}) = 22.61 \text{ h}$ and the predicted $k = 0.000303 \text{ min}^{-1}$ by QSPR, the pseudo-first-order direct photolysis rate constant of in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996)

$t_{1/2}(\text{calc}) = 15.42 \text{ h}$ direct photolysis half-life in atmospheric aerosol (QSPR, Chen et al. 2001).

Oxidation: rate constant k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated; *data at other temperatures and/or Arrhenius equation see reference:

$k(\text{calc}) < 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, $k(\text{calc}) < 1 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{\text{OH}} = (2.42 \pm 0.19) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated atmospheric lifetime $\tau \sim 1\text{d}$, and $k_{\text{O}_3} < 2 \times 10^{-9} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ $294 \pm 1 \text{ K}$ (relative rate method, Atkinson et al 1984)

$k_{\text{OH}} = (2.35 \pm 0.06) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 1 \text{ K}$ (relative rate method, Biermann et al. 1985)

$k_{\text{N}_2\text{O}_5} \sim (2 - 3) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with N_2O_5 at 298 K , the calculated lifetime $\tau \sim 10 \text{ d}$ due to night-time reaction with N_2O_5 in atmosphere (relative rate method, Pitts et al. 1985)

$k_{\text{OH}}^* = 2.17 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{\text{OH}} = (2.59 \pm 0.24) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of $\sim 11 \text{ h}$, $k_{\text{O}_3} < 3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate method, Atkinson & Aschmann 1986)

$k_{\text{N}_2\text{O}_5} = (1.4 \pm 0.2) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 at 298 K (relative rate method, Atkinson et al. 1987)

$k_{\text{OH}} = 2.17 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{O}_3} < 2 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{N}_2\text{O}_5} = 1.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 at room temp. (Atkinson & Aschmann 1987, 1988)

$k_{\text{OH}} = (22.8 - 25.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294\text{--}298 \text{ K}$ (review, Atkinson 1989)

$k_{\text{OH}}^* = 2.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 26.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}}^* = 23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , measured range $306\text{--}366 \text{ K}$ with a calculated atmospheric lifetime of 12 h based on gas-phase OH reaction (Brubaker & Hites 1998)

$k_{\text{OH}} = (2.39 \pm 0.09) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$, with a calculated tropospheric lifetime of 5.8 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ (relative rate method, Phouongphouang & Arey 2002)

Hydrolysis: not hydrolyzable (Mabey et al. 1982).

Biodegradation:

$k = 4 \times 10^{-6} \text{ g L}^{-1} \text{ d}^{-1}$ ultimate loss process (Lee & Ryan, 1976)

$k = (0.04 - 3.3) \times 10^{-6} \text{ g L}^{-1} \text{ d}^{-1}$ (Lee & Anderson 1977)

complete degradation in 8 d in gas-oil contaminated groundwater which was circulated through sand that had been inoculated with groundwater under aerobic conditions (Kappeler & Wuhrmann 1978; quoted, Howard 1989)

$k = 0.04 - 3 \text{ } \mu\text{g/L d}$ for microorganisms (Callahan et al. 1979)

$t_{1/2} = 1.9 \text{ d}$, in deeper and slowly moving contaminated water (Herbes 1981; Wakeham et al. 1983; quoted, Howard 1989);

half-lives: of $7, 24, 63$ and 1700 d in an oil polluted estuarine stream, clean estuarine stream, coastal waters, and in the Gulf stream, respectively (Lee 1977; quoted, Howard 1989)

$t_{1/2}(\text{aerobic}) = 12 \text{ h}$, based on die-away test data for an oil polluted creek (Walker & Colwell 1976)

$t_{1/2} = 480 \text{ h}$, for an estuarine river (Lee & Ryan 1976).

$t_{1/2}(\text{anaerobic}) = 25 \text{ d}$ at $\text{pH } 8$ and $t_{1/2} = 258 \text{ d}$ at $\text{pH } 5$ (Hambrick et al. 1980);

$t_{1/2} = 1.9 \text{ d}$, in deeper and slower moving contaminated water (Herbes 1981; Wakeham et al. 1983)

$k = 0.23 \text{ h}^{-1}$ (microbial degradation rate constant, Herbes et al. 1980, Hallett & Brecher 1984)

100% degradation within 7 d for an average of three static-flask screening test (Tabak et al. 1981)

$k = 3.2 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 9 \text{ h}$; $k = 7.6 \times 10^{-2} \text{ h}^{-1}$ with $t_{1/2} = 9 \text{ h}$ for mixed bacterial populations in water and sediment from the same stream (NRCC 1983)

$k = 0.14 \text{ h}^{-1}$ with $t_{1/2} = 5 \text{ h}$; $k < 4 \times 10^{-4} \text{ h}^{-1}$ with $t_{1/2} > 72 \text{ d}$ for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)

degraded completely within 1 wk by microbes in non-autoclaved samples of 0.04 mg/L in groundwater from hazardous waste site (Lee et al. 1984)

$k = 0.024 \text{ d}^{-1}$ with $t_{1/2} = 28 \text{ d}$ in groundwater with nutrients and acclimated microbes, $k = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53 \text{ d}$ in river water with acclimated microbes, and $k = 0.018 \text{ d}^{-1}$ with $t_{1/2} = 39 \text{ d}$ in river water with nutrients and acclimated microbes (Vaishnav & Babeu 1987)

$k = 0.337 \text{ d}^{-1}$ with $t_{1/2} = 2.1 \text{ d}$ for Kidman sandy loam and $k = 0.308 \text{ d}^{-1}$ with $t_{1/2} = 2.2 \text{ d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)

$t_{1/2}(\text{aerobic}) = 12\text{--}480 \text{ h}$, based on die-away test data and for estuarine river (Howard et al. 1991)

$t_{1/2}(\text{anaerobic}) = 500\text{--}6192 \text{ h}$, based on anaerobic estuarine sediment die-away test data (Howard et al. 1991)
removal rate of 2.4 and 0.43 mg (g of volatile suspended solid d) $^{-1}$, degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

Biotransformation: estimated rate constant for bacteria, $1 \times 10^{-7} \text{ ml cell}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) or Elimination (k_2) Rate Constants:

$k_1 = 197 \text{ h}^{-1}$; $k_2 = 1.667 \text{ h}^{-1}$ (*Daphnia pulex*, Southworth et al. 1978; quoted, Hawker & Connell 1986)

$\log k_2 = -0.70, -1.70 \text{ d}^{-1}$ (fish, calculated- K_{ow} , Thomann 1989)

Half-Lives in the Environment:

Air: volatility of $2.28 \times 10^4 \text{ s}$ (experimental), $7.7 \times 10^3 \text{ s}$ (calculated) for depth of water body of 22.5 m (23°C , Klöpffer et al. 1982);

estimated lifetime of $\sim 1\text{d}$ due to reaction with photochemically produced hydroxyl radical, assuming an average daytime atmospheric OH radical concn of $\sim 1 \times 10^6 \text{ molecule/cm}^3$ (Atkinson et al. 1984, 1987; quoted, Howard 1989);

calculated lifetime of $\sim 11 \text{ h}$ due to reaction with OH radical (Atkinson & Aschmann 1986);

the atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radical and with N_2O_5 can be calculated to range from ~ 4 to 13 h and $20\text{--}80 \text{ d}$, respectively (Atkinson & Aschmann 1987);

$t_{1/2} = 2.96\text{--}29.6 \text{ h}$ based on photooxidation half-life in air (Howard et al. 1991);

calculated atmospheric lifetime of 12 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface Water: $t_{1/2} = 16 \text{ h}$ (calculated for river water 1 m deep, water velocity 0.5 m/s, wind velocity 1 m/s from air-water partition coefficients (Southworth 1979; Hallett & Brecher 1984)

$t_{1/2} = 71 \text{ h}$ of photolysis in near surface water, but $t_{1/2} = 550 \text{ d}$ for a depth of 5 m (calculated from surface water in midsummer at 40°N latitude, Zepp & Schlotzhauer 1979);

calculated $t_{1/2} = 7.15 \text{ h}$, based on evaporative loss for a water depth of 1 m at 25°C (Mackay & Leinonen 1975);

an overall $t_{1/2} = 2.3 \text{ d}$ in Rhine river based on monitoring data (Zoeteman et al. 1980)

in coastal seawater mesocosm experiments: $k = 0.058 \text{ d}^{-1}$ with $t_{1/2} = 12 \text{ d}$ in winter at $3\text{--}7^\circ\text{C}$ during the periods when volatilization dominates, $k = 0.061 \text{ d}^{-1}$ with $t_{1/2} = 11.3 \text{ h}$ with HgCl_2 as poison and $k = 0.896 \text{ d}^{-1}$ corresponding to $t_{1/2} = 0.8 \text{ h}$ without poison (Wakeham et al. 1983);

$t_{1/2} = 12\text{--}480 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); photolysis $t_{1/2} = 22.81 \text{ h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: estimated $t_{1/2} = 0.6 \text{ yr}$ in the Netherlands (Zoeteman et al. 1981);

$t_{1/2} = 24\text{--}6193 \text{ h}$ based on estimated unacclimated aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{1/2} = 4.9 \text{ h}$ in oil contaminated sediment and $t_{1/2} > 88 \text{ d}$ in uncontaminated sediments (Herbes & Schwall 1978; quoted, Howard 1989);

desorption $k = 0.031 \text{ d}^{-1}$ with $t_{1/2} = 21.3 \text{ d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: an overall $t_{1/2} = 3.6 \text{ months}$ in a solid waste site (Zoeteman et al. 1981);

$t_{1/2} = 0.12\text{--}125 \text{ d}$ (Sims & Overcash 1983);

$t_{1/2} = 12 \text{ d}$ for both 5 mg/kg and 50 mg/kg added (Bulman et al. 1987);

$t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988);

$t_{1/2} > 80 \text{ d}$ (Howard 1989);

biodegradation $k = 0.337 \text{ d}^{-1}$ with $t_{1/2} = 2.1 \text{ d}$ for Kidman sandy loam soil and $k = 0.308 \text{ d}^{-1}$ with $t_{1/2} = 2.2 \text{ d}$ for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 398\text{--}1152 \text{ h}$, based on soil-die-away test data (Howard et al. 1991); $t_{1/2} = 0.02\text{--}46 \text{ wk}$, $t_{1/2} < 2.1 \text{ yr}$ (quoted, Ludington soil, Wild et al. 1991).

Biota: elimination half-lives $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes, $t_{1/2} = 2.0 \text{ d}$ from clam *Macoma balthica* (quoted, Meador et al. 1995).

TABLE 4.1.1.2.1

Reported aqueous solubilities of naphthalene at various temperatures and empirical temperature dependence equations

$$R \cdot \ln x = -\Delta H_{\text{fus}}/(T/K) + (0.000408) \cdot [(T/K) - 291.15]^2 - c + b \cdot (T/K) \quad (1)$$

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t_{1/2} + c \cdot t + d \quad (2)$$

$$R \cdot \ln x = -30.55/\theta + 28.7/(1/\theta - 1/T) + 0.31[\theta/T - 1 - \ln(\theta/T)] \quad (3)$$

$$\ln x = 1767.460/[R \cdot (T/K)] + (17.95209/R) \cdot \ln (T/K) + 1 \quad (4)$$

$$\log (S/\text{mol} \cdot \text{dm}^{-3}) = -31.24 - 143.5/(T/K) + 4.772 \cdot \ln (T/K) \quad (5)$$

1.

Hilpert 1916		Bohon & Claussen 1951		Wauchope & Getzen 1972			
shake flask-gravimetry		shake flask-UV		shake flask-UV			
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	19	25	34.4	22.2	28.8	0	13.7
25	30	0	13.74	22.2	29.1	22.2	28.3
		0.4	13.74	24.5	30.8	24.5	30.7
		0.5	13.85	24.5	30.1	25.0	31.2
		0.9	14.59	24.5	30.7	29.9	37.3
		9.4	19.62	29.9	38.1	30.3	37.8
		10	19.42	29.9	38.2	34.5	44.3
		14.9	23.43	29.9	38.3	39.3	53.3
		15.9	24.56	30.3	38.1, 37.6	40.1	55.0
		19.3	28.05	34.5	44.6, 43.8	44.7	66.2
		25.6	36.6	39.3	52.6, 52.8	50.0	82.4
		30.1	42.97	40.1	54.8	50.2	83.1
		30.2	43.87	44.7	66.0	55.6	105
		35.2	54.45	44.7	65.5	64.5	156
		36.0	54.81	44.7	65.3	73.4	239
		42.8	73.49	50.2	78.6	75	258
				55.6	106		
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$		64.5	166	temp dependence eq. 1	
		2°C	4.14	64.5	151	ln x	mole fraction
		7°C	5.77	64.5	157	$\Delta H_{\text{fus}} =$	36.36 ± 0.17
		12°C	7.24	73.4	240	$10^2 \cdot b$	1.39 ± 0.05
		17°C	8.49	73.4	247	c	13.4 ± 0.2
		22°C	10.17	73.4	244		
		27°C	12.80				
		32°C	14.23	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 36.36$			
		37°C	15.69				

(Continued)

TABLE 4.1.1.2.1 (Continued)

2.

Schwarz & Wasik 1977		Schwarz 1977		May 1980		May et al. 1983	
shake flask-fluorescence		shake flask-fluorescence		generator column-HPLC		generator column-HPLC/UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
from K _{WA} measurements							
10	18.32	8.4	17.95	8.2	16.91	8.2	16.92
12	19.87	11.1	19.1	11.5	19.23	11.5	19.25
14	21.02	14	21.2	13.4	20.37	13.4	20.39
15	22.17	17.5	24.1	15.1	21.48	15.1	21.50
16	22.56	20.2	26.54	19.3	25.79	19.3	25.81
18	23.97	23.2	28.46	23.4	29.47	23.4	29.50
19	24.61	25	30.25	25.0	31.91	25.0	31.94
20	25.51	26.3	31.79	27.0	34.15	27.0	34.18
22	27.17	29.2	34.36				
24	28.84	31.8	36.28	temp dependence eq. 2		Δ _{sol} H/(kJ mol ⁻¹) = 27.4	
25	29.61			S	μg/kg	8–32°C	
26	30.63	ΔH _{sol} /(kJ mol ⁻¹) = 22.1		a	0.0013	data fitted to eq. 3	
28	34.10	for temp 8–32°C		b	–0.0097		
30	34.61			c	0.8886		
				d	8.21		
direct measurement							
12	18.58	ΔH _{sol} /(kJ mol ⁻¹) = 26.36					
18	24.35						
25	30.0						

3.

Bennet & Canady 1984		Shaw 1989		Perez-Tejeda et al. 1990	
shake flask-UV		recommended values		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
25	31.1	0	15	5	12.3
1.90	19.2	10	19	10	20.25
10.7	17.2	20	28	15	24.35
15.4	21.66	25	31	20	28.71
21.7	26.74	30	38	25	33.71
25.2	30.75	40	61	35	41.53
30.7	40.12	50	82	35	47.55
35.1	46.36	60	130	40	55.75
39.3	54.85	70	200	data fitted to eq. 5	
44.9	68.97	75	260		
data fitted to eq. 4					
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$					
25°C					

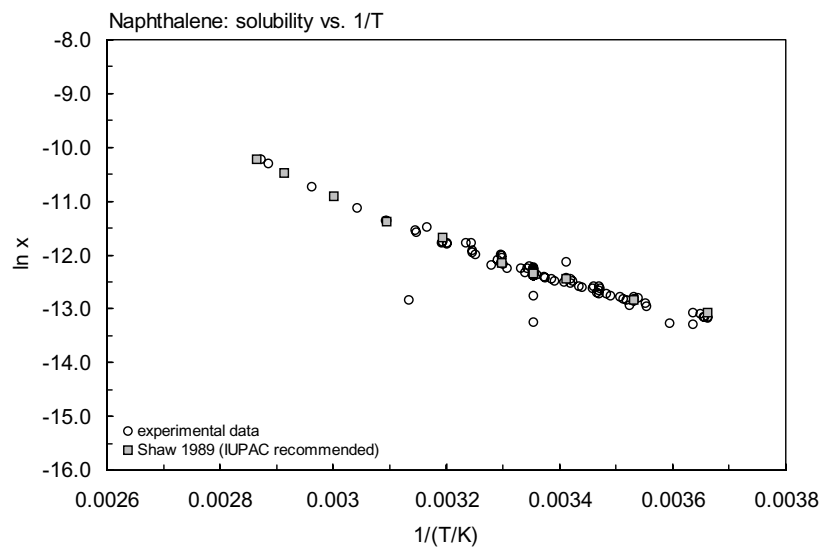


FIGURE 4.1.1.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for naphthalene.

TABLE 4.1.1.2.2
Reported vapor pressures of naphthalene at various temperatures and coefficients for vapor pressure equations

$\log P = A - B/(T/K)$
 $\log P = A - B/(C + t/^{\circ}C)$
 $\log P = A - B/(C + T/K)$
 $\log P = A - B/(T/K) - C \cdot \log (T/K)$

(1)
(2)
(3)
(4)

$\ln P = A - B/(T/K)$
 $\ln P = A - B/(C + t/^{\circ}C)$

(1a)
(2a)

1.

Swan & Mack 1925		Stull 1947		Sears & Hopke 1949		Bradley & Cleasby 1953	
effusion		summary of literature data		manometry		effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
10	2.32	52.6	133.3	10	2.053	6.7	1.627
20	8.64	74.2	666.6	20	8.533	8.1	1.88
30	23.60	85.8	1333	30	21.87	12.3	2.96
		101.7	2666			12.7	3.13
eq. 4	P/mmHg	119.3	5333	eq. 2	P/mmHg	13.85	3.506
A	595.642	130.2	7999	A	1.115	15.65	4.266
B	29.820	145.5	13332	B	108.3	16.85	4.67
C	200.682	167.7	26664	C	27	17.35	5.09
		193.2	53329			18.7	5.106
		217.9	101325			20.7	7.12
		mp/°C	80.2			eq. 1	P/mmHg
						A	10.597
						B	3783

(Continued)

TABLE 4.1.1.2.2 (Continued)

2.

Camin & Rossini 1955		Miller 1963		Fowler et al. 1968		Zwolinski & Wilhoit 1971	
manometry		Knudsen effusion		Hg manometer		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
126.325	6815	−43	0.00148	40.33	46.66	85.581	1333
130.836	8338	−33	0.00746	49.45	98.66	101.788	2666
134.548	9537	−23	0.0332	54.17	148.0	111.451	4000
138.677	10948	−13	0.1188	50.22	244.0	118.688	5333
143.930	13096			61.20	253.3	124.537	6666
155.766	19436	$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 72.67$ at 25°C		65.05	338.6	129.476	7999
161.104	22878			70.18	500.0	137.581	10666
168.540	28550			70.98	521.3	144.146	13332
175.526	34818			75.61	725.3	156.749	19998
183.336	43159			76.7	789.3	166.262	26664
191.702	53748			80.34	931.9	173.966	33331
200.471	67072					180.561	39997
216.319	98125			eq. 2	P/mmHg	191.398	53329
217.237	99729			A	9.58102	200.237	66661
217.848	101112			B	2619.91	207.760	79993
218.638	102925			C	220.651	214.343	93326
						215.569	95992
bp/°C	217.955					216.768	98659
						217.942	101325
eq. 2	P/mmHg						
A	6.84577					eq. 2	P/mmHg
B	1606.529					A	7.01063
C	187.277					B	1733.71
						C	201.859
						bp/°C	217.942
						$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) =$	
						at 25°C	72.68
						at bp	43.26

3.

Sinke 1974		Radchenko & K. 1974		Ambrose 1975		Macknick & Prausnitz 1979	
gas saturation		effusion		diaphragm gauge		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
−53.15	0.00028	9.0	2.357	263.61	0.23	7.15	1.76
−33.15	0.00837	10.7	3.113	267.98	0.40	12.8	3.133
−13.15	0.144	12.5	5.637	273.16	0.74	18.4	5.586
6.85	1.631	14.4	7.546	278.22	1.38	18.85	5.933
25	10.93	16.3	19.59	283.14	2.41	26.4	12.58
26.85	13.092	18.2	31.09	288.01	4.13	31.85	20.53
46.85	79.73	20.0	48.37	288.01	4.17	25	10.64
66.85	386.5	21.95	74.19	293.24	6.93		
80.28	999.8	23.91	112.6	293.25	6.95	eq. 1	P/mmHg
		25	12.26*	298.26	11.35	A	26.25
eq. 1	P/Pa			303.29	18.45	B	8575
A	13.83	$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 72.72$ at 25°C		308.17	28.95		
B	3817			313.24	44.73		

TABLE 4.1.1.2.2 (Continued)

Sinke 1974		Radchenko & K. 1974		Ambrose 1975		Macknick & Prausnitz 1979	
gas saturation		effusion		diaphragm gauge		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
				318.21	68.82		
		eq. 1	P/mmHg	323.14	104.14		
		A	11.7041	328.24	158.41		
		B	3798.574	333.39	237.54		
		*calcd using eq. 1		333.34	238.73		
				333.34	238.47		
				338.10	340.58		
				343.06	488.58		
				ΔH _{subl} /kJ mol ⁻¹ = 72.5 at 25°C			
4.							
de Kruif 1980		de Kruif et al. 1981					
torsion-effusion		diaphragm gauge					
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
		solid		cont'd		liquid	
257.21	0.1	274.44	0.87	340.92	421.8		
262.44	0.2	276.40	1.10	348.82	717.5	355.23	1069
265.59	0.3	279.12	1.50	350.44	790.2	356.83	1155
267.88	0.4	280.62	1.78	352.44	914.5	359.78	1328
269.68	0.5	282.73	2.24	344.72	538.0	362.77	1526
271.17	0.6	285.37	3.07	345.76	586.6	355.38	1083
272.44	0.7	285.71	3.11	328.79	159.2	372.05	2305
273.56	0.8	287.98	3.98	324.57	118.5	377.33	2899
274.55	0.9	288.11	4.02	345.92	580.4	385.20	4006
275.44	1.0	290.46	5.16	324.87	121.9	381.92	3504
		290.88	5.35	347.53	650.0	372.45	2351
ΔH _{subl} /kJ mol ⁻¹ =		292.75	6.53	347.57	653.9	368.07	1929
298.15 K	72.6	320.34	83.91	344.72	547.1	363.74	1591
253–273 K	74.4	319.87	80.76	344.86	549.1	353.57	982
		275.50	0.99	352.00	901.3	357.10	1176
		282.12	2.10	319.58	78.38	361.10	1423
		277.86	1.30	319.59	77.9	367.72	1926
		325.41	126.7	325.96	132.1	380.51	3355
		288.51	4.22	341.26	419.9	388.20	4545
		293.83	7.29	349.02	724.1	348.80	3998
		297.40	10.42	346.18	597.6	374.67	2626
		306.67	25.27	352.90	941.6	368.46	1999
		310.71	36.37	338.91	359.7	387.32	4398
		302.92	17.84	346.85	629.9	357.44	1200
		318.58	72.36	350.69	820.2	362.57	1528
		282.13	2.10	349.15	751.1	353.51	995
		277.85	1.30	341.72	441.7	353.33	985
		288.50	4.21	348.6	717.3		

(Continued)

TABLE 4.1.1.2.2 (Continued)

de Kruif 1980		de Kruif et al. 1981					
torsion-effusion		diaphragm gauge					
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
		313.96	46.87	349.24	700.9		
		313.88	48.94	345.96	599.0		
		311.49	88.77	353.14	969.3		
		317.68	66.27				
		321.31	89.40	$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} =$			
		324.05	112.0	298.15	72.5		
		339.29	361.8				

5. Colomina et al. 1982		Grayson & F. 1982		Sonnefeld et al. 1983		Van Ekeren et al. 1983	
effusion		gas saturation		gas saturation-HPLC		spinning-rotor gauge	
T/K	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
271.46	0.611	28.9	16.38	14.15	3.13	244.19	0.0163
275.08	0.94	42.7	58.33	14.15	3.24	245.31	0.0191
277.10	1.19	50	100.99	14.15	3.27	245.31	0.0192
279.93	1.63	60.2	264.32	19.49	6.0	246.59	0.0233
281.16	1.99	69.6	519.1	19.49	6.19	247.74	0.0268
282.69	2.23	79	970.5	25.05	10.1	247.74	0.0272
283.80	2.54	20	6.75	15.05	10.8	249.18	0.0373
284.63	2.80			25.05	10.4	250.45	0.04
		eq. 1a	P/mmHg	32.1	20.9	252.77	0.0554
$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 72.8$		A	31.80	32.05	21.0	255.86	0.0834
	at 25°C	B	8753	32.1	20.8		
						$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} =$	
eq. 1	P/Pa			eq. 1	P/Pa	248.51	72.92
A	14.01			A	14.299	298.15	72.92
B	3861.80			B	3960.03		

6. Sato et al. 1986		Sasse et al. 1988				Wania et al. 1994	
gas saturation-electrobalance		gas saturation				gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		solid		liquid			
24.85	10.7	-12.15	0.1653	80.16	968.85	-30.6	0.014
28.35	14.9	-12.1	0.1653	84.90	1240.4	-25.0	0.0217
30.95	19.2	-9.47	0.2266	84.93	1270.6	-20.1	0.0586
34.15	25.9	0.52	0.8199	87.16	1382.6	-14.9	0.108
41.65	52.8	10.17	2.413	84.23	1395.9	-10.0	0.2122
45.35	71.1	20.11	7.093	90.15	1590.5	-5.0	0.348
48.95	97.5	20.16	7.026			0	0.7634
49.45	101	29.98	18.265	For liquid			
51.85	124	30.03	18.80	eq. 2	P/mmHg	$\Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 73.7$	
55.35	165	40.04	44.93	A	2.25180	(-30 to 0°C)	
57.75	200	40.04	45.46	B	76.496		
		50.04	106.8	C	-25.09	eq. 1	P/Pa

TABLE 4.1.1.2.2 (Continued)

Sato et al. 1986		Sasse et al. 1988				Wania et al. 1994	
gas saturation-electrobalance		gas saturation				gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
eq. 3	P/Pa	50.04	105.2			A	13.93
A	22.892960.05	60.05	238.2			B	3851
B	4025.3560.12	60.12	232.6				
C	-102.34370.11	70.11	491.0				
		70.16	491.02				
		For solid					
		eq. 2	P/mmHg				
		A	10.05263				
		B	2907.918				
		C	236.459				

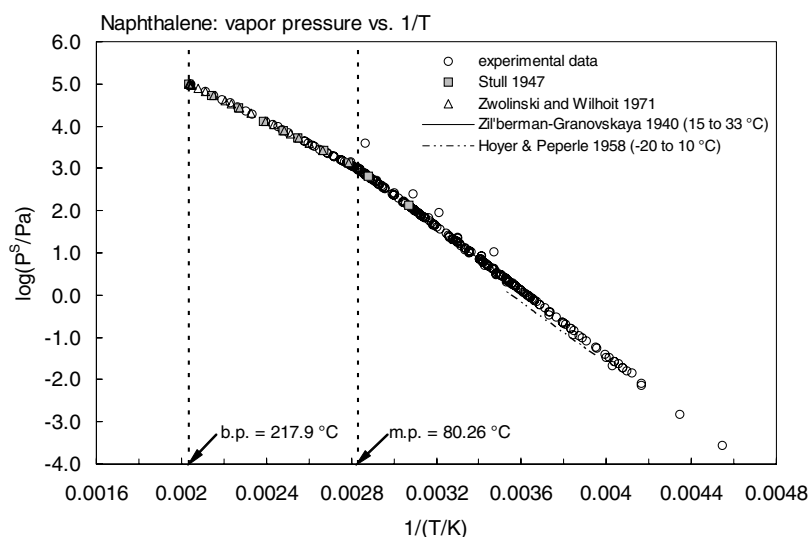


FIGURE 4.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for naphthalene.

TABLE 4.1.1.2.3

Reported Henry's law constants of naphthalene at various temperatures

Alaee et al. 1996

gas stripping-GC	
t/°C	H/(Pa m ³ /mol)
3.7	9.65
9.4	15.4
15.3	21.4
15.5	23.1
20	33.2
25	42.6
25.4	45.2
30.2	58.6

(Continued)

TABLE 4.1.1.2.3 (Continued)

Alaee et al. 1996	
gas stripping-GC	
t/°C	H/(Pa m ³ /mol)
35.5	79.1
enthalpy of volatilization: $\Delta H_{vol}/(\text{kJ}\cdot\text{mol}^{-1}) = 44.6$ at 20°C	
$\ln K_{AW} = A - B/(T/K)$	
eq. 1	K_{AW}
A	-5364.4
B	13.95

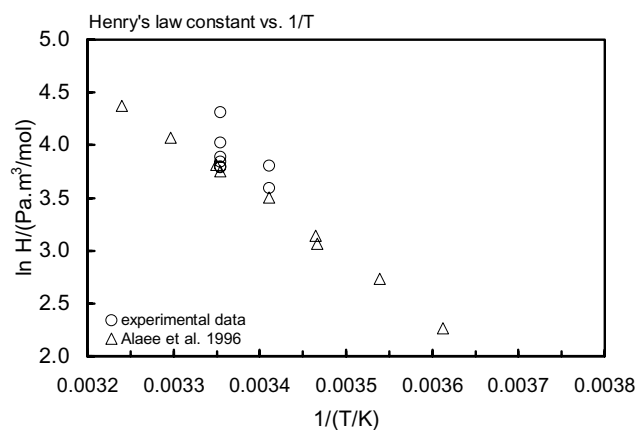
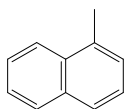


FIGURE 4.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for naphthalene.

4.1.1.3 1-Methylnaphthalene



Common Name: 1-Methylnaphthalene

Synonym: α -methylnaphthalene

Chemical Name: 1-methylnaphthalene

CAS Registry No: 90-12-0

Molecular Formula: $C_{11}H_{10}$

Molecular Weight: 142.197

Melting Point ($^{\circ}C$):

−30.43 (Lide 2003)

Boiling Point ($^{\circ}C$):

244.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.02015, 1.01649 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.0125 (Dean 1985)

1.0202 (Lide 2003)

Molar Volume (cm^3/mol):

139.4 ($20^{\circ}C$, calculated-density)

169.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

60.06, 45.48 (25° , bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.853 (Dean 1985)

4.98, 6.95; 11.92 (-32.45 , $34.25^{\circ}C$, total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

20.69, 28.82 (-32.45 , $34.25^{\circ}C$, Chickos et al. 1999)

49.3, 44.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

25.8 (shake flask-GC, Eganhouse & Calder 1976)

28.5 (shake flask-fluorescence, Mackay & Shiu 1977)

29.9* (shake flask-fluorescence, measured range 8.6 – $31.7^{\circ}C$, Schwarz & Wasik 1977)

29.5* (shake flask-fluorescence, measured range 10 – $25^{\circ}C$, Schwarz 1977)

31.7 (generator column-HPLC, Wasik et al. 1983)

27.02 (average lit. value, Pearlman et al. 1984)

30.2* ($20^{\circ}C$, shake flask-GC, measured range 20 – $70^{\circ}C$, Burris & MacIntyre 1986)

28.0 (recommended, IUPAC Solubility Data Series, Shaw 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7.165* (manometer, extrapolated-Antoine eq., Camin & Rossini 1955)

$\log(P/mmHg) = 7.03592 - 1826.948/(195.002 + t/^{\circ}C)$; temp range 142.1 – $254.4^{\circ}C$ (Antoine eq., Hg manometer, Camin & Rossini 1955)

8.95 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.06899 - 1852.674/(197.716 + t/^{\circ}C)$; temp range 130 – $305^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

66.66* ($52.8^{\circ}C$, Hg manometer, measured range 52.8 – $243.0^{\circ}C$, Myers & Fenske 1955)

7.19* (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

- $\log (P/\text{mmHg}) = 7.03592 - 1826.948/(195.002 + t/^{\circ}\text{C})$; temp range 107.68–278.32°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)
 8.82* (gas saturation-GC, Macknick & Prausnitz 1979)
 8.84 (extrapolated-Clapeyron eq., Macknick & Prausnitz 1979)
 $\log (P/\text{mmHg}) = 20.552 - 6933.2/(T/\text{K})$; temp range 5.70–38.6°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
 7221* (151.15°C, differential pressure gauge, measured range 151.15–271.70°C, Wieczorek & Kobayashi 1981)
 $\log (P/\text{atm}) = [1 - 517.727/(T/\text{K})] \times 10^{\{0.863323 - 5.26355 \times 10^{-4} \cdot (T/\text{K}) + 3.85750 \times 10^{-7} \cdot (T/\text{K})^2\}}$; temp range 278.85–593.38 K (Cox eq., Chao et al. 1983)
 8.84 (interpolated Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.15971 - 1825.586/(194.848 + t/^{\circ}\text{C})$; temp range: 142.1–245.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 7.43, 6.38 (GC-RT correlation with BP-1 column, Apolane column, Bidleman 1984)
 7.816 (extrapolated Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 7.03592 - 1826.946/(195.0 + t/^{\circ}\text{C})$; temp range 108–278°C (Antoine eq., Dean 1985, 1992)
 0.895 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.03469 - 3006.467/(T/\text{K})$; temp range 278–313 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.15928 - 1826.402/(-72.779 + T/\text{K})$; temp range 415–526 K (Antoine eq., Stephenson & Malanowski 1987)
 8.93* (pressure gauge, interpolated-Antoine eq. derived from exptl. data, temp range –14.44 to + 115°C, Sasse et al. 1988)
 $\log (P_L/\text{mmHg}) = 7.27126 - 2006.862/(212.625 + t/^{\circ}\text{C})$; temp range –14.44 to 115.1°C, (Antoine eq., pressure gauge, Sasse et al. 1998)
 7.43 (P_{GC} by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
 $\log (P/\text{mmHg}) = 29.8895 - 3.9535 \times 10^3/(T/\text{K}) - 7.2253 \cdot \log (T/\text{K}) + 1.1109 \times 10^{-11} \cdot (T/\text{K}) + 8.9552 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 243–722 K (vapor pressure eq., Yaws 1994)
 8.94, 8.93; 9.50, 8.12, 19.7; 7.42, 5.93 (quoted exptl. values; calculated; GC-RT correlation, Delle Site 1997)
 $\log (P/\text{kPa}) = 6.39609 - 2006.662/[(T/\text{K}) - 60.525]$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 6.55; 1.28 (supercooled liquid P_L ; calibrated GC-RT correlation, GC-RT correlation, Lei et al. 2002)
 $\log (P_L/\text{Pa}) = -3258/(T/\text{K}) + 11.74$; $\Delta H_{\text{vap.}} = -62.4 \text{ kJ} \cdot \text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)
 8.85* (24.05°C, transpiration method, measured range 294.1–324.2 K, Verevkin 2003)
 $\ln (P/P^{\circ}) = 298.831/R - 83537.555/R \cdot (T/\text{K}) - (78.6/R) \cdot \ln[(T/\text{K})/298.15]$; where $P^{\circ} = 101.325 \text{ kPa}$, gas constant $R = 8.31451 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ (vapor pressure eq. from transpiration measurements, temp range 294.1–324.2 K, Verevkin 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 26.3 (gas stripping, Mackay et al. 1979, 1982)
 26.3 (gas stripping-GC, Mackay et al. 1982)
 62.0 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
 36.5 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 24.3 (gas stripping-GC, Shiu & Mackay 1997)
 52.1 (gas stripping-GC, Altschuh et al. 1999)
 47.8* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)
 $\ln K_{\text{AW}} = -5821.5/(T/\text{K}) + 15.636$; $\Delta H = 48.4 \text{ kJ mol}^{-1}$; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.87 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)
 3.87 (Hansch & Leo 1979)
 3.87 (recommended, Sangster 1989, 1994)
 3.87 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.33, 3.06 (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
 3.36 (sediment from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
 2.96–3.83 (aquifer materials, Stauffer et al. 1989)

Environmental Rate Constants, k , or Half-Lives; $t_{1/2}$:

Volatilization:

Photolysis: calculated $t_{1/2} = 22$ h for direct sunlight photolysis of 50% conversion at 40°N latitude of midday in midsummer in near surface water, $t_{1/2} = 180$ d in 5-m deep inland water and $t_{1/2} = 190$ d in inland water with a suspended sediment concentration of 20 mg/L partitioning (Zepp & Schlotzhauer 1979);
 $t_{1/2} = 180$ d under summer sunlight in surface water (Mill & Mabey 1985);
 direct photolysis $t_{1/2} = 11.14$ h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).

Oxidation: rate constant k , for gas-phase second-order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 , or as indicated *data at other temperatures see original reference:

$k_{OH} = (5.30 \pm 0.48) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} < 1.3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{N_2O_5} = (3.3 \pm 0.7) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with N_2O_5 at 298 ± 2 K (relative rate method, Atkinson & Aschmann 1987, 1988)

$k_{OH} = 5.30 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989, 1990)

$k_{OH}(\text{calc}) = 59.77 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{OH} = 5.30 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $(4.09 \pm 0.20) \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at $(298 \pm 2) \text{ K}$ with a calculated tropospheric lifetime to be 2.9 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule} \cdot \text{cm}^{-3}$ (relative rate method, Phouongphouang & Arey 2002)

Hydrolysis:

Biodegradation: $k = 0.415 \text{ d}^{-1}$ with $t_{1/2} = 1.7$ d for Kidman sandy loam soil and $t_{1/2} = 0.321 \text{ d}^{-1}$ with $t_{1/2} = 2.2$ d for McLaurin sandy loam soil, all at -3.3 bar soil moisture (Park et al. 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination(k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetimes of alkyl-substituted naphthalenes due to reaction with OH radical and with N_2O_5 calculated to range from ~4 to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987);

direct photolysis $t_{1/2} = 11.14$ h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001); a calculated tropospheric lifetime to be 2.9 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule} \cdot \text{cm}^{-3}$ for the reaction with OH radical (Phouongphouang & Arey 2002).

Water: computed near-surface $t_{1/2} = 22$ h and for direct photochemical transformation at latitude 40°N, midday, midsummer, and $t_{1/2} = 80$ d with no sediment-water partitioning and $t_{1/2} = 190$ d with sediment-water partitioning for direct photolysis in 5 m deep inland water body integrated over full summer d at latitude 40°N (Zepp & Schlotzhauer 1979);

$t_{1/2} = 180$ d under summer sunlight (Mill & Mabey 1985).

Soil: biodegradation $k = 0.415 \text{ d}^{-1}$ with $t_{1/2} = 1.7$ d for Kidman sandy loam soil, $k = 0.321 \text{ d}^{-1}$ with $t_{1/2} = 2.2$ d for McLaurin sandy loam soil (Park et al. 1990).

Sediment:

Biota: elimination $t_{1/2} = 2$ d from Oyster for naphthalenes (quoted, Meador et al. 1995).

TABLE 4.1.1.3.1
Reported aqueous solubilities of 1-methylnaphthalene at various temperatures

Schwarz 1977		Schwarz & Wasik 1977		Burris & MacIntyre 1986	
shake flask-fluorescence		shake flask-fluorescence		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
8.6	19.91	10	22.75	20	30.2
14.5	22.61	14	28.44	70	87.9
17.1	22.89	20	28.44		
20.0	25.31	25	29.86		
23.0	27.59				
25.0	30.0				
26.1	30.43				
29.2	33.28				
31.7	36.26				

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 19.1$

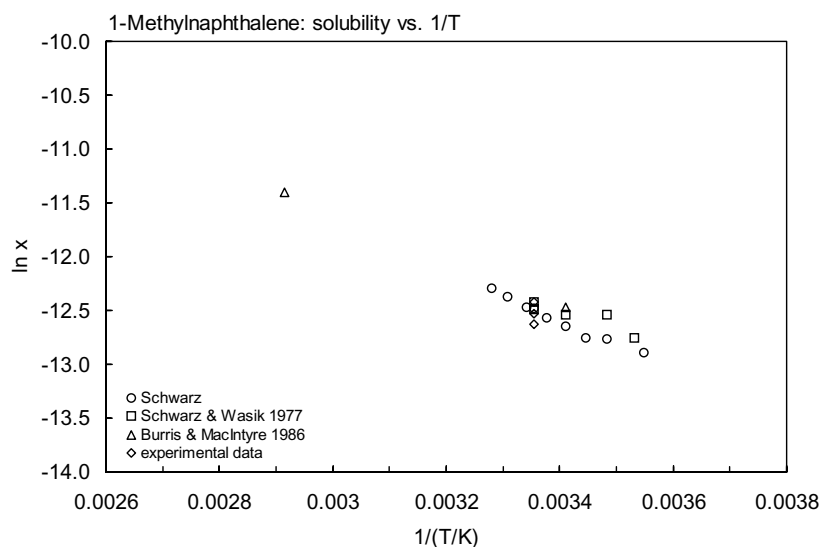


FIGURE 4.1.1.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-methylnaphthalene.

TABLE 4.1.1.3.2

Reported vapor pressures of 1-methylnaphthalene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & \ln P/P^{\circ} = A - B/(T/K) - C \cdot \ln [(T/K)/298.15] & 4(a) \end{array}$$

1.

Camin & Rossini 1955		Myers & Fenske 1955		Zwolinski & Wilhoit 1971		Macknick & Prausnitz 1979	
ebulliometry		Hg manometer		selected values		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
142.140	5524	52.8	66.66	107.68	1333	5.70	1.760
153.600	8314	63.5	133.3	123.57	2666	11.40	2.920
157.539	9510	75.8	266.6	133.66	4000	18.10	5.248
161.689	10942	83.0	400.0	141.21	5333	22.15	7.133
167.212	13088	88.9	533.3	147.319	6666	28.85	12.59
179.971	19442	93.3	666.6	152.474	7999	32.35	15.73
185.505	22881	97.1	799.9	160.932	10666	34.90	18.93
193.280	28542	103.8	1067	167.781	13332	38.60	23.46
200.536	34832	108.8	1333	180.927	19998		
208.677	43162	117.6	2000	190.846	26664	eq. 1a	P/mmHg
217.375	53762	124.4	2666	198.908	33331	A	20.552
226.498	67057	134.4	4000	205.750	39997	B	6933.2
246.243	84026	142.2	5333	217.043	53329		
243.177	98081	148.3	6666	226.250	66661		
243.949	99655	153.7	7999	234.084	79993		
244.555	101030	161.9	10666	240.938	93326		
245.326	102757	168.5	13332	242.215	95992		
		182.0	19998	243.463	98659		
eq. 2	P/mmHg	191.6	26664	244.078	99992		
A	7.03592	206.0	39997	244.685	101325		
B	1826.948	217.0	53329				
C	195.002	225.5	66661	eq. 2	P/mmHg		
		233.3	79993	A	7.03592		
$\Delta H_v/(kJ\ mol^{-1}) = 63.82$		240.0	93326	B	1826.948		
at 25°C		243.0	101325	C	195.002		
				bp/°C	244.685		
				$\Delta H_v/(kJ\ mol^{-1}) = 46.0$			
				at bp			

(Continued)

TABLE 4.1.1.3.2 (Continued)

2.

Wieczorek & Kobayashi 81		Sasse et al. 1988		Verevkin 2003	
differential pressure gauge		electronic manometer		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
151.15	7221	−14.44	0.189	20.95	6.86
158.75	9929	−9.64	0.317	24.05	8.85
166.42	12812	10.14	23386	27.05	11.17
175.40	16969	20.18	6.093	30.15	14.29
182.48	21024	30.15	13.73	33.15	17.51
189.45	25738	40.04	28.40	35.15	20.29
196.03	30891	49.90	56.53	36.15	22.51
202.35	36636	59.89	107	38.05	25.25
210.18	44906	69.98	194	39.05	26.72
217.70	54250	79.94	35.42	42.15	32.68
225.93	66313	89.99	579	45.15	41.63
233.82	79716	100.06	950	47.15	53.96
240.26	92116	110.04	1507	51.05	67.87
243.27	98620	115.10	1888		
244.60	101629			eq. 4a	P/kPa
254.66	126232	eq. 2	P/mmHg	P ^o	101.325 kPa
263.69	151814	A	7.27126	A	298.831/R
271.70	177915	B	2006.862	B	83537.555/R
		C	212.625	C	78.6/R
data fitted to				R = 8.314 J K ^{−1} mol ^{−1}	
Chebyshev polynomial		$\Delta H_v/(kJ\ mol^{-1}) = 60.58$		$\Delta H_v/(kJ\ mol^{-1}) = 60.7$	
temp range 424–593 K		at 25°C		at 25°C	

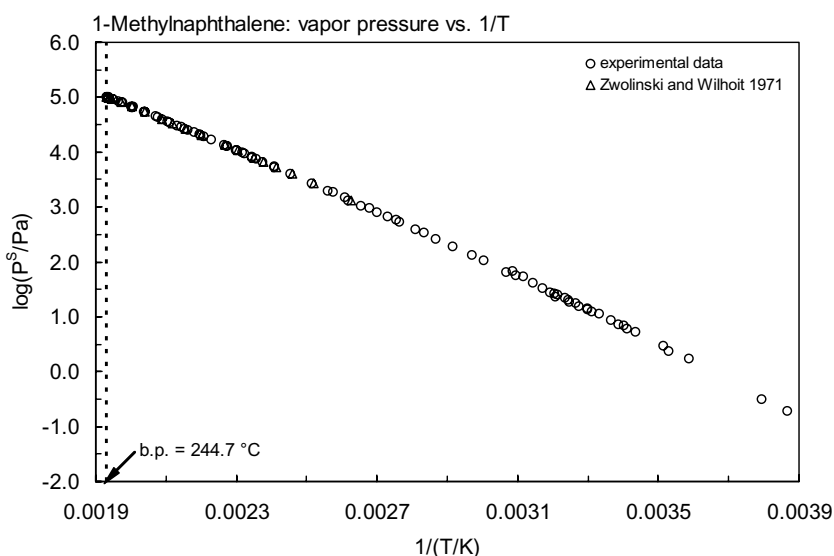


FIGURE 4.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 1-methylnaphthalene.

TABLE 4.1.1.3.3

Reported Henry's law constants of 1-methylnaphthalene at various temperatures and temperature dependence equations

Bamford et al. 1999		
gas stripping-GC/MS		
t/°C	H/(Pa m ³ /mol)	H/(Pa m ³ /mol)
		average
4.1	9.41, 10.7	10.1
11.0	16.6, 18.2	17.4
18.0	27.8, 30.8	29.2
25.0	44.8, 51.0	47.8
31.0	65.7, 78.2	71.7
$\ln K_{AW} = A - B/(T/K)$		
A	15.636	
B	5821.5	
enthalpy, entropy change:		
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 48.4 \pm 1.4$		
$\Delta S/(\text{J}\cdot\text{K}^{-1}\text{ mol}^{-1}) = 130$		
at 25°C		

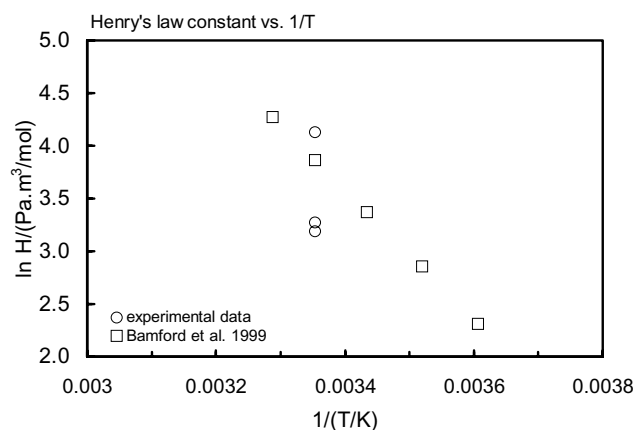
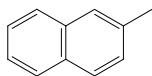


FIGURE 4.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for 1-methylnaphthalene.

4.1.1.4 2-Methylnaphthalene



Common Name: 2-Methylnaphthalene

Synonym: β -methylnaphthalene

Chemical Name: 2-methylnaphthalene

CAS Registry No: 91-57-6

Molecular Formula: $C_{11}H_{10}$

Molecular Weight: 142.197

Melting Point ($^{\circ}C$):

34.6 (Weast 1972–73; Lide 2003)

Boiling Point ($^{\circ}C$):

241.1 (Weast 1977; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0058 (Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

141.4 ($20^{\circ}C$, calculated-density)

169.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

59.40, 45.20 (25° , bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.924 (Parks & Huffman 1931)

5.61, 12.13; 17.74 (15.35, $34.25^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

39.25 (Tsonopoulos & Prausnitz 1971)

19.43, 39.43 (15.35, $34.25^{\circ}C$, Chickos et al. 1999)

58.87, 44.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.805 (mp at $34.6^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

24.6 (shake flask-GC, Eganhouse & Calder 1976)

25.4 (shake flask-fluorescence, Mackay & Shiu 1977)

20.0 (Vozňáková et al. 1978)

25.6 (average lit. value, Pearlman et al. 1984)

27.3 (generator column-HPLC, Vadas et al. 1991)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9.07* (Hg manometer, extrapolated-Antoine eq., Camin & Rossini 1955)

$\log (P/mmHg) = 7.06850 - 1840.268/(198.395 + t/^{\circ}C)$; temp range 139.1 – $242^{\circ}C$ (Antoine eq., Hg manometer, Camin & Rossini 1955)

10.67 (calculated by formula, Dreisbach 1955)

$\log (P/mmHg) = 7.06850 - 1840.268/(198.395 + t/^{\circ}C)$, temp range 130 – $300^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

9.07* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 7.06850 - 1840.268/(198.395 + t/^{\circ}C)$; temp range 104.85 – $274.3^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

9.07 (extrapolated-Antoine eq., Boublik et al. 1973)

5.60 ($20^{\circ}C$, Vozňáková et al. 1978)

8629* ($151.26^{\circ}C$, differential pressure gauge, measured range 151.26 – $279.81^{\circ}C$, Wiczorek & Kobayashi 1981)

$\log (P/atm) = [1 - 514.242/(T/K)] \times 10^4 \{0.879050 - 5.85793 \times 10^{-4} \cdot (T/K) + 4.19235 \times 10^{-7} \cdot (T/K)^2\}$; temp range 378.0 – $629.32 K$ (Cox eq., Chao et al. 1983)

9.08 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.19638 - 1842.831/(198.692 + t/^{\circ}\text{C})$; temp range 139.2–241.76°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6.31 (GC-RT correlation, supercooled liquid, Bidleman 1984)

9.033 (extrapolated, Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.0685 - 1840.268/(198.4 + t/^{\circ}\text{C})$; temp range 105–274°C (Antoine eq., Dean 1985, 1992)

9.33 (extrapolated from Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.21475 - 1858.19/(-72.479 + T/\text{K})$; temp range 423–515 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 56.2052 - 5.2563 \times 10^3/(T/\text{K}) - 16.195 \cdot \log (T/\text{K}) + 8.1583 \times 10^{-11} \cdot (T/\text{K}) + 3.0253 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 308–761 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

32.23 (wetted-wall column-GC, Fendinger & Glotfelty 1990)

50.6 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

20.265* (26°C EPICS-GC, Hansen et al. 1993)

46.0 (gas stripping-HPLC/fluor., De Maagd et al. 1998)

62.0 (gas stripping-GC, Altschuh et al. 1999)

51.3* (gas stripping-GC; Bamford et al. 1999)

$\ln K_{AW} = -5099.83/(T/\text{K}) + 13.23$; $\Delta H = 42.4 \text{ kJ mol}^{-1}$; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

18620 (20°C, selected value based on Hansen et al. 1993 data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 2.245 - 399/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.864 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

3.86 (Hansch & Leo 1979)

4.11 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)

3.70 (HPLC- k' correlation, Hanai et al. 1981)

4.01 (HPLC-RT correlation, Eadsforth 1986)

4.09 (HPLC-RT correlation, Wang et al. 1986)

4.00 (recommended, Sangster 1989)

3.86 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

2.61 (quoted from Davies & Dobbs 1984, Sabljic 1987)

2.65 (calculated-MCI χ , Sabljic 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

3.93 (natural sediments, average sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)

3.40 (sediment 4.02% from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)

3.719; 3.72, 3.71 (sediment: concn ratio $C_{\text{sed}}/C_{\text{w}}$; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2}$ (calc) = 54 h for direct sunlight photolysis at 40°N latitude of midday in midsummer in near surface water, $t_{1/2}$ = 410 d in inland water and $t_{1/2}$ = 440 d in inland water with sediment partitioning (Zepp & Schlotzhauer 1979);

$t_{1/2}$ = 410 d under summer sunlight in surface water (Mill & Mabey 1985);

$k = 0.042 \text{ h}^{-1}$ with $t_{1/2}$ = 6.4 h in distilled water (Fukuda et al. 1988);

direct photolysis $t_{1/2}$ = 9.23 h predicted - QSPR, in atmospheric aerosol (Chen et al. 2001).

Hydrolysis:

Oxidation: rate constant, k for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (5.23 \pm 0.42) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime of ~5 h, and

$k_{\text{O}_3} < 4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate, Atkinson & Aschmann 1986)

$k_{\text{N}_2\text{O}_5} = (4.2 \pm 0.9) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with N_2O_5 at $298 \pm 2 \text{ K}$ (relative rate method, Atkinson & Aschmann 1987)

$k_{\text{OH}} = 5.23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{O}_3} < 0.4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{N}_2\text{O}_5} = 4.2 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 at room temp. (Atkinson & Aschmann 1987, 1988)

$k_{\text{OH}} = 52.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 57.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}} = (4.86 \pm 0.25) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ with a calculated tropospheric lifetime to be 3.4 h using a global tropospheric 12-h daytime average OH radical concn of $2.0 \times 10^6 \text{ molecule/cm}^3$ (relative rate method, Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated atmospheric lifetime of ~4 h due to reaction with OH radical (Atkinson & Aschmann 1986)

atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radicals and with N_2O_5 can be calculated to range from ~4 to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987);

direct photolysis $t_{1/2} = 9.23 \text{ h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001);

a calculated tropospheric lifetime to be 3.4 h using a global tropospheric 12-h daytime average OH radical concn of $2.0 \times 10^6 \text{ molecule/cm}^3$ for the reaction with OH radical (Phousong-phouang & Arey 2002).

Surface water: computed near-surface $t_{1/2} = 54 \text{ h}$ and for direct photochemical transformation at latitude 40°N , midday, midsummer; $t_{1/2} = 410 \text{ d}$ with no sediment-water partitioning and $t_{1/2} = 440 \text{ d}$ with sediment-water partitioning by direct photolysis in a 5-m deep Inland Water Body (Zepp & Schlotzhauer 1979);

$t_{1/2} = 410 \text{ d}$ under summer sunlight (Mill & Mabey 1985);

rate constants and half-lives: $k = 0.064 \text{ d}^{-1}$, $t_{1/2} = 11 \text{ d}$ in spring at $8\text{--}16^\circ\text{C}$, $k = 0.687 \text{ d}^{-1}$, $t_{1/2} = 1.0 \text{ d}$ in summer at $20\text{--}22^\circ\text{C}$, $k = 0.054 \text{ d}^{-1}$, $t_{1/2} = 13 \text{ d}$ in winter at $3\text{--}7^\circ\text{C}$ for the periods when volatilization appears to dominate, and $k = 0.046 \text{ d}^{-1}$, $t_{1/2} = 15.1 \text{ d}$ with HgCl_2 as poison, and $k = 0.954 \text{ d}^{-1}$, $t_{1/2} = 0.7 \text{ d}$ without poison in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

TABLE 4.1.1.4.1

Reported vapor pressures of 2-methylnaphthalene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Wieczorek & Kobayashi 1981	
ebulliometry		selected values		differential pressure gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
139.193	5536	104.85	1333	151.26	8629
145.431	6951	120.68	2666	158.72	10992
150.655	8339	130.73	4000	164.34	13183

TABLE 4.1.1.4.1 (Continued)

Camin & Rossini 1955		Zwolinski & Wilhoit 1971		Wieczorek & Kobayashi 1981	
ebulliometry		selected values		differential pressure gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
154.676	9539	138.25	5333	169.89	15615
158.689	10942	144.329	6666	175.93	18756
164.155	13100	149.459	7999	181.84	22550
176.722	19433	157.872	10666	189.18	27850
182.322	22882	164.486	13332	196.20	33812
190.033	28551	177.752	19998	202.04	39538
197.234	34820	187.610	26664	209.49	48007
205.329	43163	195.619	33331	217.00	57974
213.963	53782	202.414	39997	225.34	70794
223.026	67089	213.626	53329	232.47	83506
239.613	98125	222.764	66661	239.90	96992
240.336	99734	230.537	79993	246.90	114865
240.957	101114	237.336	93326	254.69	134992
241.760	102929	238.602	95992	263.24	160539
		239.840	98659	271.29	188158
eq. 2	P/mmHg	240.449	99992	279.81	221176
A	7.06850	241.052	101325		
B	1840.268				
C	198.395	eq. 2	P/mmHg	exptl data fitted to Chebyshev polynomial temp range 424–639 K	
bp/°C	241.052	A	7.06850		
		B	1840.268		
		C	198.395		
		bp/°C	241.052		

$\Delta H_v/(\text{kJ mol}^{-1}) = 46.0$
at bp

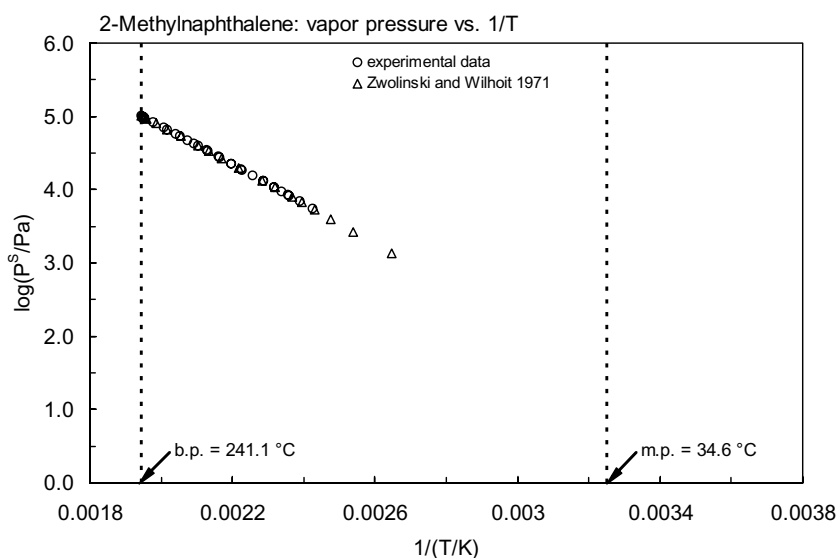


FIGURE 4.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylnaphthalene.

TABLE 4.1.1.4.2

Reported Henry's law constants of 2-methylnaphthalene at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1) \quad \log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \quad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4) \quad \ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

Hansen et al. 1993

Bamford et al. 1999

EPICS-GC

gas stripping-GC/MS

t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	H/(Pa m ³ /mol)
				average
26.0	20.265	4.1	10.5, 16.2	13.0
35.8	22.900	11.0	18.2, 24.4	21.0
46.0	26.243	18.0	28.8, 38.3	33.2
		25.0	42.1, 62.5	51.3
eq. 4	H/(Pa m ³ /mol)	31.0	56.2, 95.5	73.3
A	7.0 ± 0.14			
B	1234 ± 44	eq. 1	K _{AW}	
		A	13.2307	
		B	5100	
		enthalpy, entropy change:		
		$\Delta H/(\text{kJ} \cdot \text{mol}^{-1}) = 42.4 \pm 4.2$		
		$\Delta S/(\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}) = 110$		
		at 25°C		

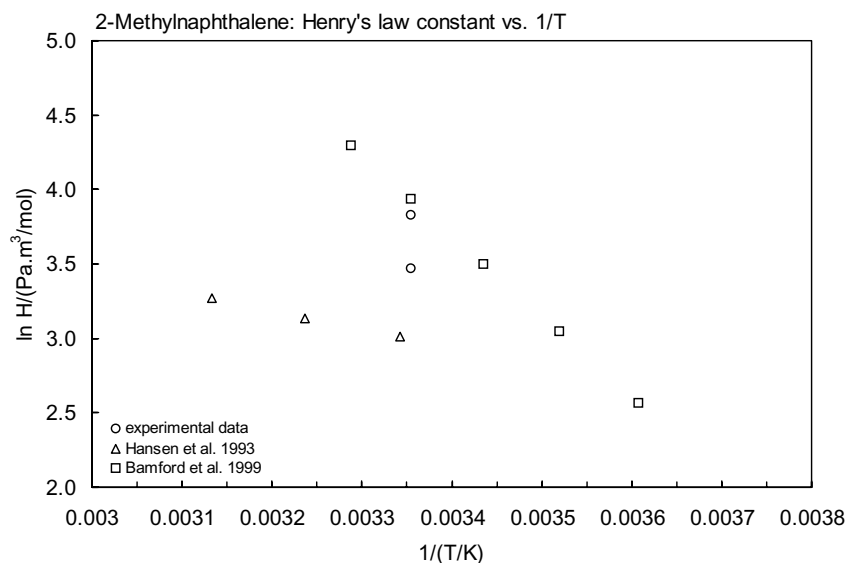
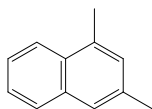


FIGURE 4.1.1.4.2 Logarithm of Henry's law constant versus reciprocal temperature for 2-methylnaphthalene.

4.1.1.5 1,3-Dimethylnaphthalene



Common Name: 1,3-Dimethylnaphthalene

Synonym:

Chemical Name: 1,3-dimethylnaphthalene

CAS Registry No: 575-41-7

Molecular Formula: $C_{12}H_{12}$

Molecular Weight: 156.223

Melting Point ($^{\circ}C$):

−6.0 (Weast 1982–83; Dean 1985; Lide 2003)

Boiling Point ($^{\circ}C$):

263 (Dreisbach 1955; Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0063, 1.0026 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.0144 (Weast 1982–83; Dean 1985; Lide 2003)

Molar Volume (cm^3/mol):

154.0 ($20^{\circ}C$, calculated-density)

192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

69.58, 48.69 ($25^{\circ}C$, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

8.00 (shake flask-fluorescence, Mackay & Shiu 1977)

7.81 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.947 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.0469 - 1845.6/(180.0 + t/^{\circ}C)$; temp range 150 – $313^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [1 - 540.353/(T/K)] \times 10^{\{1.72680 - 7.87991 \times 10^{-4} \cdot (T/K) + 42.8535 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 400.0 – $541.0 K$ (Cox eq., Chao et al. 1983)

6.950 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.6347 - 2295.4/(232.4 + t/^{\circ}C)$; temp range 20 – $148^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.2698 - 2076.0/(210 + t/^{\circ}C)$; temp range 148 – $310^{\circ}C$ (Antoine eq., Dean 1985, 1992)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

71.03 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.421 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

4.42 (Hansch & Leo 1979)

4.42 (recommended, Sangster 1993)

4.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 , or as indicated *data at other temperatures see original reference:

$k_{OH} = (7.49 \pm 0.39) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(298 \pm 2) \text{ K}$ with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ (relative rate method, Phouongphouang & Arey 2002)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ for the reaction with OH radical (Phouongphouang & Arey 2002).

Surface water:

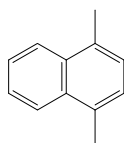
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

4.1.1.6 1,4-Dimethylnaphthalene



Common Name: 1,4-Dimethylnaphthalene

Synonym:

Chemical Name: 1,4-dimethylnaphthalene

CAS Registry No: 571-58-4

Molecular Formula: $C_{12}H_{12}$

Molecular Weight: 156.223

Melting Point ($^{\circ}C$):

7.60 (Lide 2003)

Boiling Point ($^{\circ}C$):

268 (Dreisbach 1955, Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0166, 1.0129 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.0166 (Weast 1982–83)

Molar Volume (cm^3/mol):

153.7 ($20^{\circ}C$, calculated-density)

192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.315, 48.62 ($25^{\circ}C$, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.6 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

37.87, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

11.4 (shake flask-fluorescence, Mackay & Shiu 1977)

11.40 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.55 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.0527 - 1869.0/(180.0 + t/^{\circ}C)$; temp range 155 – $310^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [1 - 544.363/(T/K)] \times 10^{\{1.57594 - 8.55425 \times 10^{-4} \cdot (T/K) + 51.4189 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 397.0 – $544 K$ (Cox eq., Chao et al. 1983)

2.27 (calculated-TSA, Amidon & Anik 1981; selected, Ma et al. 1990)

4.50 (interpolated, Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.6347 - 2345.8/(232.6 + t/^{\circ}C)$; temp range 20 – $148^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.2698 - 2076.0/(210 + t/^{\circ}C)$; temp range 148 – $310^{\circ}C$ (Antoine eq., Dean 1985, 1992)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

48.84 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.372 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

4.37 (Hansch & Leo 1979)

4.37 (recommended, Sangster 1989, 1993)

4.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 , or as indicated *data at other temperatures see original reference:

$k_{OH} = (5.79 \pm 0.36) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(298 \pm 2)K$ with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ (relative rate method, Phousongphouang & Arey 2002)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:

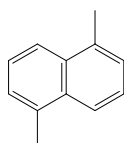
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

4.1.1.7 1,5-Dimethylnaphthalene



Common Name: 1,5-Dimethylnaphthalene

Synonym:

Chemical Name: 1,5-dimethylnaphthalene

CAS Registry No: 571-61-9

Molecular Formula: $C_{12}H_{12}$

Molecular Weight: 156.223

Melting Point ($^{\circ}C$):

82 (Dreisbach 1955; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

265 (Dreisbach 1955; Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.276 (mp at $82^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.74 (shake flask-GC, Eganhouse & Calder 1976)

3.38 (shake flask-fluorescence, Mackay & Shiu 1977)

3.12 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations.):

$\log(P/mmHg) = 7.0493 - 1855.0/(180.0 + t/^{\circ}C)$; temp range 150 – $313^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1.93; 0.513 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -3346/(T/K) + 11.51$; $\Delta H_{vap} = -64.1$ kJ \cdot mol $^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

35.5 (gas stripping-fluorescence, Mackay et al. 1982)

61.8 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

36.3 (gas stripping, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.38 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

4.38 (Hansch & Leo 1979)

4.38 (recommended, Sangster 1989, 1993)

4.38 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 , or as indicated *data at other temperatures see original reference:

$k_{\text{OH}} = (6.01 \pm 0.35) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(298 \pm 2) \text{ K}$ with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ (relative rate method, Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: a calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:

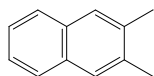
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

4.1.1.8 2,3-Dimethylnaphthalene



Common Name: 2,3-Dimethylnaphthalene

Synonym: guaiene

Chemical Name: 2,3-dimethylnaphthalene

CAS Registry No: 581-40-8

Molecular Formula: $C_{12}H_{12}$

Molecular Weight: 156.223

Melting Point ($^{\circ}C$):

105 (Dreisbach 1955; Weast 1972–73; Lide 2003)

Boiling Point ($^{\circ}C$):

268 (Dreisbach 1955; Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.003 (Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

155.8 ($20^{\circ}C$, calculated-density)

192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.315, 48.97 ($25^{\circ}C$, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.10 (Ruelle & Kesselring 1997)

15.9 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

42.06, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.164 (mp at $105^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.99 (shake flask-GC, Eganhouse & Calder 1976)

3.0 (shake flask-fluorescence, Mackay & Shiu 1977)

2.50 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.55 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.0527 - 1869.0/(180.0 + t/^{\circ}C)$; temp range $155-315^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1.86 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 631.969/(T/K)] \times 10^{\{1.09999 - 10.2378 \times 10^{-4} \cdot (T/K) + 11.3931 \times 10^{-7} \cdot (T/K)^2\}}$; temp range $333.15-408.15 K$ (Cox eq., Chao et al. 1983)

0.91 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.27335 - 1383.083/(141.333 + t/^{\circ}C)$; temp range $105-135^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.543 (interpolated, Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.40396 - 2111.9/(201.1 + t/^{\circ}C)$; temp range $20-155^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.0527 - 1869/(180 + t/^{\circ}C)$; temp range $155-315^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.437 (Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.635 - 4172.6/(T/K)$; temp range $278-301 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.97875 - 2959.733/(-59.936 + T/K)$; temp range $333-373 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.18084 - 1544.764/(-116.821 + T/K)$; temp range $378-408 K$ (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 38.92 (calculated-P/C, Eastcott et al. 1988)
- 92.16, 64.9 (quoted, calculated-bond contribution method, Meylan & Howard 1991)
- 59.9 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 4.396 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)
- 4.40 (Hansch & Leo 1979)
- 4.40 (recommended, Sangster 1993)
- 4.40 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (7.68 \pm 0.48) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, with a calculated atmospheric lifetime of $\sim 4 \text{ h}$, and

$k_{\text{O}_3} < 4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate method, Atkinson & Aschmann 1986)

$k_{\text{N}_2\text{O}_5} = (5.7 \pm 1.9) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 at $298 \pm 2 \text{ K}$ (relative rate method, Atkinson & Aschmann 1987)

$k_{\text{O}_3} < 0.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} = 7.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{N}_2\text{O}_5} = 5.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 at room temp. (Atkinson & Aschmann 1987, 1988)

$k_{\text{OH}} = (76.8 \pm 4.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (Atkinson 1989)

$k_{\text{OH}} = 77 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{\text{OH}} = 100.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}} = (6.15 \pm 0.47) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(298 \pm 2) \text{ K}$ using a relative rate method with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ (Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated atmospheric lifetime of $\sim 4 \text{ h}$ due to reaction with OH radical (Atkinson & Aschmann 1986); the atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radicals and with N_2O_5 can be calculated to range from ~ 4 to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987);

calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:

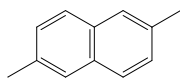
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

4.1.1.9 2,6-Dimethylnaphthalene



Common Name: 2,6-Dimethylnaphthalene

Synonym:

Chemical Name: 2,6-dimethylnaphthalene

CAS Registry No: 581-42-0

Molecular Formula: $C_{12}H_{12}$

Molecular Weight: 156.223

Melting Point ($^{\circ}C$):

112 (Lide 2003)

Boiling Point ($^{\circ}C$):

262 (Dreisbach 1955; Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.003, 0.999 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.142 (Dean 1985)

Molar Volume (cm^3/mol):

155.8 (calculated-density)

192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

69.45, 48.70 ($25^{\circ}C$, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.27 (Tsonopoulos & Prausnitz 1971)

25.06 (calorimetry, Osborn & Douslin 1975; quoted, Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

63.18 (Tsonopoulos & Prausnitz 1971)

65.39, 45.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.140 (mp at $112^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.30 (shake flask-GC, Eganhouse & Calder 1976)

2.0 (shake flask-fluorescence, Mackay & Shiu 1977)

1.72 (average lit. value, Pearlman et al. 1984)

0.997 (generator column-HPLC, Vadas et al. 1991)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

20.41 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.0460 - 1841.0/(180.0 + t/^{\circ}C)$; temp range $150-310^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

0.75 (calculated-TSA, Amidon & Anik 1981)

1.38 (extrapolated- Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 687.081/(T/K)] \times 10^4 \{1.14901 - 11.9220 \times 10^{-4} \cdot (T/K) + 17.3468 \times 10^{-7} \cdot (T/K)^2\}$; temp range $328.15-418.15 K$ (Cox eq., Chao et al. 1983)

1.41 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.19014 - 1325.209/(139.781 + t/^{\circ}C)$; temp range $111-145^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

2.036 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.3968 - 2080.3/(200.8 + t/^{\circ}C)$; temp range $20-150^{\circ}C$ (Antoine eq., Dean 1992)

$\log(P/mmHg) = 7.0460 - 1841/(180 + t/^{\circ}C)$; temp range $150-310^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.378 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.290 - 3047.828/(T/K)$; temp range $333-368 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 8.45107 - 2512.509/(-89.765 + T/\text{K})$; temp range 384–418 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.18084 - 1320.21/(-133.876 + T/\text{K})$; temp range 384–418 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -6.9795 - 2.9488 \times 10^3/(T/\text{K}) + 7.4483 \cdot \log (T/\text{K}) - 1.15821 \times 10^{-2} \cdot (T/\text{K}) + 4.3391 \times 10^{-6} (T/\text{K})^2$; temp range 383–777 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

121 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.313 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

4.31 (Hansch & Leo 1979)

4.38 (calculated-fragment const., Yalkowsky & Valvani 1979, 1980)

4.31 (recommended, Sangster 1989, 1993)

4.31 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant in distilled water $k = 0.045 \text{ h}^{-1}$ with $t_{1/2} = 15.5 \text{ h}$ (Fukuda et al. 1988).

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 , or as indicated *data at other temperatures see original reference:

$k_{OH} = (6.65 \pm 0.35) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(298 \pm 2) \text{ K}$ with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ (relative rate method, Phoussongphouang & Arey 2002)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: a calculated tropospheric lifetime to be 1.9–2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ for the reaction with OH radical (Phoussongphouang & Arey 2002).

Surface water:

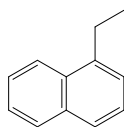
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995)

4.1.1.10 1-Ethyl-naphthalene



Common Name: 1-Ethyl-naphthalene

Synonym: α -ethyl-naphthalene

Chemical Name: 1-ethyl-naphthalene

CAS Registry No: 1127-76-0

Molecular Formula: $C_{12}H_{12}$

Molecular Weight: 156.223

Melting Point ($^{\circ}C$):

−13.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

258.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.00816, 1.00446 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.0082 (Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

155.0 ($20^{\circ}C$, calculated-density)

192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

67.42, 46.92 ($25^{\circ}C$, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

10.7 (shake flask-fluorescence, Mackay & Shiu 1977)

10.0* (shake flask-fluorescence, Schwarz & Wasik 1977)

10.0* (shake flask-fluorescence, Schwarz 1977)

11.58 (generator column-HPLC, Wasik et al. 1981)

10.31 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

133.3* ($70.0^{\circ}C$, summary of literature data, temp range 70.0 – $258.1^{\circ}C$, Stull 1947)

3.0 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.9599 - 1791.4/(180.5 + t/^{\circ}C)$; temp range 145 – $310^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

2.51* (extrapolated from liquid state, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 7.03159 - 1841.320/(185.28 + t/^{\circ}C)$; temp range 120 – $292^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/atm) = [1 - 531.480/(T/K)] \times 10^{0.923623 - 6.97505 \times 10^{-4} \cdot (T/K) + 5.07450 \times 10^{-7} \cdot (T/K)^2}$; temp range 393.15 – 565.45 K (Cox eq., Chao et al. 1983)

2.51 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.15645 - 1841.32/(-87.87 + T/K)$; temp range 393 – 565 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 7.5650 - 3.7597 \times 10^3/(T/K) + 2.6035 \cdot \log(T/K) - 1.1581 \times 10^{-2} \cdot (T/K) + 5.1365 \times 10^{-6} \cdot (T/K)^2$; temp range 259 – 776 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 14.8 (calculated-P/C, Eastcott et al. 1988)
- 36.7 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 69.4 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 4.39 (calculated-fragment const., Yalkowsky & Valvani 1979, 1980)
- 4.38 (calculated-fragment const., Yalkowsky et al. 1983)
- 4.42 (calculated-solvatochromic parameters and V_{I} , Kamlet et al. 1988)
- 4.40 (recommended, Sangster 1989, 1994)
- 4.44 (calculated-molar volume, Wang et al. 1992)
- 4.8016 (calculated-UNIFAC group contribution, Chen et al. 1993)
- 4.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 3.77 (sediment, HPLC- k' correlation, Vowles & Mantoura 1987)
- 3.89 (HPLC-capacity factor correlation, Hodson & Williams 1988)
- 3.78 (calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 , or as indicated *data at other temperatures see original reference:

$k_{\text{OH}} = (3.64 \pm 0.41) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(298 \pm 2)\text{K}$ with a calculated tropospheric lifetime to be 3.8 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ (relative rate method, Phoungphouang & Arey 2002)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: a calculated tropospheric lifetime to be 3.8 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^6 \text{ molecule cm}^{-3}$ for the reaction with OH radical (Phoungphouang & Arey 2002).

Surface water:

Groundwater:

Sediment:

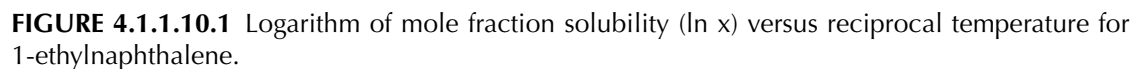
Soil:

Biota: elimination $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

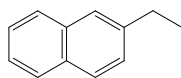
TABLE 4.1.1.10.1

Reported aqueous solubilities and vapor pressures of 1-ethylnaphthalene at various temperatures

Aqueous solubility				Vapor pressure			
Schwarz 1977		Schwarz & Wasik 1977		Stull 1947		Zwolinski & Wilhoit 1971	
shake flask-fluorescence		shake flask-fluorescence		summary of literature data		selected values	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
8.6	8.124	10	8.1	70.0	133.3	120.0	1333
11.1	8.124	14	8.1	101.4	666.6	136.04	2666
14.0	8.28	20	10	116.8	1333	146.22	4000
17.1	8.593	25	10	133.8	2666	153.85	5333
20.0	8.436			152.0	5333	160.01	6666
23.0	8.593			164.1	7999	165.22	7999
25.0	10.0			180.0	13332	173.76	10666
26.1	9.842			204.6	26664	180.67	13332
31.7	11.72			230.8	53329	193.94	19998
				258.1	101325	203.96	26664
						212.10	33331
				mp/°C	–27	219.01	39997
						230.41	53329
						239.71	66661
						247.62	79993
						254.54	93326
						255.83	95992
						257.09	98659
						258.94	101325
						log P = A – B/(C + t/°C)	
						P/mmHg	
						A	7.03159
						B	1841.320
						C	185.28
						bp/°C	258.33
						$\Delta H_v/(kJ\ mol^{-1}) =$	
						at 25°C	–
						at bp	48.1



4.1.1.11 2-Ethyl-naphthalene



Common Name: 2-Ethyl-naphthalene

Synonym: β -ethyl-naphthalene

Chemical Name: 2-ethyl-naphthalene

CAS Registry No: 939-27-5

Molecular Formula: $C_{12}H_{12}$

Molecular Weight: 156.223

Melting Point ($^{\circ}C$):

−7.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

258 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9922 (Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

157.4 ($20^{\circ}C$, calculated from density)

192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

66.99, 47.33 (25° , bp, Dreisbach 1955)

64.7 (Lei et al. 2002)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

7.97 (shake flask-GC, Eganhouse & Calder 1976)

7.97 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3.76 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 8.0819 - 1886.0/(191.0 + t/^{\circ}C)$; temp range 145–300 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

3.24* (extrapolated from liq. state, Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981)

$\log(P/mmHg) = 7.07566 - 1880.73/(191.41 + t/^{\circ}C)$; temp range 119.14–291.9 $^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

4.21* (extrapolated exptl. data, Macknick & Prausnitz 1979; quoted, Mackay & Shiu 1981)

$\log(P/mmHg) = 21.485 - 7435.9/(T/K)$; temp range 13.05–45.1 $^{\circ}C$ (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)

$\log(P/atm) = [1 - 531.189/(T/K)] \times 10^{\{0.871612 - 5.23140 \times 10^{-4} \cdot (T/K) + 3.70623 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 286.2–565.05 K (Cox eq., Chao et al. 1983)

4.21 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.46683 - 3232.791/(T/K)$; temp range 286–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.20056 - 1880.73/(-82.74 + T/K)$; temp range 393–565 K (Antoine eq.-II, Stephenson & Malanowski 1987)

3.71* (pressure gauge in vacuum cell, interpolated-Antoine eq. derived from exptl. data, temp range, −4.65–125 $^{\circ}C$, Sasse et al. 1988)

$\log(P_L/mmHg) = 6.83511 - 1799.779/(189.505 + t/^{\circ}C)$; temp range −4.65 to 125.09 $^{\circ}C$ (Antoine eq., pressure gauge, Sasse et al. 1988)

$\log(P/kPa) = 7.46683 - 3232.79/(T/K)$; temp range 5–50 $^{\circ}C$ (regression eq. from literature data, Shiu & Ma 2000)

2.56; 0.633 (supercooled liquid P_L ; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -3381/(T/K) + 11.75$; $\Delta H_{vap} = -64.7 kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol at 25°C):

- 82.2 (calculated-P/C, Mackay & Shiu 1981)
 63.2 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
 54.5 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:

- 4.377 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)
 4.43 (HPLC-k' correlation, Vowles & Mantoura 1987)
 4.38 (recommended, Sangster 1989, 1994)
 4.38 (recommended, Hansch et al. 1995)
 4.00 (HPLC-k' correlation, Ritter et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

- 3.76 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
 3.76 (calculated-MCI ¹χ, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: k = 0.038 h⁻¹ in distilled water with t_{1/2} = 18.4 h (Fukuda et al. 1988).

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃, or as indicated *data at other temperatures see original reference:

k_{OH} = (4.02 ± 0.55) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at (298 ± 2) K with a calculated tropospheric lifetime to be 3.5 h using a global tropospheric 12-h daytime average OH radical concentration of 2.0 × 10⁶ molecule cm⁻³ (relative rate method, Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: t_{1/2} = 18.4 h in distilled water (Fukuda et al. 1988).

Groundwater:

Sediment:

Soil:

Biota: elimination t_{1/2} = 2 d from Oyster for naphthalenes (quoted, Meador et al. 1995).

TABLE 4.1.1.11.1

Reported vapor pressures of 2-ethylnaphthalene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
Zwolinski & Wilhoit 1971	Macknick & Prausnitz 1979	Sasse et al. 1988	
selected values	gas saturation	electronic manometer	
t/°C	P/Pa	t/°C	P/Pa
119.14	1333	13.05	1.533
135.28	2666	17.90	2.213

TABLE 4.1.1.11.1 (Continued)

Zwolinski & Wilhoit 1971		Macknick & Prausnitz 1979		Sasse et al. 1988	
selected values		gas saturation		electronic manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
145.52	4000	22.90	3.40	10.17	0.880
153.19	5333	29.50	6.213	20.08	2.426
159.38	6666	34.85	9.799	20.16	2.40
164.61	7999	39.40	13.16	30.11	6.05
173.19	10666	45.10	20.0	40.01	13.33
180.13	13332			49.93	27.33
193.45	19998	eq. 1a	P/mmHg	59.92	54.26
203.49	26664	A	21.485	69.96	103.6
211.65	33331	B	7435.9	79.98	187.9
218.57	39997			90.01	326.8
230.00	53329			100.08	551.8
239.31	66661			110.08	898.1
247.22	79993			120.02	1420
254.15	93326			125.09	1771
255.44	94659				
255.83	95992			eq. 2	P/mmHg
256.70	98659			A	6.83541
257.32	99992			B	1799.779
257.93	101325			C	189.505
eq. 2	P/mmHg				
A	7.07566				
B	1880.73				
C	191.41				
bp/°C	257.93				
$\Delta H_v/(\text{kJ mol}^{-1}) = 48.1$					
at bp					

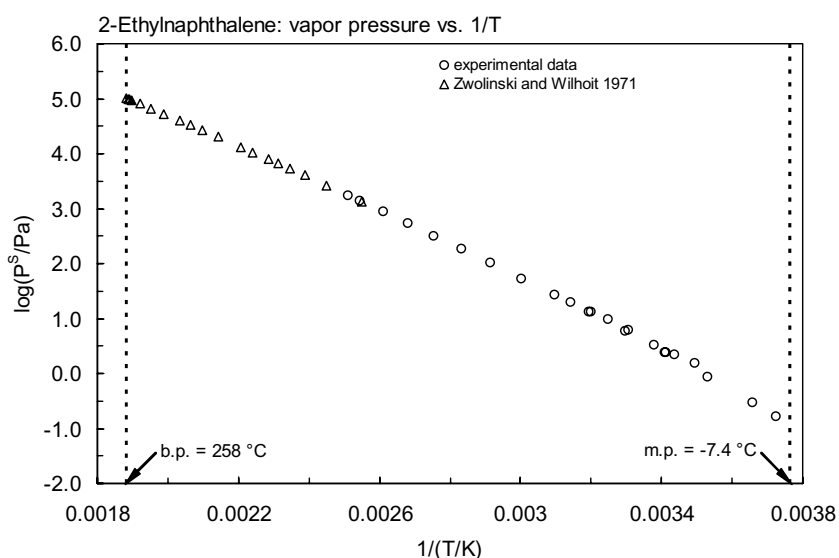
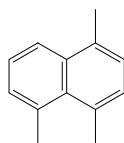


FIGURE 4.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for 2-ethylanthracene.

4.1.1.12 1,4,5-Trimethylnaphthalene



Common Name: 1,4,5-Trimethylnaphthalene

Synonym:

Chemical Name: 1,4,5-trimethylnaphthalene

CAS Registry No: 2131-41-1

Molecular Formula: $C_{13}H_{14}$

Molecular Weight: 170.250

Melting Point ($^{\circ}C$):

63 (Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Zwolinski & Wilhoit 1971)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

169.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

214.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.424 (mp at $63^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.10 (shake flask-fluorescence, Mackay & Shiu 1977)

2.04 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.681 (supercooled liquid P_L , Chao et al. 1983)

$\log(P_L/atm) = [1 - 558.187/(T/K)] \times 10^4 \{0.998467 - 7.03095 \times 10^{-4} \cdot (T/K) + 1.71801 \times 10^{-7} \cdot (T/K)^2\}$; temp range 415.15–558.15 K (Cox eq., Chao et al. 1983)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

23.50 (calculated-P/C, Eastcott et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.90 (calculated-fragment const., Yalkowsky & Valvani 1979, 1980)

4.79 (calculated-solubility and mp, Mackay et al. 1980)

4.94 (calculated-solvatochromic parameters and intrinsic molar volume V_I , Kamlet et al. 1988)

5.10 ± 0.50 (recommended, Sangster 1989)

4.91 (calculated-molar volume, Wang et al. 1992)

5.6829 (calculated-UNIFAC group contribution, Chen et al. 1993)

4.79 (recommended, Sangster 1993)

4.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

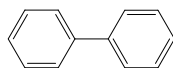
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 2$ d from Oyster for naphthalenes (quoted, Meador et al. 1995).

4.1.1.13 Biphenyl



Common Name: Biphenyl

Synonym: diphenyl, phenylbenzene

Chemical Name: biphenyl

CAS Registry No: 92-52-4

Molecular Formula: $C_{12}H_{10}$

Molecular Weight: 154.207

Melting Point ($^{\circ}C$):

68.93 (Lide 2003)

Boiling Point ($^{\circ}C$):

256.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.866 (Weast 1982–1983)

1.04 (Lide 2003)

Molar Volume (cm^3/mol):

148.3 ($20^{\circ}C$, calculated-density)

184.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.58 (Parks & Huffman 1931)

18.66 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

51.05 (Miller et al. 1984)

54.81, 59.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.371 (mp at $68.93^{\circ}C$)

0.35 (Mackay et al. 1980, 1983; Shiu & Mackay 1986; Shiu et al. 1987)

0.381 (calculated, $\Delta S_{fus} = 54\ J/mol\ K$, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5.94 (shake flask-UV, Andrews & Keefer 1949)

7.48* (shake flask-UV, measured range 0.4 – $42.8^{\circ}C$, Bohon & Claussen 1951)

3.87 (shake flask-UV, Sahyun 1966)

7.08* (shake flask-UV, measured range 0 – $64.5^{\circ}C$, Wauchope & Getzen 1972)

$R \cdot \ln x = -4520/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 298.15]^2 - 20.8 + 0.0273 \cdot (T/K)$, temp range 24.6 – $73.4^{\circ}C$
(shake flask-UV measurements, Wauchope & Getzen 1972)

7.45 (shake flask-GC, Eganhouse & Calder 1976)

7.0 (shake flask-fluorescence, Mackay & Shiu 1977)

8.50 (shake flask-nephelometry, Hollifield 1979)

7.51 (shake flask-LSC, Banerjee et al. 1980)

8.09 (TLC-RT correlation, Bruggeman et al. 1982)

6.71 (generator column-GC/ECD, Miller et al. 1984, 1985; quoted, Hawker 1989b)

7.09 (recommended, Pearlman et al. 1984)

7.05 (vapor saturation-UV, Akiyoshi et al. 1987)

6.5 ($29^{\circ}C$, shake flask-GC/FID; Stucki & Alexander 1987)

7.20, 7.55 (generator column-HPLC/UV, Billington et al. 1988)

10.67 (calculated average of HPLC-RI, Brodsky & Ballschmiter 1988)

7.2* (recommended, IUPAC Solubility Data Series, Shaw 1989)

$\log [S_L/(mol/L)] = 1.872 - 973.4/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -1.5792 - 3669.26/(T/K)$, temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

5.37, 5.32 (generator column-GC/ECD, different flow rates, Oleszek-Kudlak et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 7933* (162.5°C, isoteniscope-manometer, measured range 162.5–255.2°C, Chipman & Peltier 1929)
 104* (69.20°C, temp range 69.20–271.2°C, Cunningham 1930; quoted, Boublik et al. 1984)
 133.3* (70.6°C, summary of literature data, temp range 70.6–254.0°C, Stull 1947)
 1.30 (effusion method, Bright 1951)
 $\log(P/\text{mmHg}) = 10.38 - 3799/(T/K)$; temp range 4.0–34.5°C (Antoine eq., effusion, Bright 1951)
 0.031 (manometry, Augood et al. 1953; selected, Bidleman 1984)
 1.273* (effusion method, Bradley & Cleasby 1953; selected, Bidleman 1984; Neely 1983; Erickson 1986)
 $\log(P/\text{cmHg}) = 11.282 - 4263/(T/K)$; temp range 15.05–40.55°C (Antoine eq., Bradley & Cleasby 1953)
 $\log(P/\text{mmHg}) = [-0.2185 \times 12910.0/(T/K)] + 8.218583$; temp range 70.6–254.9°C (Antoine eq., Weast 1972–73)
 7.60 (selected P_L , Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1982; Bopp 1983)
 1.41* (effusion method, interpolated-Antoine eq., measured range 24.9–50.33°C, Radchenko & Kitiagorodskii 1974; selected, Bidleman 1984)
 $\log(P/\text{mmHg}) = 12.6789 - 4367.436/(T/K)$; temp range 24.9–50.33°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)
 16.0* (53.05°C, gas saturation-GC, measured range 53.05–81.05°C, Sharma & Palmer 1974)
 2040* (123.0°C, pressure transducer, measured range 123.0–327.55°C, Nasir et al. 1980)
 1.40 (HPLC-RT correlation, Swann et al. 1983)
 $\log(P/\text{atm}) = [1 - 528.437/(T/K)] \times 10^4 \{0.821410 - 2.73337 \times 10^{-4} \cdot (T/K) + 1.02285 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 342.35–673.15 K (Cox eq., Chao et al. 1983)
 5.608 (P_L supercooled liquid converted from literature P_S with ΔS_{fus} , Bidleman 1984)
 3.35, 3.41 (P_{GC} by GC-RT correlation with octadecane as reference standard, different columns, BP-1 column, Apolane-87 column, Bidleman 1984)
 $\log(P/\text{kPa}) = 6.36895 - 1997.558/(202.608 + t/^\circ\text{C})$; temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 1.19 ± 0.03; 1.03, 1.29, 0.579, 0.969 (gas saturation-GC; quoted lit. values Burkhard et al. 1984, 1985b)
 1.15* (24.7°C, gas saturation-GC/FID, measured range 5.2–24.7°C, Burkhard et al. 1984)
 $\log(P/\text{Pa}) = 14.840 - 4402.1/(T/K)$; temp range 5.2–24.7°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)
 0.423, 0.703, 0.594 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)
 2.03 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)
 $\log(P/\text{mmHg}) = 7.24541 - 1998.725/(202.733 + t/^\circ\text{C})$; temp range 69–271°C (Antoine eq., Dean 1985, 1992)
 5.61; 6.62 (supercooled liquid P_L , quoted lit.; GC-RT correlation, Foreman & Bidleman 1985)
 2.43; 6.90 (selected P_S ; supercooled liq. P_L , Shiu & Mackay 1986; Shiu et al. 1987; Sklarew & Girvin 1987)
 1.443; 1.23 (P_S , interpolated - Antoine equations; Stephenson & Malanowski 1987)
 $\log(P_S/\text{kPa}) = 11.71929 - 4143.054/(T/K)$; temp range 297–324 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_S/\text{kPa}) = 28.5175 - 21141.5/(374.85 + T/K)$; temp range 283–342 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.37526 - 1794.8/(-74.85 + T/K)$; temp range 390–563 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 3.35 (P_{GC} by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
 $\log(P/\text{mmHg}) = 53.0479 - 5.3509 \times 10^3/(T/K) - 14.955 \cdot \log(T/K) + 2.1039 \times 10^{-9} \cdot (T/K) + 2.4345 \times 10^{-6} \cdot (T/K)^2$; temp range 342–789 K (vapor pressure eq., Yaws 1994)
 0.422–2.54; 2.03–7.04 (quoted range of lit. P_S values; lit. P_L values, Delle Site 1997)
 5.31; 2.02 (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)
 $\log(P_S/\text{Pa}) = 11.05 - 3201/(T/K)$ (solid, Passivirta et al. 1999)
 $\log(P_L/\text{Pa}) = 8.20 - 2228/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log(P/\text{kPa}) = 14.840 - 4402.1/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 3.63; 0.822 (supercooled liquid P_L , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
 $\log(P_L/\text{Pa}) = -3265/(T/K) + 11.51$; $\Delta H_{\text{vap}} = -62.5 \text{ kJ} \cdot \text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 41.34 (gas stripping-GC, Mackay et al. 1979)
- 30.4 (gas stripping-GC, Mackay et al. 1980)
- 11.55 (gas stripping-GC, Warner et al. 1987)
- 19.57 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
- 86.5 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
- 31.20 (gas stripping-GC, Shiu & Mackay 1997)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 6.33 - 1255/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.16 (shake flask-UV, Rogers & Cammarata 1969)
- 4.09 (shake flask, Leo et al. 1971; Hansch & Leo 1979)
- 4.04 (shake flask, Hansch et al. 1973)
- 4.17, 4.09, 3.16, 4.04 (Neely et al. 1974; Hansch & Leo 1979)
- 3.95 (HPLC- k' correlation, Rekker & De Kort 1979)
- 3.75 (HPLC-RT correlation, Veith et al. 1979a)
- 4.04 (shake flask-HPLC, Banerjee et al. 1980)
- 3.88 (lit. average, Kenaga & Goring 1980; Freitag et al. 1985)
- 4.10 (RP-TLC- k' correlation, Bruggeman et al. 1982)
- 4.08 (HPLC- k' correlation, Hammers et al. 1982)
- 3.70 (HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)
- 3.16–4.09, 3.91 (shake flask, range, average, Eadsforth & Moser, 1983)
- 3.91–4.15, 4.05 (HPLC, range, average, Eadsforth & Moser 1983)
- 4.03 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
- 3.93 (HPLC correlation; Harnisch et al. 1983)
- 3.76 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 3.89 (generator column-HPLC, Woodburn et al. 1984)
- 3.79 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 4.11–4.13 (HPLC-RV correlation, quoted exptl., Garst 1984)
- 4.10 (HPLC-RV correlation, Garst & Wilson 1984)
- 4.05 (HPLC-RT correlation, Eadsforth 1986)
- 3.81 (shake flask-GC, Menges & Armstrong 1991)
- 4.13 (HPLC-RT correlation, Wang et al. 1986)
- 3.63 (HPLC- k' correlation, De Kock & Lord 1987)
- 3.89 (generator column-GC, Doucette & Andren 1987, 1988)
- 4.14, 4.06, 4.00, 3.94 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
- 3.69 (HPLC-RT correlation, Doucette & Andren 1988)
- 3.75 (HPLC-RT correlation, Sherblom & Eganhouse 1988)
- 4.008; 4.10 (slow stirring-GC; calculated- π const., De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 3.98 (recommended, Sangster 1989, 1993)
- 4.29 (dual-mode centrifugal partition chromatography, Gluck & Martin 1990)
- 4.26 (HPLC- k' correlation, Noegrohati & Hammers 1992)
- 4.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 6.92, 6.09; 6.09 (0, 20°C , multi-column GC- k' correlation; calculated at 20°C , Zhang et al. 1999)
- 6.15 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 2.64 (trout, calculated- k_1/k_2 , Neely et al. 1974)
- 3.12 (rainbow trout, Veith et al. 1979; Veith & Kosian 1983)
- 2.53 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 2.73, 2.45, 3.41 (algae, fish, activated sludge, Freitag et al. 1985; selected, Halfon & Reggiani 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.15 (soil, Kenaga 1980)
 3.0, 3.27 (Aldrich humic acid, reversed phase separation, Landrum et al. 1984)
 3.57, 3.77 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with 9.6 mg/L DOC: Landrum et al. 1984)
 5.58, 4.04 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 mg/L DOC, Landrum et al. 1984)
 5.68, 5.34, 5.23, 3.57 (humic materials in natural water: Huron River 6.7% DOC spring, Grand River 10.7% DOC spring, Lake Michigan 4.7% DOC spring, Lake Erie 9.6% DOC spring, RP-HPLC separation method, Landrum et al. 1984)
 3.52, 2.94 (Apison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium, Southworth & Keller 1986)
 3.40 (calculated, soil, Chou & Griffin 1987)
 3.04, 3.32, 3.26, 3.04, 3.08 (5 soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
 4.20; 3.30 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
 3.03, 3.12 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average values, Delle Site 2001)

Sorption Partition Coefficient, $\log K_p$:

- 2.146 (lake sediment, calculated- K_{OW} , f_{OC} , Formica et al. 1988)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

- Volatilization/Evaporation: $t_{1/2} = 7.52$ d evaporation from water depth of 1 m (Mackay & Leinonen 1975), rate of volatilization $k = 0.92$ g m^{-2} h^{-1} (Metcalf et al. 1988)
 Photolysis: $k = 5.1 \times 10^{-4}$ h^{-1} to 7.4×10^{-3} h^{-1} with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988);
 photodegradation $k = 5.1 \times 10^{-4}$ min^{-1} and $t_{1/2} = 22.61$ h in methanol-water (3:7, v/v) with initial concentration of 16.2 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991).
 Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH} = (8.06 \pm 0.77) \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} with an estimated lifetime of ~3 d, and $k_{O_3} < 2.0 \times 10^{-19}$ cm^3 molecule $^{-1}$ s^{-1} at 294 ± 1 K (relative rate method, Atkinson et al. 1984)
 $k_{OH} = (8.5 \pm 0.8) \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} at 295 K (relative rate method, Atkinson & Aschmann 1985)
 $k_{OH} = (7 \pm 2) \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1985)
 $k_{OH}(calc) = 7.9 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} , $k_{OH}(obs.) = (5.8 - 8.2) \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} with a calculated tropospheric lifetime of 3 d (Atkinson 1987a)
 $k_{OH}(calc) = 7.1 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} , $k_{OH}(obs.) = 7.0 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} (SAR structure-activity relationship, Atkinson 1987b)
 $k_{O_3} < 2 \times 10^{-19}$ cm^3 molecule $^{-1}$ s^{-1} ; $k_{OH} = 7.0 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} ; $k_{N_2O_5} < 2.0 \times 10^{-19}$ cm^3 molecule $^{-1}$ s^{-1} for reaction with N_2O_5 at room temp. (Atkinson & Aschmann 1988)
 $k_{OH}^* = 7.2 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} at 298 K (recommended, Atkinson 1989)
 $k_{OH}(calc) = 6.44 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} (molecular orbital calculations, Klamt 1993)
 $k_{OH}(exptl) = 7.2 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} , $k_{OH}(calc) = 6.7 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} with a calculated tropospheric lifetime of 2.0 d (Kwok et al. 1995)

Hydrolysis:

- Biodegradation: 100% degraded by activated sludge in 47 h cycle (Monsanto Co. 1972);
 $k = 109$ yr^{-1} in the water column and $k = 1090$ yr^{-1} in the sediment, microbial degradation pseudo first-order rate constant (Wong & Kaiser 1975; selected, Neely 1981);
 $k = 9.3-9.8$ $nmol$ L^{-1} d^{-1} with an initial biphenyl concentration of 4.4-4.7 $\mu mol/L$, and $k = 3.2$ $nmol$ L^{-1} d^{-1} with initial concentration of 2.9 $\mu mol/L$, rate of biodegradation in water from Port Valdez (estimated, Reichardt et al. 1981)
 $t_{1/2} = 1.5$ d, estimated by using water die-away test (Bailey et al. 1983)
 $t_{1/2}(aq. aerobic) = 36-168$ h, based on river die-away test data and activated sludge screening test data (Howard et al. 1991)
 $t_{1/2}(aq. anaerobic) = 144-672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

removal rate of 5.3 and 0.52 mg (g of volatile suspended solid d)⁻¹, degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

Biotransformation

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 6.79 \text{ h}^{-1}$; $k_2 = 0.0155 \text{ h}^{-1}$ (trout muscle, Neely et al. 1974; Neely 1979)

$k_1 = 6.8 \text{ h}^{-1}$; $1/k_2 = 65 \text{ h}$ (trout, quoted, Hawker & Connell 1985)

$\log k_1 = 2.21 \text{ d}^{-1}$; $\log 1/k_2 = 0.43 \text{ d}$ (fish, Connell & Hawker 1988)

$\log k_2 = -0.43 \text{ d}^{-1}$ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air: calculated lifetime of ~3 d due to reaction with OH radical, assuming an average daytime atmospheric OH radical concn of $\sim 1 \times 10^6 \text{ molecule/cm}^3$ (Atkinson et al. 1984);

estimated atmospheric lifetime of ~2.7 d due to reaction with the OH radical for a 24-h average OH radical concn of $5 \times 10^5 \text{ cm}^{-3}$ (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 9 d due to the rate constants of gas-phase reaction with OH radical (Atkinson 1987);

$t_{1/2} = 7.8\text{--}110 \text{ h}$, based on photooxidation half-life in air (Howard et al. 1991);

tropospheric lifetime of 2.0 d based on the experimentally determined rate constant for gas phase reaction with OH radical for biphenyl (Kwok et al. 1995).

Surface water: $t_{1/2} \sim 1.5 \text{ d}$ in river water (Bailey et al. 1983);

$t_{1/2} = 36\text{--}168 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

photolysis $t_{1/2} = 19.18 \text{ min}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2} = 72\text{--}336 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 36\text{--}168 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota: estimated $t_{1/2} = 29 \text{ h}$ from fish in simulated ecosystem (Neely 1980).

TABLE 4.1.1.13.1

Reported aqueous solubilities of biphenyl at various temperatures

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
			experimental		smoothed		
0.40	2.83	24.6	7.13	0	2.64	0	2.72
2.4	2.97	24.6	7.29	24.6	6.96	10	4.1
5.2	3.38	24.6	7.35	25	7.08	20	6.3
7.6	3.64	29.9	8.77	29.9	8.73	25	7.2
10	4.06	29.9	8.64	30.3	8.88	30	9.1
12.6	4.58	29.9	8.95	38.4	12.7	40	14.4
14.9	5.11	30.3	8.55	40.1	13.8	50	22
15.9	5.27	30.3	8.54	47.5	19.5	69	37
25	7.48	30.3	8.48	50	22.0		
25.6	7.78	38.4	13.2	50.1	22.1		
30.1	9.64	38.4	13.3	50.2	22.2		
30.4	9.58	38.4	13.5	54.7	27.7		
33.3	11.0	40.1	13.1	59.2	34.8		
34.9	11.9	40.1	13.4	60.5	37.2		
36	12.5	40.1	13.4	64.5	45.9		
42.8	17.2	47.5	18.8				

(Continued)

TABLE 4.1.1.13.1 (Continued)

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
for supercooled liquid:		47.5	19.0	temp dependence eq. 1			
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$		47.5	18.7	$\ln x$	mole fraction		
at 275 K	7.03	50.1	20.6	ΔH_{fus}	18.9 ± 0.50		
280 K	10.13	50.1	21.6	$10^2 \cdot b$	2.73 ± 0.12		
285 K	11.25	50.1	21.8	c	20.8 ± 0.4		
290 K	12.55	50.2	20.7				
295 K	13.43	50.2	21.8				
300 K	15.02	54.7	28.3				
305 K	18.58	54.7	28.8				
310 K	21.42	59.2	36.4				
315 K	21.09	59.2	36.3				
		59.2	36.0				
		60.5	40.4				
		64.5	43.7, 44.7				
		64.5	46.5				
		$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.91$					

Empirical temperature dependence equations:

Wauchope & Getzen (1972): $R \cdot \ln x = -[H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K)$ (1)

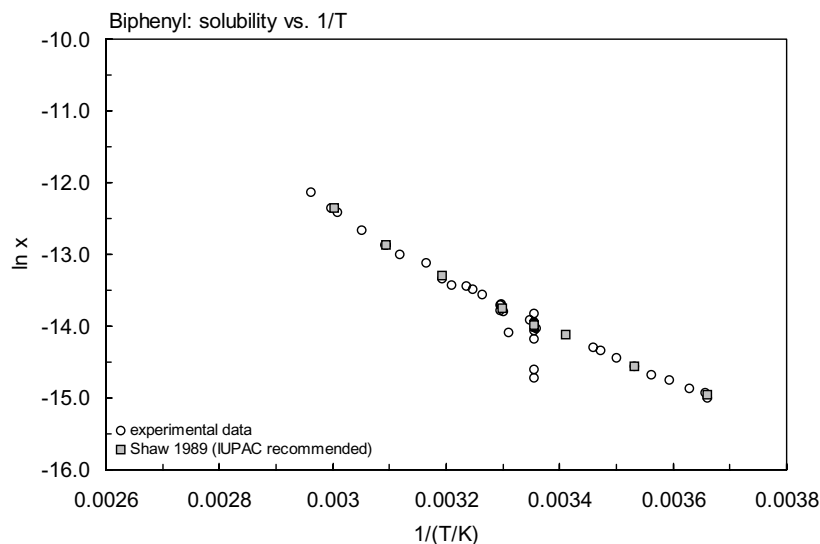


FIGURE 4.1.1.13.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for biphenyl.

TABLE 4.1.1.13.2

Reported vapor pressures of biphenyl at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K)^2 & (5) & & \end{aligned}$$

1.

Chipman & Peltier 1929		Stull 1947		Bright 1951		Bradley & Cleasby 1953				
isoteniscope-manometer		summary of literature data		effusion		effusion				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa			
162.5	7933	70.6	133.3	Data presented in graph		15.05	0.416			
172.3	10959	101.8	666.6	25	0.579	20.7	0.7786			
177.7	12799	117.0	1333	(interpolated)		24.7	1.2252			
183.5	15705	134.2	2666	eq. 1	P/mmHg	24.0	1.1825			
191.6	19972	152.5	5333	A	10.38	24.1	1.184			
198.75	24691	165.2	7999	B	3799	27.05	1.600			
293.8	28504	180.7	13332	temp range 4.9–34.5°C		29.15	2.053			
211.25	34677	204.2	26664			32.45	2.973			
220.05	43756	229.4	53329	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 72.80$		35.05	3.866			
229.8	56329	254.0	101325			37.9	5.160			
238.2	68901	mp/°C	69.5			40.55	6.693			
247.7	85580					23.05	1.027			
253.7	98019					36.5	1.533			
255.2	101178					31.25	2.546			
						35.9	4.133			
bp/°C	266.25					eq. 1	P/mmHg			
$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 44.99$										
at bp										
eq. 5	P/mmHg					temp range 15–41°C				
A	7.0220									
B	1723									
C	245700									
temp range 162–322°C										

2.

Radchenko & K. 1974		Nasir et al. 1980		Burkhard et al. 1984		Cunningham 1930	
Knudsen effusion		pressure transducer		gas saturation-GC		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.9	1.433	123.0	2040	5.2	0.106	69.20	104
31.75	2.976	143.81	4773	14.9	0.361	93.3	413
33.7	3.734	164.69	9962	24.7	1.15	148.7	4833
35.5	4.538	181.28	16447	eq. 1	P/Pa	160.0	7239
37.6	5.726	200.87	28599			171.1	10548
39.57	6.913	223.66	51518			182.2	15031
41.52	8.26	245.65	86254			193.3	21098

(Continued)

TABLE 4.1.1.13.2 (Continued)

2.

Radchenko & K. 1974		Nasir et al. 1980		Burkhard et al. 1984		Cunningham 1930	
Knudsen effusion		pressure transducer		gas saturation-GC		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
43.48	10.26	257.91	111343			204.4	28958
45.45	12.35	274.09	154493			215.6	39093
47.4	15.49	296.14	235345			226.7	51986
50.0	19.46	315.19	329300			237.8	68051
		327.55	400175			248.9	88252
eq. 1	P/mmHg					255.3	101353
A	12.6789	data fitted to Chebyshev polynomial				260.0	112384
B	4367.436					271.2	142032
for temp range 24.9–50°C							
Sharma & Palmer 1974						eq. 2	P/kPa
gas saturation-GC						A	6.36895
t/°C	P/Pa					B	1997.558
53.05	16.0					C	202.608
61.05	34.66					bp/°C	255.208
71.95	92.0						
81.05	220.0						

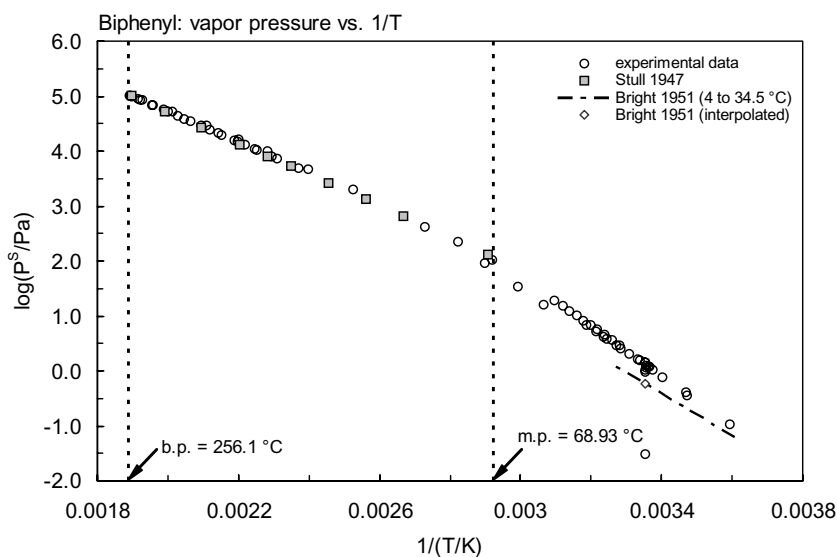
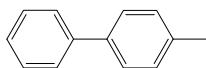


FIGURE 4.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for biphenyl.

4.1.1.14 4-Methylbiphenyl

Common Name: 4-Methylbiphenyl

Synonym: 4-phenyltoluene

Chemical Name: 4-methylbiphenyl

CAS Registry No: 644-08-6

Molecular Formula: $C_{13}H_{12}$

Molecular Weight: 168.234

Melting Point ($^{\circ}C$):

49.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

267.5 (2003)

Density (g/cm^3 at $20^{\circ}C$):

1.015 ($27^{\circ}C$, Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

165.7 ($27^{\circ}C$, calculated-density)

206.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.575 (mp at $49.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations.):

1.834, 4.05, 7.03 (4.9 , 25 , $40^{\circ}C$, generator column-HPLC/GC, Doucette & Andren 1988a)

$S/(mol/L) = 9.18 \times 10^{-6} \exp(0.038 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range 4.9 – $40^{\circ}C$, Doucette & Andren 1988a); or

$\log x = -1436/(T/K) - 1.541$; temp. range 4.9 – $40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.63 (generator column-HPLC/GC, calculated-group contribution, TSA, Doucette & Andren 1987)

4.63 (recommended, Sangster 1989, 1994)

4.63 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

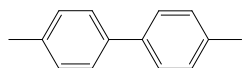
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.1.15 4,4'-Dimethylbiphenyl



Common Name: 4,4'-Dimethylbiphenyl

Synonym: 4,4'-dimethyl-1,1'-biphenyl

Chemical Name: 4,4'-dimethylbiphenyl

CAS Registry No: 613-33-2

Molecular Formula: $C_{14}H_{14}$

Molecular Weight: 182.261

Melting Point ($^{\circ}C$):

125 (Weast 1982–83; Ruelle & Kesselring 1997; Lide 2003)

Boiling Point ($^{\circ}C$):

295 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

194.0 (Ruelle & Kesselring 1997)

229.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S = 56$ J/mol K), F: 0.104 (mp at $125^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations.):

0.0687, 0.175, 0.441 (4.9, 25, $40^{\circ}C$, generator column-GC, Doucette & Andren 1988a)

$S/(mol/L) = 2.90 \times 10^{-7} \exp(0.052 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range 4 – $40^{\circ}C$, Doucette & Andren 1988a)

$\log x = -1913/(T/K) - 1.288$; temp. range 4.9 – $40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

0.931 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.09 (generator column-GC/ECD, Doucette & Andren 1987)

5.09 (recommended, Sangster 1989, 1994)

5.09 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

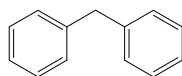
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.1.16 Diphenylmethane



Common Name: Diphenylmethane

Synonym: diphenyl methane, 1,1'-methylenebis-benzene

Chemical Name: diphenylmethane

CAS Registry No: 101-81-5

Molecular Formula: $C_{13}H_{12}$

Molecular Weight: 168.234

Melting Point ($^{\circ}C$):

25.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

265 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.00592, 1.00192 ($20^{\circ}C$, $25^{\circ}C$. Dreisbach 1955)

1.001 ($26^{\circ}C$ Lide 2003)

Molar Volume (cm^3/mol):

168.1 ($27^{\circ}C$, from density, Stephenson & Malanowski 1987)

167.2 ($20^{\circ}C$, calculated-density)

206.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

64.02 (Bright 1951)

66.845, 45.34 ($25^{\circ}C$, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.28 (Dreisbach 1955)

18.58 (Parks & Huffman 1931; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

61.92 (Stephenson & Malanowski 1987)

62.34, 62.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K, F: 0.991 (mp at $25.4^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

14.10 (shake flask/UV, Andrews and Keefer 1949)

16.40 (Deno & Berkheimer 1960)

3.76 (Lu et al. 1978)

3.00 (shake flask-nephelometry, Hollifield 1979)

16.19 (lit. mean, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

133.3* ($76.0^{\circ}C$, summary of literature data, temp range 76.0 – $264.5^{\circ}C$, Stull 1947)

1.09 (effusion method, interpolated from reported Antoine eq., Bright 1951)

$\log(P/mmHg) = 9.12 - 3341/(T/K)$; temp range 5.1 – $26.5^{\circ}C$ (Antoine eq., effusion, Bright 1951)

2.266 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.16125 - 1944.42/(190.0 + t/^{\circ}C)$; temp range 150 – $310^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

3904* ($151.49^{\circ}C$, static-differential pressure gauge, measured range 151.49 – $336.32^{\circ}C$, Wiecezorek & Kobayashi 1980)

0.0452 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.94201 - 1668.355/(186.212 + t/^{\circ}C)$; temp range 217.5 – $282.2^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

13100* (457.95 K, vapor-liquid equilibrium, measured range 457.95–581.85 K, Klara et al. 1987)
 0.052 (extrapolated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.291 - 1261/(105 + t/^{\circ}\text{C})$; temp range 217–282°C (Antoine eq., Dean 1985, 1992)
 0.0885 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.8765 - 1707.9/(-101.15 + T/\text{K})$; temp range 295–383 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.28615 - 1944.42/(-83.15 + T/\text{K})$; temp range 423–583 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 50.8894 - 5.2749 \times 10^3/(T/\text{K}) - 14.246 \cdot \log(T/\text{K}) - 4.2994 \times 10^{-10} \cdot (T/\text{K}) + 2.4197 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 298–768 K (vapor pressure eq., Yaws 1994)
 1.456* (22.25°C, transpiration-GC, measured range –0.95 to 22.25°C, Verevkin 1999)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.931 (calculated-P/C, Mackay et al. 1992)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.14 (Hansch & Leo 1979)
 4.22 (HPLC-RT correlation, Burkhard et al. 1985)
 4.33 (HPLC-RT correlation, Eadsforth 1986)
 4.14 (recommended, Sangster 1989, 1994)
 4.14 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 4.1.1.16.1

Reported vapor pressures of diphenylmethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Stull 1947	Bright 1951	Wieczorek & Kobayashi 1980	Verevkin 1999				
summary of literature data	effusion method	static-differential pressure gauge	transpiration-GC				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa		
76.0	133.3	Data presented in graph		151.49	3904	−0.95	0.07946
107.4	666.6			151.77	3929	5.15	0.1584
122.8	1333			158.06	4942	10.15	0.3261
138.8	2666	eq. 1	P/mmHg	164.06	6182	15.05	0.6196
157.8	5333	A	9.12	170.31	7799	18.65	0.9556
170.2	7999	B	3341	176.25	9487	22.25	1.456
186.3	13332	temp range 5.1–26.5°C		182.32	11487		
210.7	26664			189.57	14279	eq. 1a	P/Pa
237.5	53329	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 64.015$		196.01	17435	A	36.43
264.5	101325			202.69	21342	B	10639

TABLE 4.1.1.16.1 (Continued)

Stull 1947		Bright 1951		Wieczorek & Kobayashi 1980		Verevkin 1999	
summary of literature data		effusion method		static-differential pressure gauge		transpiration-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
mp/°C	26.5			209.7	26436	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 88.48$	
				217.16	32381	at 284.3 K	
				225.99	41037	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 87.63$	
				232.67	58832	at 298.15 K	
				247.79	70500		
		Klara et al. 1987		255.23	83501	30.25	3.099
		vapor-liquid equilibrium		263.79	100021	35.05	4.653
		T/K		264.36	100938	40.05	7.019
		P/Pa		272.29	119269	44.95	10.19
		457.95	13100	280.24	137819	55.05	21.63
		488.05	31000	288.0	1377.37	60.05	30.55
		527.25	82720	295.97	162025	65.15	47.05
		560.95	168900	303.88	186511	70.15	67.41
		581.85	250200	311.45	218741		
				320.63	253090	eq. 1a	P/Pa
				336.32	298026	A	27.43
						B	7981.2
				fitted to Chebyshev Polynomial		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 66.36$	
				at 323.3 K			
				$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 67.83$			
				at 298.15 K			

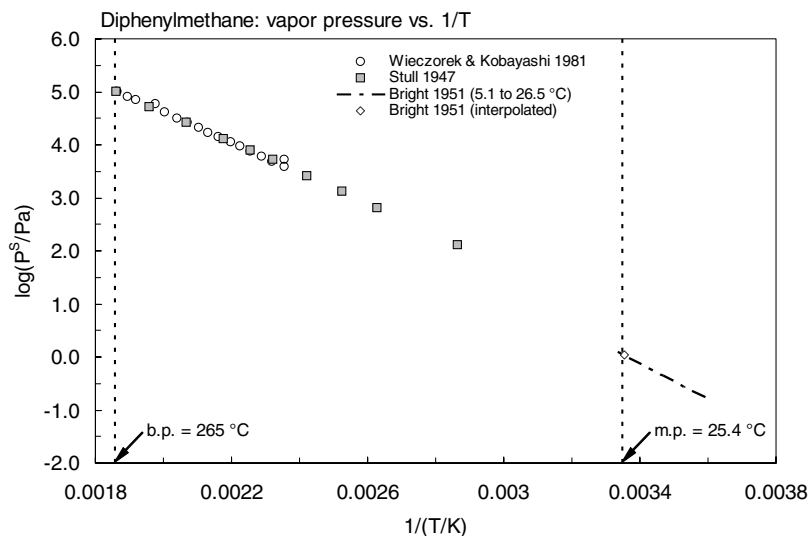
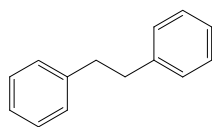


FIGURE 4.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for diphenylmethane.

4.1.1.17 Bibenzyl



Common Name: Bibenzyl

Synonym: 1,2-Diphenylethane, dibenzyl, 1,1'-(1,2-ethanediyl) bis-benzene

Chemical Name: 1,2-diphenylethane

CAS Registry No: 103-29-7

Molecular Formula: $C_{14}H_{14}$

Molecular Weight: 182.261

Melting Point ($^{\circ}C$):

52.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

284 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9780 ($25^{\circ}C$ Lide 2003)

Molar Volume (cm^3/mol):

190.2 ($60^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

186.4 ($25^{\circ}C$, calculated-density)

229.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.43 (Parks & Huffman 1931)

30.54 (Stephenson & Malanowski 1987)

22.73 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

94.14 (Stephenson & Malanowski 1987)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S = 56\ J/mol\ K$, F: 0.537 (mp at $52.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.37 (shake flask-UV, Andrews & Keefer 1950b)

4.37 (quoted, Pearlman et al. 1984)

1.89; 0.44 (generator column-HPLC/UV; HPLC-RT correlation, Swann et al. 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

133.3* ($86.8^{\circ}C$, summary of literature data, temp range 86.8 – $284.0^{\circ}C$, Stull 1947)

0.198 (effusion method, interpolated from reported Antoine eq., Bright 1951)

$\log(P/mmHg) = 9.86 - 3783/(T/K)$; temp range 17.1 – $44.2^{\circ}C$ (Antoine eq., effusion, Bright 1951)

17.1* ($60^{\circ}C$, inclined piston, measured range 60 – $140^{\circ}C$, Osborn & Scott 1980)

$\log(P/atm) = [1 - 547.288/(T/K)] \times 10^{\{0.914704 - 6.08831 \times 10^{-4} \cdot (T/K) + 5.11258 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 333.15 – $413.15\ K$, (Cox eq., Chao et al. 1983)

0.406 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.319 - 4386/(T/K)$, temp range 286 – $308\ K$, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.93271 - 2636.21/(-22.009 + T/K)$; temp range 369 – $557\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 48.5573 - 5.2841 \times 10^3/(T/K) - 13.41 \cdot \log(T/K) - 1.0073 \times 10^{-9} \cdot (T/K) + 2.1338 \times 10^{-6} \cdot (T/K)^2$; temp range 324 – $780\ K$ (vapor pressure eq., Yaws 1994)

0.734; 0.249 (supercooled liquid P_L , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -3522/(T/K) + 11.67$; $\Delta H_{vap} = -67.4\ kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 4.79, 4.82 (Hansch & Leo 1979)
- 4.76 (quoted, HPLC- k' correlation, Hammers et al. 1982)
- 3.67 (HPLC-RT correlation, Swann et al. 1983)
- 4.60 (HPLC-RT correlation, Webster et al. 1985)
- 4.71 (HPLC-RT correlation, Eadsworth 1986)
- 4.70 ± 0.20 (recommended, Sangster 1989)
- 4.79 (recommended, Sangster 1993)
- 4.79 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 4.1.1.17.1

Reported vapor pressures of bibenzyl at various temperatures and the coefficients for the vapor pressure equations

	$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)	
	$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)	
	$\log P = A - B/(C + T/K)$	(3)			
	$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)			
Stull 1947		Bright 1951		Osborn & Scott 1980	
summary of literature data		effusion method		inclined piston	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
86.8	133.3	Data presented in graph		60	17.1
119.8	666.6			65	24.1
136.0	1333			70	34.0
153.7	2666			75	47.7
173.7	5333	eq. 1	P/mmHg	80	65.9
186.0	7999	A	9.56	85	89.7
202.8	13332	B	3783	90	121.2
227.8	26664	temp range 17.1–44.2°C		95	161.9
255.0	53329	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 72.38$		100	213.6
284.0	101325			105	280.1
				110	364.2
				115	469.8
mp/°C	51.5			120	602.4
				125	761.8
				130	961.1
				135	1202.7
				140	1498
data fitted to a 4–constant vapor pressure eq.					

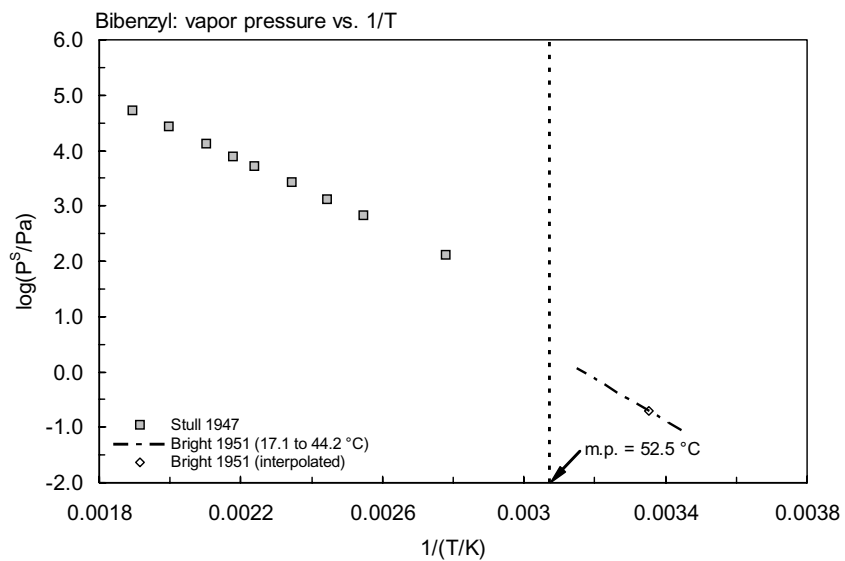
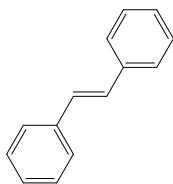


FIGURE 4.1.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for bibenzyl.

4.1.1.18 *trans*-Stilbene

Common Name: *trans*-1,2-Diphenylethene

Synonym: *trans*-stilbene, *trans*-diphenylethylene, E-stilbene

Chemical Name: *trans*-1,2-diphenylethene

CAS Registry No: 103-30-0

Molecular Formula: C₁₄H₁₂

Molecular Weight: 180.245

Melting Point (°C):

124.2 (Lide 2003)

Boiling Point (°C):

307 (Lide 2003)

Density (g/cm³ at 20°C):

0.9707 (Weast 1982–83; Lide 2003)

Molar Volume (cm³/mol):

185.0 (Ruelle & Kesselring 1997)

185.7 (20°C, calculated-density)

221.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

100.7 (Van Ekeren et al. 1983)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.125 (Stephenson & Malanowski 1987)

27.40 (Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

76.73 (Stephenson & Malanowski 1987)

68.81, 69.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.106 (mp at 124.2°C)

Water Solubility (g/m³ or mg/L at 25°C):

0.29 (shake flask-UV, Andrews & Keefer 1950)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (113.2°C, summary of literature data, temp range 113.2–306.5°C, Stull 1947)

0.00764* (manometer-spinning rotor friction gauge, torsion mass loss effusion, measured range 297.45–364.5 K, Van Ekeren et al. 1983)

0.0274 (34.65°C, effusion-quartz crystal microbalance, Offringa et al. 1983)

0.00647 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_s/kPa) = 12.25604 – 5201.358/(T/K); temp range 298–343 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.97928 – 2610.05/(–54.759 + T/K); temp range 419–580 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

log (P/mmHg) = 68.6303 – 6.3776 × 10³/(T/K) – 21.015 · log (T/K) + 5.7813 × 10^{–3} · (T/K) + 1.8334 × 10^{–12} · (T/K)²; temp range 397–820 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{ow}:

4.81 (Hansch & Leo 1979)

- 4.81 (recommended, Sangster 1989)
 4.81 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 7.48 (calculated- S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 4.1.1.18.1

Reported vapor pressures of *trans*-stilbene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}C) & (2) & \ln P = A - B/(C + t/^{\circ}C) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

Stull 1947		Van Ekeren et al. 1983					
Summary of literature data		Spinning rotor fraction gauge		Torsion mass loss effusion		Static method	
t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa
113.2	133.3	24.3	0.00704	44.97	0.100	69.17	1.43
145.8	666.6	24.3	0.00699	50.78	0.200	69.45	1.44
161.0	1333	24.3	0.00715	54.27	0.300	71.25	1.83
179.8	2666	24.43	0.0693	56.80	0.400	71.52	1.80
199.0	5333	27.24	0.0102	60.43	0.600	72.2	1.94
211.5	7999	27.24	0.0104	64.14	0.900	73.70	2.25
227.4	13332	27.24	0.0105	65.11	1.00	74.18	2.39
251.7	26664	30.65	0.0151	69.45	1.44	75.73	2.81
287.3	53329	30.65	0.015	71.25	1.83	75.83	2.80
306.5	101325	32.03	0.0196	71.25	1.80	75.86	2.83
mp/ $^{\circ}C$	124	32.03	0.0195	72.2	1.94	77.15	3.10
		34.96	0.0287	73.7	2.25	78.27	3.55
		34.96	0.0288	74.18	2.39	8.06	4.34
		34.96	0.0289	75.73	2.81	80.39	4.39
		37.33	0.0386	75.86	2.83	81.79	5.07
		37.33	0.0387	76.88	3.10	83.36	5.84
		40.61	0.0584	78.27	3.55	85.04	6.86
		40.61	0.0585	80.79	4.39	86.35	7.71
		43.32	0.0792	81.79	5.07	86.38	7.74
		25	0.00765	83.36	5.84	86.51	7.90
				85.04	6.86	87.35	8.47
				86.35	7.71	89.74	10.57
				86.51	7.90	90.43	11.22
				87.35	8.47	91.35	12.20
				89.74	10.57		
				90.43	11.22		
				91.35	12.20		
				$\Delta H_{fus} = 100.17 \text{ kJ/mol}$			
				at 331.64 K			

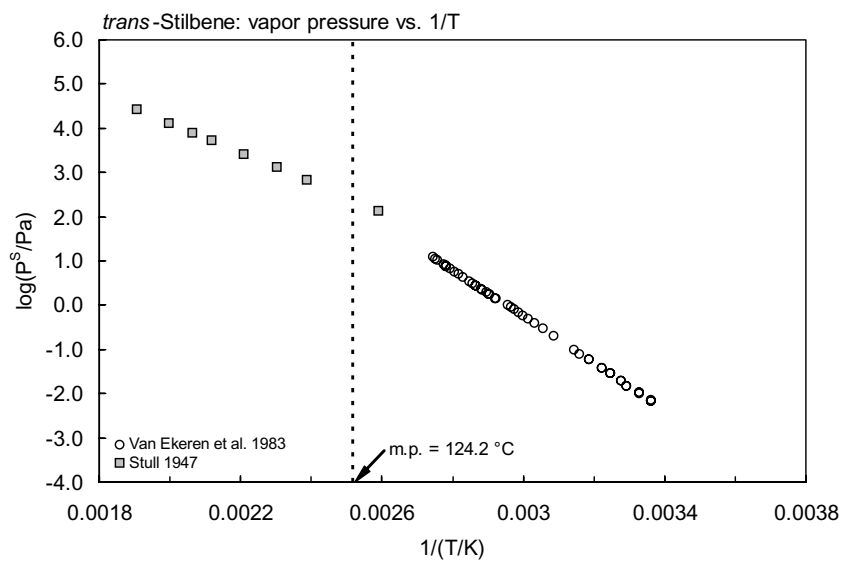
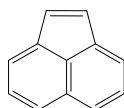


FIGURE 4.1.18.1 Logarithm of vapor pressure versus reciprocal temperature for *trans*-stilbene.

4.1.1.19 Acenaphthylene



Common Name: Acenaphthylene

Synonym:

Chemical Name: acenaphthylene

CAS Registry No: 208-96-8

Molecular Formula: $C_{12}H_8$

Molecular Weight: 152.192

Melting Point ($^{\circ}C$):

91.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

280 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.899 (Dean 1985)

0.8987 ($17^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

141.2 (Ruelle & Kesselring 1997)

167.1 ($17^{\circ}C$, calculated-density)

165.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.96 (Ruelle & Kesselring 1997)

1.4, 6.95, 10.96; 12.36 (-156.55 , 88.45 , $88.85^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

30.3 (Passivirta et al. 1999)

42.4, 37.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.221 (mp at $91.8^{\circ}C$)

0.458 (calculated, $\Delta S_{fus} = 30.3\ J/mol\ K$, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

3.93 (misquoted from Mackay & Shiu 1977)

16.1 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

$\log [S_L/(mol/L)] = 1.315 - 573.5/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.893* (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)

$\log (P/Pa) = 12.768 - 3821.55/(T/K)$; temp range 10 – $50^{\circ}C$ (Antoine eq., Sonnefeld et al. 1983)

0.893 (generator column-HPLC, Wasik et al. 1983)

1.105 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 9.500 - 3714/(T/K)$; temp range 286 – $318\ K$ (Antoine eq., Stephenson & Malanowski 1987)

0.90 (selected, Mackay et al. 1992, 1996; quoted, Shiu & Mackay 1997)

0.90; 1.97 (quoted solid P_s from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 11.11 - 3201/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.53 - 2751/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11.55 (gas stripping-GC, Warner et al. 1987)

11.40 (wetted-wall column-GC, Fendinger & Glotfelty 1990)

12.7* (gas stripping-GC, measured range 4.1 – $31^{\circ}C$, Bamford et al. 1999)

$\ln K_{AW} = -6278.6/(T/K) + 15.757$; $\Delta H = 52.2 \text{ kJ mol}^{-1}$; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

$\log [H/(\text{Pa m}^3/\text{mol})] = 8.22 - 2178/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.07 (calculated as per Leo et al. 1971)
- 3.94 (Yalkowsky & Valvani 1979)
- 3.72 (calculated-fragment const., Mabey et al. 1982)
- 4.08 (selected, Mills et al. 1982)
- 4.06 (calculated-molar refraction MR, Yoshida et al. 1983)
- 3.90 (calculated-MCI χ as per Rekker & De Kort 1979, Ruepert et al. 1985)
- 3.55 (HPLC-RT correlation, Chin et al. 1986)
- 4.07–4.10; 4.08 (quoted lit. range; lit. mean, Meadors et al. 1995)
- 4.00; 3.67 (quoted lit.; calculated, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 3.0 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 2.58 (Isnard & Lambert 1988)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 3.83, 3.75 (soil, RP-HPLC correlation on CIHAC, on PIHAC, Szabo et al. 1990b)
- 4.91–5.21; 3.60–3.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 4.96; 5.05, 5.14, 5.45 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: not environmentally significant (Mabey et al. 1982);

$t_{1/2} = 0.7 \text{ h}$ on silica gel, $t_{1/2} = 2.2 \text{ h}$ on alumina and $t_{1/2} = 44 \text{ h}$ on fly ash for different atmospheric particulate substrates determined in the rotary photoreactor (appr. 25 $\mu\text{g/g}$ on substrate) (Behymer & Hites 1985); direct photolysis $t_{1/2} = 9.08 \text{ h}$ (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).

Photodegradation $k = 3 \times 10^{-5} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 5 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (calculated, Mabey et al. 1982)

$k_{O_3} \sim 5.50 \times 10^{-16} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$, $k_{OH} = (11.0 \pm 0.1) \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ and $k_{NO_3} = (54 \pm 0.8) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate methods, Atkinson & Aschmann 1988)

$k_{OH} = 11.0 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at 296 K (Atkinson 1989)

$k_{OH} = 12.4 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at $296 \pm 2 \text{ K}$ with a atmospheric lifetime of 1.1 h assuming an average ambient 12-h daytime OH radical concn of $2 \times 10^6 \text{ molecule/cm}^3$; $k_{O_3} = 1.60 \times 10^{-16} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at 296 K with lifetime of 2.5 h assuming ambient O_3 concn of $7 \times 10^{11} \text{ molecule/cm}^3$ (relative rate method, Reisen & Arey 2002)

Hydrolysis: not hydrolyzable (Mabey et al. 1982; Howard et al. 1991).

Biodegradation: > 98% degradation within 7 d, based on domestic sewer for an average of three static-flask screening test (Tabak et al. 1981);

aerobic $t_{1/2} = 1020\text{--}1440 \text{ h}$, based on soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

anaerobic $t_{1/2} = 4080\text{--}5760 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $k = 3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$, estimated rate constant for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.191\text{--}1.27$ h, based on photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Atmospheric lifetime of 1.1 h and 2.5 h due to reaction with OH and O₃ at 296 K, respectively (Reisens & Arey 2002)

Surface water: $t_{1/2} = 1020\text{--}1440$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Kincannon & Lin 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 2040\text{--}2880$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 1020\text{--}1440$ h, based on soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);
 $t_{1/2} > 50$ d (Ryan et al. 1988).

Biota: elimination $t_{1/2} = 1$ d from rainbow trout (quoted, Meador et al. 1995).

TABLE 4.1.1.19.1

Reported vapor pressures and Henry's law constants of acenaphthylene at various temperatures and the coefficients for the vapor pressure equations

Vapor pressure		Henry's law constant		
Sonnefeld et al. 1983		Bamford et al. 1999		
gas saturation-HPLC		gas stripping-GC/MS		
t/°C	P/Pa	t/°C	H/(Pa m³/mol)	H/(Pa m³/mol)
				average
11.20	0.206	4.1	1.98, 2.87	2.38
11.20	0.205	11.0	3.76, 4.86	4.27
11.20	0.216	18.0	6.67, 8.33	7.46
20.56	0.590	25.0	10.9, 14.6	12.7
20.56	0.585	31.0	16.2, 23.7	19.6
20.56	0.588			
30.40	1.50	ln K _{AW} = A – B/(T/K)		
30.40	1.54	A	15.7566	
30.40	1.52	B	6278.6	
39.05	3.30			
39.05	3.41	enthalpy, entropy change:		
39.05	3.27	ΔH/(kJ·mol ⁻¹) = 52.2 ± 3.3		
39.05	3.34	ΔS/(J·K ⁻¹ mol ⁻¹) = 131		
25.0	0.89	at 25°C		
log P/Pa = A – B/(T/K)				
A	12.768			
B	3821.55			

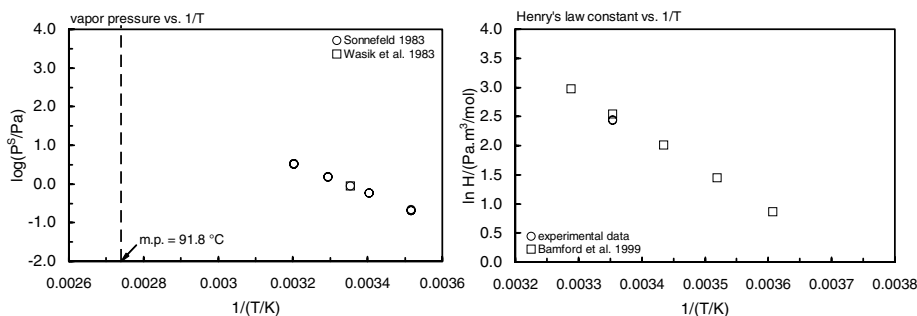
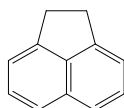


FIGURE 4.1.1.19.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for acenaphthylene.

4.1.1.20 Acenaphthene



Common Name: Acenaphthene

Synonym: 1,8-hydroacenaphthylene, ethylenenaphthalene, periethylenenaphthalene, 1,2-dihydro-acenaphthalene

Chemical Name: 1,8-hydroacenaphthylene

CAS Registry No: 83-32-9

Molecular Formula: $C_{12}H_{10}$

Molecular Weight: 154.207

Melting Point ($^{\circ}C$):

93.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

279 (Weast 1982–82; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.069 ($95^{\circ}C$, Dean 1985)

1.222 (Lide 2003)

Molar Volume (cm^3/mol):

126.2 ($20^{\circ}C$, calculated-density)

173.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

84.68 (Radchenko & Kitiagorodskii 1974)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.88 (differential calorimetry, Wauchope & Getzen 1972)

21.46 (calorimetry, Osborn & Douslin 1975; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

60.25 (Wauchope & Getzen 1972)

59.83 (Casellato et al. 1973)

56.90 (Ubbelohde 1978)

58.55, 41.09 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{\text{fus}} = 56\ J/mol\ K$), F : 0.213 (mp at $93.4^{\circ}C$)

0.197 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6.14 (Deno & Berkheimer 1960)

3.88* (shake flask-UV, measured range $0-74.7^{\circ}C$, Wauchope & Getzen 1972)

$R \cdot \ln x = -5230/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 17.1 + 0.0186 \cdot (T/K)$; temp range $22.2-73.4^{\circ}C$ (shake flask-UV measurements, Wauchope & Getzen 1972)

3.59 (shake flask-UV, Vesala 1974)

3.47 (shake flask-GC, Eganhouse & Calder 1976)

3.93 (shake flask-fluorescence, Mackay & Shiu 1977)

7.37 (shake flask-LSC, Banerjee et al. 1980)

2.42 (shake flask-GC, Rossi & Thomas 1981)

4.47 (average lit. value, Pearlman et al. 1984)

4.16 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

3.8* (recommended, IUPAC Solubility Data Series, Shaw 1989)

3.88 (shake flask-HPLC, Haines & Sandler 1995)

$\log [S_L/(mol/L)] = 2.505 - 1127/(T/K)$ (supercooled liquid S_L , Passivirta et al. 1999)

$\ln x = 0.684974 - 4541.77/(T/K)$; temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 2560* (147.2°C, static isoteniscope method, measured range 147.2–287.8°C, Mortimer & Murphy 1923)
 $\log (P/\text{mmHg}) = 8.033 - 2835/(T/K)$; temp range 147.2–287.8°C (Antoine eq. static isoteniscope method, Mortimer & Murphy 1923)
- 666.6* (114.8°C, summary of literature data, temp range 114.8–277.5°C, Stull 1947)
- 0.207 (Hoyer & Peperle 1958)
 $\log (P/\text{mmHg}) = 11.50 - 4264/(T/K)$; temp range –15 to 30°C (Knudsen effusion method, Hoyer & Peperle 1958)
- 4.02 (extrapolated-Antoine eq., Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 13078.5/(T/K)] + 8.069478$; temp range 114.8–277.5°C (Antoine eq., Weast 1972–73)
- 3.07 (extrapolated-Antoine eq., liquid state P_L , Boublik et al. 1973)
- 8.622* (54.1°C, effusion method, measured range 54.1–83.45°C, Radchenko & Kitiagorodskii 1974)
 $\log (P/\text{mmHg}) = 12.2930 - 4422.921/(T/K)$; temp range 54.10–83.15°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)
- 0.373* (manometry-extrapolated, measured range 65–140°C, Osborn & Douslin 1975)
- 0.287* (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)
 $\log (P/\text{Pa}) = 14.669 - 4535.39/(T/K)$; temp range 10–50°C (Antoine eq., gas saturation, Sonnefeld et al. 1983)
- 0.287 (gas saturation/generator column-HPLC, Wasik et al. 1983)
- 3.03, 1.48 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P_L/\text{kPa}) = 6.84571 - 2527.716/(244.912 + t/^\circ\text{C})$; temp range 147.2–287.8°C (Antoine eq. from reported exptl. data of Mortimer & Murphy 1923, Boublik et al. 1984)
- $\log (P_L/\text{kPa}) = 6.38504 - 2102.491/(203.124 + t/^\circ\text{C})$; temp range 95–140°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1966, Boublik et al. 1984)
- 3.07 (extrapolated from liquid state P_L , Dean 1985)
 $\log (P/\text{mmHg}) = 7.72819 - 2534.234/(245.576 + t/^\circ\text{C})$; temp range 147–187°C (Antoine eq., Dean 1985, 1992)
- $\log (P/\text{mmHg}) = 8.033 - 2834.99/(T/K)$; temp range 147–288°C (Antoine eq., Dean 1985, 1992)
- 0.237, 0.319 (19.95°C, 26.85°C, gas saturation-GC, Sato al. 1986)
- 0.427* (gas saturation, interpolated-Antoine eq., temp range 20–169°C, Sato al. 1986)
 $\ln (P/\text{Pa}) = 22.9288 - 5183.86/(T/K - 80.153)$; temp range: 293.1–342 K (Antoine eq., gas saturation, Sato et al. 1986)
- 0.311 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_S/\text{kPa}) = 10.883 - 4290.5/(T/K)$; temp range 290–311 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_S/\text{kPa}) = 9.4944 - 3248.008/(-48.055 + T/K)$; temp range 338–366 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.3519 - 2082.356/(-71.578 + T/K)$; temp range 368–413 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 7.30401 - 2975/(10.674 + T/K)$; temp range 388–552 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- 0.336, 0.211, 0.383; 0.287; 0.375; 0.377, 0.122, 0.306, 0.862 (quoted lit. values: effusion method; gas saturation-HPLC; calculated, Delle Site 1997)
- 0.30; 1.52 (quoted solid P_S from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F , Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 11.20 - 3492/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 8.13 - 2367/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
- $\log (P/\text{kPa}) = 10.883 - 4290.5/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 1.52; 0.428 (supercooled liquid P_L , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
 $\log (P_L/\text{Pa}) = -3337/(T/K) + 11.37$; $\Delta H_v = -63.9 \text{ kJ}\cdot\text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 14.79 (gas stripping-GC, Mackay et al. 1979)
- 15.7 (gas stripping-GC, Mackay & Shiu 1981; Mackay et al. 1982)
- 24.42 (gas stripping-GC, Warner et al. 1987)

- 6.45 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
 9.17 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
 16.20 (gas stripping-fluorescence, Shiu & Mackay 1997)
 18.5* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)
 $\ln K_{AW} = -6242.48/(T/K) + 16.0$, $\Delta H = 51.9 \text{ kJ mol}^{-1}$; measured range 4.1–31°C, (gas stripping-GC, Bamford et al. 1999)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 5.63 - 1240/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated:

- 3.92 (shake flask-LSC, Veith et al. 1979, 1980)
 3.92; 4.49 (shake flask-GC; RP-HPLC-RT correlation; Veith et al. 1980)
 3.92 (23°C, shake flask, Banerjee et al. 1980)
 3.92 (recommended, Sangster 1989, 1993)
 3.92 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 6.31 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 2.59 (bluegill sunfish, Veith et al. 1979, 1980)
 2.59 (bluegill sunfish, Barrows et al. 1980)
 2.59 (bluegill sunfish, Davies & Dobbs, 1984)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 5.38 (sediments average, Kayal & Connell 1990)
 3.79 (RP-HPLC correlation on CIHAC, Szabo 1990b)
 3.59 (RP-HPLC correlation on PIHAC, Szabo 1990b; quoted, Pussemier et al. 1990)
 3.58; 3.79 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.40–5.33; 3.80–5.40 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
 4.79; 4.89, 4.31, 4.20 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: half-lives on different atmospheric substrates determined in the rotary photoreactor (appr. 25 µg/g on substrate): $t_{1/2} = 2.0 \text{ h}$ on silica gel, $t_{1/2} = 2.2 \text{ h}$ on alumina and $t_{1/2} = 44 \text{ h}$ on fly ash (Behymer & Hites 1985);
 $k = 0.23 \text{ h}^{-1}$ in distilled water with $t_{1/2} = 3 \text{ h}$ (Fukuda et al. 1988);
 direct photolysis $t_{1/2} = 7.67 \text{ h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).

Hydrolysis: not hydrolyzable (Mabey et al. 1982).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for singlet O_2 , $k = 8000 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k_{OH}(\text{exptl}) = 1.03 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.49 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1988)

$k_{O_3} < 5.0 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = (1.03 \pm 0.13) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{NO_3} = (4.6 \pm 2.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate methods, Atkinson & Aschmann 1988)

$k_{OH} = (103 - 58.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296–300 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 84.03 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{OH}^* = 58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 325–365 K with a calculated atmospheric lifetime of 4.9 h based on gas-phase OH reaction (Brubaker & Hites 1998)

$k_{OH} = 8.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ with a atmospheric lifetime of 1.8 h assuming an average ambient 12-h daytime OH radical concn of $2 \times 10^6 \text{ molecule/cm}^3$ (Reisen & Arey 2002)

Biodegradation: significant degradation within 7 d for a domestic sewer test (Tabak et al. 1981);

aerobic $t_{1/2} = 295\text{--}2448 \text{ h}$, based on aerobic soil column test data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

anaerobic $t_{1/2} = 1180\text{--}9792$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: 3×10^{-9} mL cell $^{-1}$ h $^{-1}$, estimated bacterial transformation rate constant (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Sorption (k_1)-Desorption (k_2) Rate constants: desorption rate constant of 0.018 d $^{-1}$ with $t_{1/2} = 38.5$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Half-Lives in the Environment:

Air: $t_{1/2} = 0.879\text{--}8.79$ h, based on estimated photooxidation half-life in air (Howard et al. 1991);
calculated atmospheric lifetime of 4.9 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: $t_{1/2} = 3\text{--}300$ h, based on photolysis half-life in water (Howard et al. 1991).

Groundwater: $t_{1/2} = 590\text{--}4896$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption $t_{1/2} = 38.5$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} = 295\text{--}2448$ h, based on aerobic soil column test data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988).

Biota: $t_{1/2} < 1.0$ d in the tissue of bluegill sunfish (Veith et al. 1980).

TABLE 4.1.1.20.1
Reported aqueous solubilities of acenaphthene at various temperatures

Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV				IUPAC recommended	
t/°C	S/g·m $^{-3}$	t/°C	S/g·m $^{-3}$	t/°C	S/g·m $^{-3}$
	experimental		smoothed data		
22.2	3.57	0	1.45	0	1.5
30.0	4.76	22.2	3.46	20	3.2
30.0	4.60	25.0	3.88	25	3.8
30.0	4.72	30.0	4.80	30	4.8
34.5	6.00	34.5	5.83	40	7.4
34.5	5.68	39.3	7.20	50	9.2
34.5	5.75	44.7	9.20	60	19
39.3	6.80	50	11.9	70	32
39.3	7.10	50.1	11.9	75	43
39.3	7.00	55.6	15.6		
44.7	9.40	64.5	24.3		
44.7	9.40	65.2	25.2		
44.7	9.30	69.8	32.1		
50.1	12.5	71.9	35.9		
50.1	12.4	73.4	39.0		
50.1	12.4	74.7	41.8		
55.6	15.8	75.0	42.5		
55.6	16.3				
55.6	15.9				
64.5	25.9	temp dependence eq. 1			
64.5	27.8	ln x	mole fraction		
65.2	23.7	ΔH_{fus}	21.88 ± 0.21		
65.2	23.4	$10^2 \cdot b$	1.86 ± 0.11		
65.2	22.8	c	20.8 ± 0.4		
69.8	30.1				
69.8	34.3				

TABLE 4.1.1.20.1 (Continued)

Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV				IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
69.8	33.6				
71.9	35.2				
73.4	39.1				
79.4	40.1				
74.7	40.8				
74.7	39.3				

$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 21.88$

Empirical temperature dependence equations:
Wauchope & Getzen (1972): $R \cdot \ln x = -[H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K)$ (1)

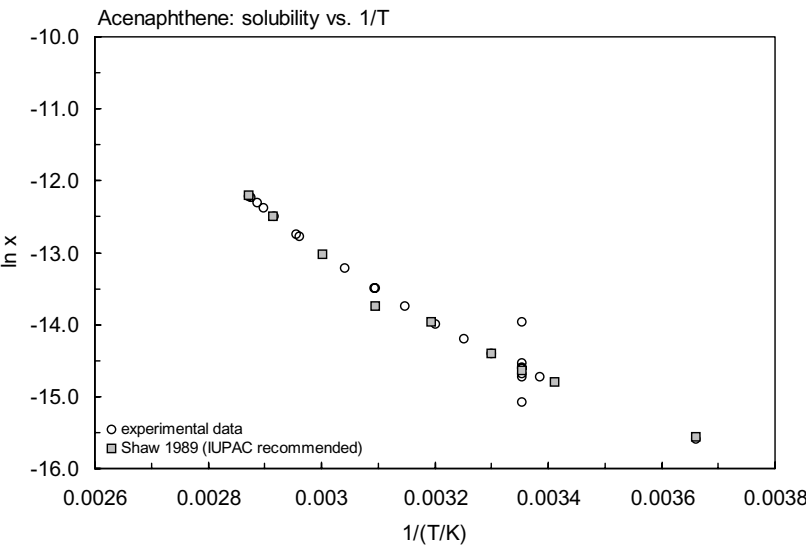


FIGURE 4.1.1.20.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for acenaphthene.

TABLE 4.1.1.20.2

Reported vapor pressures of acenaphthene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

1.

Mortimer & Murphy 1923		Stull 1947		Hoyer & Peperle 1958		Radchenko & K. 1974	
static isoteniscope method		summary of literature data		effusion		effusion method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
147.2	2560	114.8	666.6	data presented as		54.1	8.622
182.4	8479	131.2	1333	eq. 1	P/mmHg	57.85	10.576
182.4	8479	148.7	2666	A	11.50	58.95	13.180
210.2	19732	168.2	5333	B	4264	61.3	16.545
210.4	19865	181.2	7999	temp range -15–35°C		64.55	20.438
227.2	31277	197.5	13332	$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 83.26$		67.25	26.757
233.2	36264	222.1	26664			69.5	31.304
246.2	49943	250.0	53329			71.8	37.77
246.6	50383	277.5	101325			73.65	47.22
247.0	51049					76.0	57.23
252.4	57929	mp/°C	55			78.05	67.66
252.5	57955					80.5	82.045
264.4	76047					83.45	130.30
264.4	76460						
275.3	97779					eq. 1	P/mmHg
275.4	97779					A	12.2930
275.4	97779					B	4222.924
286.8	124030						
287.0	124296						
287.8	125723						
eq. 1	P/mmHg						
A	8.033						
B	2835						
temp range 147–288°C							

2.

Osborn & Douslin 1975		Sonnefeld et al. 1983		Sato et al. 1986	
inclined-piston manometry		gas saturation-HPLC		gas saturation-electrobalance	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
solid					
65.0	25.865	10.87	0.048	19.95	0.237
70.0	30.797	10.87	0.0504	26.85	0.519
75.0	46.796	10.87	0.0515	30.85	0.792
80.0	70.526	20.45	0.167	35.75	1.30
85.0	104.92	20.45	0.161	37.95	1.60
90.0	153.45	20.45	10.66	43.35	3.21
92.0	185.05	30.15	0.539	45.35	4.21
92.5	195.05	30.15	0.512	48.35	5.76

TABLE 4.1.1.20.2 (Continued)

Osborn & Douslin 1975		Sonnefeld et al. 1983		Sato et al. 1986	
inclined-piston manometry		gas saturation-HPLC		gas saturation-electrobalance	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
liquid		32.15	0.580	51.85	7.68
95.0	214.91	38.9	1.35	58.05	9.72
100.0	281.04	38.9	1.32	60.25	12.0
105.0	364.23	38.9	1.32	63.65	15.6
110.0	468.35	25	0.287	68.85	23.5
115.0	597.94				
120.0	755.39	eq. 1	P/Pa	eq. 3	P/Pa
125.0	948.97	A	14.385	A	22.9288
130.0	1184	B	4616.07	B	5183.86
135.0	1469			C	-80.153
140.0	1809				

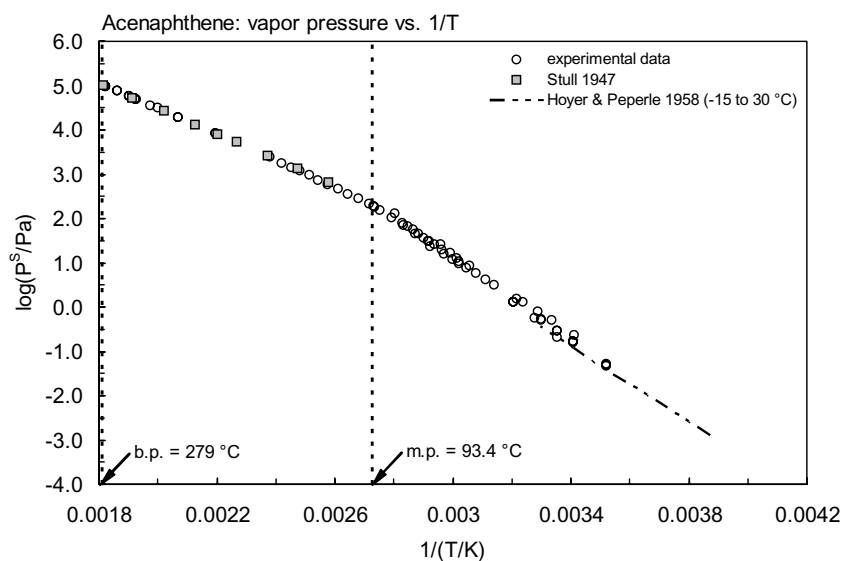


FIGURE 4.1.1.20.2 Logarithm of vapor pressure versus reciprocal temperature for acenaphthene.

TABLE 4.1.1.20.3

Reported Henry's law constants of acenaphthene at various temperatures

Bamford et al. 1999		
gas stripping–GC/MS		
t/°C	H/(Pa m ³ /mol)	H/(Pa m ³ /mol)
		average
4.1	3.27, 3.79	3.52
11.0	5.98, 6.62	6.29
18.0	10.5, 11.4	10.9
25.0	17.5, 19.6	18.5
31.0	26.5, 30.8	28.6

$\ln K_{AW} = A - B/(T/K)$
 K_{AW}
A 15.997
B 6242.5
enthalpy, entropy change:
 $\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 51.9 \pm 1.3$
 $\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 133$
at 25°C

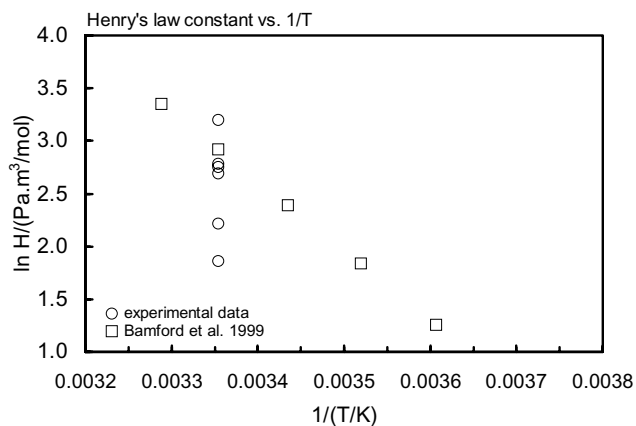
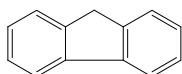


FIGURE 4.1.1.20.3 Logarithm of Henry's law constant versus reciprocal temperature for acenaphthene.

4.1.1.21 Fluorene



Common Name: Fluorene

Synonym: 2,3-benzindene, diphenylenemethane, 9H-fluorene

Chemical Name: diphenylenemethane

CAS Registry No: 86-73-7

Molecular Formula: $C_{13}H_{10}$

Molecular Weight: 166.218

Melting Point ($^{\circ}C$):

114.77 (Lide 2003)

Boiling Point ($^{\circ}C$):

295 (Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.203 ($0^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

138.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

187.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.54 (Wauchope & Getzen 1972)

19.58 (Osborn & Douslin 1975; Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

50.63 (Wauchope & Getzen 1972)

48.53 (Casellato et al. 1973)

50.48, 51.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

50.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.132 (mp at $114.77^{\circ}C$)

0.161 (calculated, $\Delta S_{fus} = 50.5 J/mol K$, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.90 (Pierotti et al. 1959)

1.66 (shake flask, binding to bovine serum albumin, Sahyun 1966)

1.90* (shake flask-UV, measured range 24.6 – $73.4^{\circ}C$, Wauchope & Getzen 1972)

$R \cdot \ln x = -4670/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 24.2 + 0.0309 \cdot (T/K)$; temp range 24.6 – $73.4^{\circ}C$ (shake flask-UV measurements, Wauchope & Getzen 1972)

1.98 (shake flask-fluorescence, Mackay & Shiu 1977)

1.68* (generator column-HPLC, measured range 6.6 – $31^{\circ}C$, May et al. 1978)

$S/(\mu g/kg) = 324.0 + 5.413 \cdot (t/^{\circ}C) + 0.8059 \cdot (t/^{\circ}C)^2 + 0.0025 \cdot (t/^{\circ}C)^3$; temp range 4 – $29^{\circ}C$ (generator column-HPLC/UV, May et al. 1978)

1.62* ($24^{\circ}C$, generator column-HPLC, measured range 279.75 – $304.25 K$, May et al. 1983)

1.68 (generator column-HPLC, Wasik et al. 1983)

1.83 (average lit. value, Pearlman et al. 1984)

1.90 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

1.96 (generator column-HPLC/UV, Billington et al. 1988)

1.9* (recommended, IUPAC Solubility Data Series, Shaw 1989)

2.23 (generator column-HPLC, Vadas et al. 1991)

$\log [S_L/(mol/L)] = 1.664 - 1024/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = 0.82861 - 4824/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 2400* (161.0°C, static isoteniscope method, measured range 161.0–300.4°C, Mortimer & Murphy 1923)
 $\log (P/\text{mmHg}) = 8.059 - 2957/(T/K)$; temp range 161–300.4°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)
- 666.6* (129.3°C, summary of literature data, temp range 129.3–295.0°C, Stull 1947)
- 0.087* (effusion method, measured range 33.3–49.55°C, Bradley & Cleasby 1953)
 $\log (P/\text{cmHg}) = 10.325 - 4324/(T/K)$; temp range 33.3–49.55°C (Antoine eq., Bradley & Cleasby 1953)
- 1.66 (extrapolated-Antoine eq., liquid state P_L , Weast 1972-73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 13682.8/(T/K)] + 8.18894$; temp range 129.3–295°C (Antoine eq., Weast 1972-73)
- 1.13 (extrapolated-Antoine eq., liquid state P_L , Boublik et al. 1973)
- 1.133 (extrapolated-Antoine eq., supercooled liquid P_L , Dean 1985)
- 0.127* (static method-manometry, measured range 75.8–114°C, Osborn & Douslin 1975)
- 0.0946 (Irwin 1982)
- 0.080* (gas saturation-HPLC/UV, measured range 10–50°C, Sonnefeld et al. 1983)
 $\log (P/\text{Pa}) = 14.385 - 4616.07/(T/K)$; temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)
- 0.080 (generator column-HPLC, Wasik et al. 1983)
- 0.473, 0.380 (P_{GC} by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
 $\log (P/\text{kPa}) = 2.88490 - 2635.371/(243.022 + t/^\circ\text{C})$; temp range 161–300.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 0.403 (Yamasaki et al. 1984)
 $\log (P/\text{mmHg}) = 7.7619 - 2637.1/(243.2 + t/^\circ\text{C})$; temp range 161–300°C (Antoine eq., Dean 1985, 1992)
- 0.0875* (gas saturation, interpolated-Antoine eq. derived from exptl. data, temp range 34–72°C, Sato et al. 1986)
 $\ln (P/\text{Pa}) = 17.0935 - 2815.52/(T/K - 153.984)$; temp range 307.7–347.5 K (Antoine eq., gas saturation, Sato et al. 1986)
- 0.088 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 10.449 - 4324/(T/K)$; temp range 306–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 10.04542 - 4122.908/(T/K)$; temp range 348–388 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.31368 - 4133.08/(86.582 + T/K)$; temp range 402–568 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- 0.0850*, 0.566 (pressure gauge in vacuum cell: solid P_s , supercooled liquid P_L , extrapolated for 25°C from reported Antoine eq., measured temp range 30.03–154.81°C, Sasse et al. 1988)
 $\log (P_s/\text{mmHg}) = 11.64431 - 4268.644/(262.656 + t/^\circ\text{C})$; temp range: 30.03–100.08°C (Antoine eq., pressure gauge, Sasse et al. 1988)
 $\log (P_L/\text{mmHg}) = 7.74839 - 2641.73/(230.963 + t/^\circ\text{C})$; temp range 110.06–154.83°C (Antoine eq., pressure gauge, Sasse et al. 1988)
- 0.474 (P_{GC} by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
- 0.793, 0.652 (supercooled P_L converted from literature P_s with different ΔS_{fus} values, Hinckley et al. 1990)
 $\log (P/\text{mmHg}) = 53.9382 - 5.322 \times 10^3/(T/K) - 16.059 \cdot \log (T/K) + 4.5696 \times 10^{-3} \cdot (T/K) + 8.1430 \times 10^{-13} \cdot (T/K)^2$; temp range 388–870 K (vapor pressure eq., Yaws 1994)
- 0.407 (supercooled liquid P_L , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
- 0.0575, 0.0885; 0.080; 0.0851 (quoted exptl.: effusion method; gas saturation; manometry, Delle Site 1997)
- 0.0792, 0.243; 0.00594, 0.00477 (quoted lit.; calculated; GC-RT correlation, Delle Site 1997)
- 0.72; 0.116 (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_s with fugacity ratio F , Passivirta et al. 1999)
 $\log (P_s/\text{Pa}) = 11.27 - 3638/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 8.63 - 2614/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P/\text{Pa}) = 14.385 - 4616.07/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.526; 0.194 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
 $\log (P_L/\text{Pa}) = -3492/(T/K) + 11.43$; $\Delta H_{vap} = -66.9 \text{ kJ} \cdot \text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

0.086* (25.05°C, transpiration method, measured range 288.7–359.2 K, Verevkin 2004)

$\ln (P/\text{Pa}) = 298.47/R - 95086.65/[R(T/K)] - (30.2/R) \cdot \ln [(T/K)/298.15]$; temp range 288.7–359.2 K (transpiration method, Verevkin 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7.75 (batch stripping, Mackay & Shiu 1981)

10.13 (batch stripping, Mackay et al. 1982)

11.85 (batch stripping, Warner et al. 1987)

6.45 (wetted-wall column, Fendinger & Glotfelty 1990)

9.75 (gas stripping-fluorescence, Shiu & Mackay 1997)

6.50 (gas stripping-HPLC/fluorescence, De Maagd et al. 1998)

9.81* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)

$\ln K_{\text{AW}} = -5869.62/(T/K) + 14.193$; $\Delta H = 48.8 \text{ kJ mol}^{-1}$; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

$\log (H/(\text{Pa m}^3/\text{mol})) = 6.97 - 1590/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.18 (Hansch & Leo 1979)

4.12 (Chou & Jurs 1979)

4.18 (HPLC- k' correlation, Rekker & De Kort 1979)

3.91 (HPLC- k' correlation, Hanai et al. 1981)

4.18 (RP-TLC- k' correlation, Bruggeman et al. 1982)

4.18 (shake flask-UV, Yalkowsky et al. 1983b)

4.23 (HPLC-RT correlation, Rapaport et al. 1984)

4.18 (shake flask-GC, Haky & Leja 1986)

4.10 (RP-HPLC-RT correlation, Chin et al. 1986)

4.23 (HPLC-RT correlation, Wang et al. 1986)

4.13 (TLC-RT correlation, De Voogt et al. 1990)

4.18 (recommended, Sangster 1993)

4.18 (recommended, Hansch et al. 1995)

4.32 ± 0.19 , 3.68 ± 0.62 (HPLC- k' correlation: ODS column; Diol column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:

6.68 (calculated, Finizio et al. 1997)

6.79*; 6.59 (generator column-GC; calculated- $C_{\text{O}}/C_{\text{A}}$, measured range 0–40°C, Harner & Bidleman 1998)

$\log K_{\text{OA}} = -7.74 + 4332/(T/K)$; temp range 0–40°C (generator column-GC, Harner & Bidleman 1998)

6.83, 6.79 (calculated- S_{oct} and vapor pressure P , quoted lit., Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

3.67 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

2.70 (*Daphnia magna*, Newsted & Giesy 1987)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.95; 3.87 (Aldrich and Fluka humic acids, observed; predicted, Chin et al. 1989)

5.47 (sediments average, Kayal & Connell 1990)

3.76 (RP-HPLC correlation, Pussemier et al. 1990)

4.15, 4.21 (RP-HPLC correlation on CIHAC, on PIHAC, Szabo 1990b)

4.68 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)

3.24–5.75; 4.10–5.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

4.81; 4.93, 4.24, 4.63 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

- 3.95 (Askov soil, a Danish Agricultural soil, Sverdrup et al. 2002)
 3.93–6.19 (sediment/water, initial-final values of 5–100 d contact time, gas-purge technique-HPLC/fluor., ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: half-lives on different atmospheric particulate substrates determined in rotary photoreactor (approx. 25 $\mu\text{g/g}$ on substrate): $t_{1/2} = 110$ h on silica gel, $t_{1/2} = 62$ h on alumina and $t_{1/2} = 37$ h on fly ash (Behymer & Hites 1985);

photolysis rate $k < 2 \times 10^{-5} \text{ s}^{-1}$ with $t_{1/2} > 1.6$ d (Kwok et al. 1997);

direct photolysis $t_{1/2} = 7.69$ h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001)

Photodegradation $k = 9.0 \times 10^{-7} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 , or as indicated *data at other temperatures and/or the Arrhenius expression see reference:

$k(\text{calc}) < 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 3 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{\text{OH}}(\text{calc}) = 13.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (SAR structure-activity relationship, Arey et al. 1989, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 9.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculation, Klamt 1996)

$k_{\text{OH}}(\text{exptl}) = (16 \pm 5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 9.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 9$ h; $k_{\text{NO}_3}(\text{exptl}) = (3.5 \pm 1.2) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 1.3$ d; and $k_{\text{O}_3}(\text{exptl}) < 2 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau > 82$ d at 297 ± 2 K (relative rate method; calculated-SAR structure-activity relationship, Kwok et al. 1997)

$k_{\text{OH}}^* = 23 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 306–366 K with a calculated atmospheric lifetime of 22 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: significant degradation with gradual adaptation within 7 d for an average of three static-flask screening test (Tabak et al. 1981);

nonautoclaved groundwater samples of approx. 0.06 mg/L are degraded at rates of about 30% per week by microbes (Lee et al. 1984);

$t_{1/2}(\text{aq. aerobic}) = 768\text{--}1440$ h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 3072\text{--}5760$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated rate constant for bacteria, $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 12.3 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.051 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 6.81\text{--}68.1$ h, based on reported rate constant for reaction with hydroxyl radical in air (Howard et al. 1991);

photolysis $t_{1/2} > 1.6$ d; calculated tropospheric lifetimes of 9 h, 1.3 d and > 82 d due to reactions with OH radical, NO_3 radical and O_3 , respectively, at room temp. (Kwok et al. 1997);

calculated atmospheric lifetime of 22 h based on gas-phase reactions with OH radical (Brubaker & Hites 1998).

Surface water: $t_{1/2} = 768\text{--}1440$ h, based on aerobic soil die-away test data (Howard et al. 1991).

Groundwater: $t_{1/2} = 1536\text{--}2880$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 768\text{--}1440$ h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988).

Biota: elimination $t_{1/2} = 7$ d from rainbow trout (quoted, Meador et al. 1995).

TABLE 4.1.1.21.1

Reported aqueous solubilities of fluorene at various temperatures

Wauchope & Getzen 1972				May 1980, 1983		Shaw 1989	
shake flask-UV				generator column-HPLC		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
	experimental		smoothed				
24.6	1.93	0	0.66	6.60	0.7184	0	0.70
24.6	1.87	24.6	1.86	13.2	0.9673	25	1.90
24.6	1.88	25	1.90	18.0	1.203	30	2.40
29.9	2.41	29.9	2.37	24.0	1.616	40	3.80
29.9	2.33	30.3	2.41	27.0	1.845	50	6.30
29.9	2.34	38.4	3.53	31.1	2.248	60	10
30.3	2.10	40.1	3.84			70	19
30.3	2.25	47.5	5.54				
30.3	2.23	50	6.29	temp dependence eq. 2			
38.4	3.72	50.1	6.32	S	μg/kg		
38.4	3.73	50.2	6.35	a	0.0185		
40.1	3.88	54.7	8.02	b	0.4543		
40.1	3.84, 3.85	59.2	10.2	c	22.76		
47.5	5.59, 5.62	60.5	10.9	d	543.3		
47.5	5.68	65.1	14.1				
50.1	6.31, 6.42	70.7	19.2	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 32.97$			
50.1	6.54	71.9	20.6	measured between 5–30°C			
50.2	6.27	73.4	22.5				
54.7	8.31, 8.41	75	24.7				
54.7	8.56						
59.2	10.5						
60.5	10.7	temp dependence eq. 1					
60.5	11.0	ln x	mole fraction				
60.5	11.6	ΔH_{fus}	19.54 ± 0.13				
65.1	14.2	$10^2 \cdot b$	3.09 ± 0.1				
65.1	14.1	c	24.2 ± 0.3				
70.7	18.5						
70.7	18.9						
71.9	18.8						
73.4	21.5						

 $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 19.54$

Empirical temperature dependence equations:

$$\text{Wauchope \& Getzen (1972): } R \cdot \ln x = -[H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K) \quad (1)$$

$$\text{May et al. (1978): } -S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t_{1/2} + c \cdot t + d \quad (2)$$

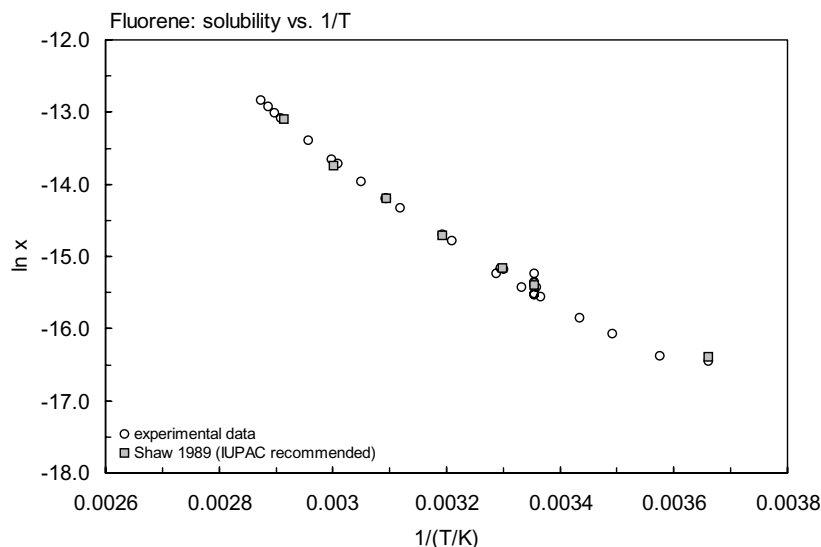


FIGURE 4.1.1.21.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for fluorene.

TABLE 4.1.1.21.2

Reported vapor pressures of fluorene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K)$$

$$\log P = A - B/(C + t/^{\circ}\text{C})$$

$$\log P = A - B/(C + T/K)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K)$$

(1)

(2)

(3)

(4)

$$\ln P = A - B/(T/K)$$

$$\ln P = A - B/(C + t/^{\circ}\text{C})$$

(1a)

(2a)

$$\ln P = A/R - B/[R(T/K)] - (C/R) \cdot \ln [(T/K)/298.15]; R - \text{gas constant}$$

(5)

1.

Mortimer & Murphy 1923		Stull 1947		Bradley & Cleasby 1953		Osborn & Douslin 1975	
isoteniscope-Hg manometer		summary of literature data		effusion		manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
161.0	2400	129.3	666.6	33.3	0.2186	75.0	15.065
202.5	9266	146.0	1333	37.2	0.3333	80.0	22.264
203.0	9399	164.2	2666	40.3	0.4573	85.0	32.263
240.0	27398	185.2	5333	45.0	0.7239	90.0	47.462
241.4	27784	197.8	7999	49.25	1.0906	95.0	68.26
276.6	64995	214.7	13332	34.85	0.2600	100.0	99.19
277.1	65421	240.3	26664	38.45	0.3746	105.0	141.45
295.6	98499	268.6	53329	42.45	0.5546	110.0	199.98
295.7	98499	295.0	101325	47.75	0.9439	114.0	259.04
295.7	98499			49.55	1.1106		
299.8	107231	mp/°C	113				
300.4	108298						
				eq. 1	P/mmHg	triple point	387.943 K
				A	10.325		
				B	4324	ΔH _{subl} /(kJ mol ⁻¹) = 81.76	
eq. 1	P/mmHg			temp range 33–50°C			at bp

TABLE 4.1.1.21.2 (Continued)

Mortimer & Murphy 1923		Stull 1947		Bradley & Cleasby 1953		Osborn & Douslin 1975	
isoteniscope-Hg manometer		summary of literature data		effusion		manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
A	8.059					$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 19.58$	
B	2957					$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 62.17$	
temp range 161–300°C						at bp	
2.							
Sonnefeld et al. 1983		Sato et al. 1986		Sasse et al. 1988		Verevkin 2004	
gas saturation–HPLC		gas saturation–electrobalance		electronic manometry		transpiration	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
				solid			
10.5	0.0132	34.55	0.297	30.03	0.157	288.8	0.028
10.5	0.0133	36.35	0.360	39.92	0.184	290.4	0.034
10.5	0.013	41.15	0.620	49.88	1.241	292.4	0.044
20.4	0.0425	47.45	1.21	59.92	3.426	289.6	0.031
20.4	0.0438	49.85	1.53	60.03	3.533	296.2	0.067
20.4	0.0451	52.35	1.95	69.93	8.746	298.2	0.086
30.0	0.147	55.45	2.60	79.96	20.67	300.2	0.112
29.97	0.153	57.35	3.07	79.98	20.80	302.2	0.132
29.97	0.146	58.75	3.88	89.99	46.26	304.3	0.166
38.85	0.387	63.25	4.78	89.99	46.40	306.3	0.218
38.85	0.384	64.55	5.88	100.04	97.86	308.3	0.268
38.85	0.382	67.25	7.38	100.08	98.93	310.2	0.328
38.9	0.387	69.75	9.13			313.3	0.449
38.9	0.393	71.25	10.2	eq. 2	P/mmHg	314.3	0.507
25.0	0.080	74.35	13.0	A	11.64431	315.3	0.545
				B	4268.664	317.3	0.666
eq. 1	P/Pa	eq. 3	P/Pa	C	262.656	320.3	0.930
A	14.385	A	17.0935	temp range: 30–100.08°C		323.4	1.245
B	4616.07	B	2815.52			326.5	1.645
		C	–153.984	liquid		329.3	2.223
				110.06	212.5	332.3	3.103
				120.04	352.0	335.3	3.867
				120.04	353.0	338.2	4.838
				129.97	568.6	341.2	6.552
				139.95	894.3	344.2	8.417
				149.86	1369	347.1	11.190
				154.81	1683	350.3	14.497
						353.2	18.302
				eq. 2	P/mmHg	356.3	23.900
				A	7.94839	359.2	30.456
				B	2641.73		
				C	230.963	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.08$	
				temp range: 110–155°C		eq. 5	P/Pa
						A	298.47
						B	95086.65
						C	30.2

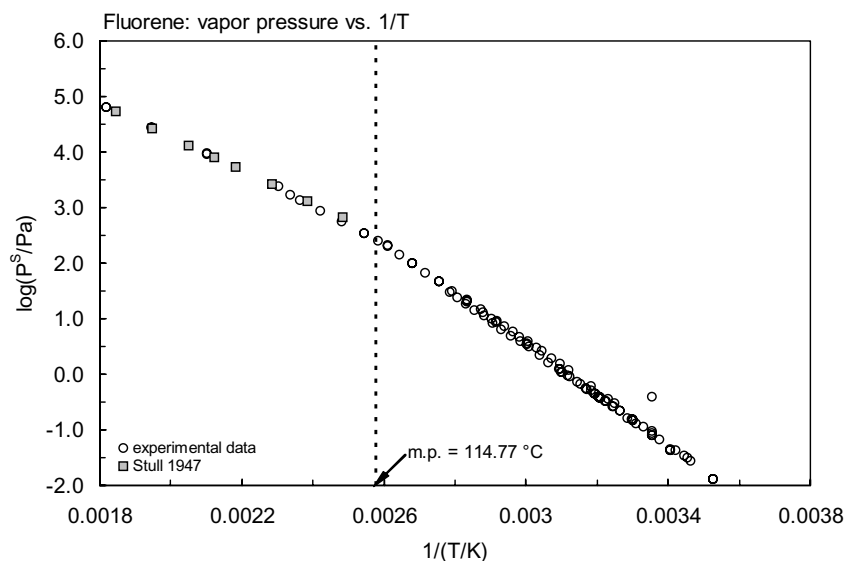


FIGURE 4.1.1.21.2 Logarithm of vapor pressure versus reciprocal temperature for fluorene.

TABLE 4.1.1.21.3

Reported Henry's law constants and octanol–air partition coefficients of fluorene at various temperatures and temperature dependence equations

Henry's law constant			log K _{OA}	
Bamford et al. 1999			Harner & Bidleman 1998	
gas stripping-GC/MS			generator column-GC/FID	
t/°C	H/(Pa m³/mol)	H/(Pa m³/mol)	t/°C	log K _{OA}
		average		
4.1	1.96, 2.14	2.05	0	8.134
11.0	3.44, 3.65	3.54	10	7.501
18.0	5.81, 6.12	5.96	20	7.130
25.0	9.49, 10.1	9.81	30	6.516
31.0	14.1, 15.4	14.8	40	6.093
			25(exptl)	6.79
			25(calc)	6.59
ln K _{AW} = A – B/(T/K)			log K _{OA} = A + B/(T/K)	
eq. 1	K _{AW}		A	–7.74
A	14.193		B	4332
B	5870			
enthalpy, entropy change:			enthalpy of phase change	
ΔH/(kJ·mol ^{–1}) = 48.8 ± 0.8			ΔH _{OA} /(kJ mol ^{–1}) = 82.9	
ΔS/(J·K ^{–1} mol ^{–1}) = 118				
at 25°C				

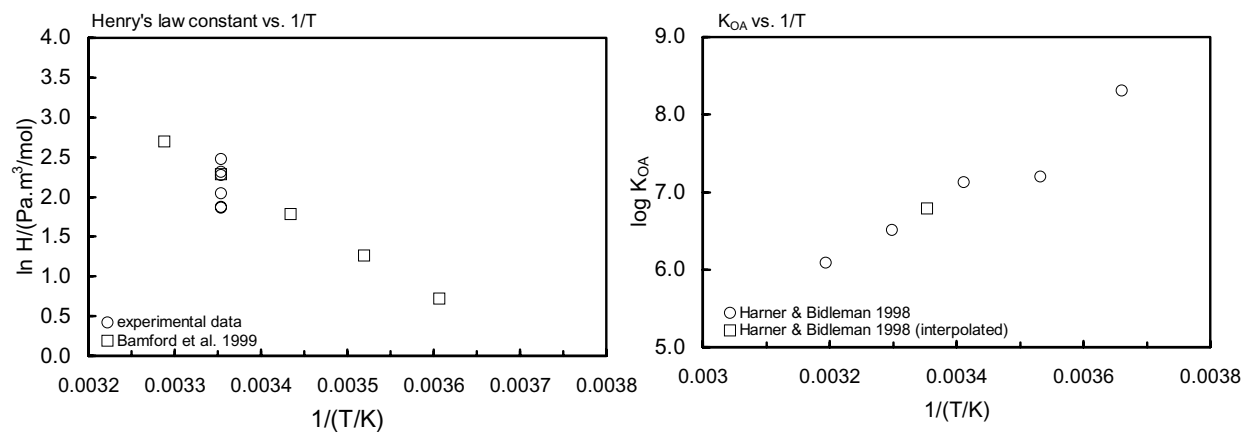
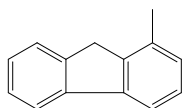


FIGURE 4.1.1.21.3 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for fluorene.

4.1.1.22 1-Methylfluorene



Common Name: 1-Methylfluorene

Synonym:

Chemical Name: 1-methylfluorene

CAS Registry No: 1730-37-6

Molecular Formula: $C_{14}H_{12}$

Molecular Weight: 180.245

Melting Point ($^{\circ}C$):

87 (Lide 2003)

Boiling Point ($^{\circ}C$):

318 (Weast 1982)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

177.1 (Ruelle & Kesselring 1997)

210.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.246 (mp at $87^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.092, 4.867 (measured, supercooled liquid value, Miller et al. 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

0.136; 0.0708 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -3711/(T/K) + 11.58$; $\Delta H_{vap} = -71.1 kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

0.032 (24.95 $^{\circ}C$, transpiration method, measured range 298.1–375.3 K, Verevkin 2004)

$\ln (P_S/Pa) = 311.78/R - 101590.4/[R(T/K)] - (35.1/R) \cdot \ln [(T/K)/298.15]$; temp range 298.1–359.2 K (solid, transpiration method, Verevkin 2004)

$\ln (P_L/Pa) = 330.39/R - 104778.1/[R(T/K)] - (87.5/R) \cdot \ln [(T/K)/298.15]$; temp range 361.2–375.3 K (liquid, transpiration method, Verevkin 2004)

Henry's Law Constant ($Pa m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.97 (calculated, Miller et al. 1985)

4.63 (calculated-solvatochromic parameters and V_L , Kamlet et al. 1988)

5.7640 (calculated-UNIFAC group contribution, Chen et al. 1993)

4.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

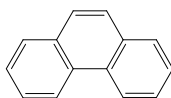
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.1.23 Phenanthrene



Common Name: Phenanthrene

Synonym: *o*-diphenyleneethylene, phenanthren

Chemical Name: phenanthrene

CAS Registry No: 85-01-8

Molecular Formula: $C_{14}H_{10}$

Molecular Weight: 178.229

Melting Point ($^{\circ}C$):

99.24 (Lide 2003)

Boiling Point ($^{\circ}C$):

340 (Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.174 (Dean 1985)

0.980 ($4^{\circ}C$, Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

182.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

199.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.62 (Parks & Huffman 1931; Tsonopoulos & Prausnitz 1971; Fu & Luthy 1985)

16.28 (differential calorimetry, Wauchope & Getzen 1972)

16.44 (calorimetry, Osborn & Douslin 1975)

0.22, 16.46; 15.58 (74.35, $99.25^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

42.68 (Wauchope & Getzen 1972)

45.19 (Casellato et al. 1973)

50.63 (Ubbelohde 1978)

47.70 (De Kruif 1980)

44.83, 44.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.187 (mp at $99.24^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.65 (shake flask-nephelometry, Davis & Parker 1942)

1.60 ($27^{\circ}C$, nephelometry, Davis et al. 1942)

0.994 (shake flask-UV, Andrews & Keefer 1949)

1.60 (shake flask-UV, Kleven 1950)

1.18 (Pierotti et al. 1959)

0.71 (shake flask, binding to bovine serum albumin, Sahyun 1966)

1.60 (shake flask-UV/fluorescence, Barone et al. 1967)

2.67 ($20^{\circ}C$, shake flask-UV, Eisenbrand & Baumann 1970)

1.18* (shake flask-UV, measured range 24.6 – $73.4^{\circ}C$, Wauchope & Getzen 1972)

$R \cdot \ln x = -3890/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 27.9 + 0.0374 \cdot (T/K)$; temp range 24.6 – $73.4^{\circ}C$
(shake flask-UV measurements, Wauchope & Getzen 1972)

3.03, 2.85 ($20^{\circ}C$, HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)

1.21 (shake flask-UV, Vesala 1974)

1.07 (shake flask-GC, Eganhouse & Calder 1976)

1.29 (shake flask-fluorescence, Mackay & Shiu 1977)

1.002 (Rossi 1977; Neff 1979)

1.151* (shake flask-UV, measured range 8.4 – $31.8^{\circ}C$, Schwarz 1977)

- 1.002* (generator column-HPLC/UV, measured range 4–29°C, May et al. 1978, 1983)
 $S/(\mu\text{g/kg}) = 324.0 + 5.413 \cdot (t/^\circ) + 0.8059 \cdot (t/^\circ\text{C})^2 + 0.0025 \cdot (t/^\circ\text{C})^3$; temp range 4–29°C (generator column-HPLC/UV, May et al. 1978)
- 0.955* (24.3°C, generator column-HPLC, measured range 4.0–29.9°C, May 1980)
- 0.816 (quoted, Verschueren 1983)
- 1.0 (generator column-HPLC/UV, Wasik et al. 1983)
- 1.28 (average lit. value, Pearlman et al. 1984)
- 1.29 (generator column-HPLC/fluorescence, Walters & Luthy 1984)
- 1.10* (generator column-HPLC/UV, measured range 4.6–25.3°C, Whitehouse 1984)
- 1.69 (29°C, shake flask-GC/FID, Stucki & Alexander 1987)
- 0.0446 (vapor saturation-UV, Akiyoshi et al. 1987)
- 1.08 (generator column-HPLC, Billington et al. 1988)
- 1.10* (recommended, IUPAC Solubility Data Series, Shaw 1989)
- 1.0 (generator column-HPLC, Vadas et al. 1991)
- 1.03 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
- 0.823 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
- 1.20 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)
- $\log S_L (\text{mol/L}) = 0.930 - 861.6/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
- $\ln x = -2.546051 - 4053/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 7773* (230°C, isoteniscope-Hg, measured range 230–340°C, Nelson & Senseman 1922)
- 3626* (203.6°C, isoteniscope-Hg manometer, measured range 203.6–346.8°C, Mortimer & Murphy 1923)
- $\log (P/\text{mmHg}) = 7.771 - 2990/(T/K)$; temp range 203.6–346.8°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)
- 133.3* (118.2°C, summary of literature data, temp range 118.2–340.2°C, Stull 1947)
- 0.0997 (effusion method, Inokuchi et al. 1952)
- 0.0227* (effusion method, Bradley & Cleasby 1953)
- $\log (P/\text{cmHg}) = 10.388 - 4519/(T/K)$; temp range 36.7–49.65°C (Antoine eq., Bradley & Cleasby 1953)
- $\log (P/\text{mmHg}) = 16.0 - 5008/(T/K)$; temp range 0–60°C (Knudsen effusion method, Hoyer & Peperle 1958)
- 0.464 (extrapolated from Antoine eq. of liquid state P_L , Weast 1972–73)
- $\log (P/\text{mmHg}) = [-0.2185 \times 14184.0/(T/K)] + 7.936781$; temp range 118.2–340°C (Antoine eq., Weast 1972–73)
- 0.159 (extrapolated from Antoine eq. of liquid state P_L , Boublik et al. 1973)
- 30.4* (100.0°C, inclined-piston manometry, measured range 100.0–150.0°C, Osborn & Douslin 1975)
- 0.0187 (lit. average-interpolated, API 1979)
- 0.0263* (gas saturation, Macknick & Prausnitz 1979)
- 0.0267 (extrapolated-Clapeyron eq., Macknick & Prausnitz 1979)
- $\log (P/\text{mmHg}) = 26.648 - 10484/(T/K)$; temp range 51.6–90.3°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
- 0.018* (effusion, De Kruif 1980)
- 0.0161* (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
- $\log (P/\text{Pa}) = 14.852 - 4962.77/(T/K)$; temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)
- 0.016 (generator column-HPLC/UV, Wasik et al. 1983)
- 0.111, 0.0688 (P_{GC} by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
- 0.134 (supercooled liquid P_L converted from literature P_s , Bidleman 1984)
- $\log (P_L/\text{kPa}) = 6.61335 - 2593.134/(224.402 + t/^\circ\text{C})$; temp range 203.6–346.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P_L/\text{kPa}) = 6.01392 - 2039.351/(168.569 + t/^\circ\text{C})$; temp range 230–340°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P/\text{mmHg}) = 7.26082 - 2379.04/(203.76 + t/^\circ\text{C})$; temp range 176–379°C (Antoine eq., Dean 1985, 1992)
- 0.070 (Yamasaki et al. 1984)
- 0.0149 (selected, Howard et al. 1986)

- 0.012* (gas saturation, extrapolated-Antoine eq. from exptl. data, temp range 49–74°C, Sato et al. 1986)
 $\ln (P/\text{Pa}) = 20.3950 - 2931.20/(T/\text{K} - 139.743)$; temp range: 322.9–347.8 K (Antoine eq., gas saturation, Sato et al. 1986)
- 0.025 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 10.305 - 4444/(T/\text{K})$; temp range 296–315 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 10.70162 - 4554.38/(T/\text{K})$; temp range 313–363 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.64812 - 2513.134/(-65.345 + T/\text{K})$; temp range 373–423 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.17186 - 3235.19/(12.908 + T/\text{K})$; temp range 391–613 K (Antoine eq., Stephenson & Malanowski 1987)
- 0.0127, 0.0827 (literature mean P_s , supercooled liquid P_L , Bidleman & Foreman 1987)
- 0.111, 0.0556 (P_{GC} , GC-RT correlation with different reference standards, Hinckley et al. 1990)
- 0.134, 0.10 (supercooled liquid P_L converted from literature P_s with different ΔS_{fus} values, Hinckley et al. 1990)
 $\log (P_L/\text{Pa}) = 11.46 - 3716/(T/\text{K})$ (GC-RT correlation, Hinckley et al. 1990)
 $\log (P/\text{mmHg}) = 50.2858 - 5.7409 \times 10^3/(T/\text{K}) - 13.935 \cdot \log (T/\text{K}) - 8.852 \times 10^{-10} \cdot (T/\text{K}) + 2.11343 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 372–869 K (vapor pressure eq., Yaws 1994)
- 0.0708 (supercooled liquid P_L , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
- 0.0251, 0.0227, 0.018, 0.0186; 0.0267, 0.0161 (quoted exptl.: effusion method, gas saturation, Delle Site 1997)
- 0.0288, 0.0227, 0.0181; 0.0196, 0.0122, 0.0173 (quoted lit.: calculated; from GC-RT correlation, Delle Site 1997)
- 0.0197* (Knudsen effusion/thermogravimetry technique, extrapolated Clausius-Clapeyron eq., Oja & Suuberg 1998)
 $\log (P/\text{Pa}) = 34.387 - 11423/(T/\text{K})$; temp range: 303–333 K (Clausius-Clapeyron eq., Knudsen effusion, Oja & Suuberg 1998)
- 0.115; 0.0306 (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_s with fugacity ratio F , Passivirta et al. 1999)
 $\log (P_s/\text{Pa}) = 11.38 - 3842/(T/\text{K})$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 9.07 - 2982/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)
- 0.0163 \pm 0.004 (gas saturation-HPLC/fluorescence; de Seze et al. 2000)
 $\log (P/\text{Pa}) = 14.852 - 4962.77/(T/\text{K})$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.0799; 0.0475 (supercooled liquid P_L , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
 $\log (P_L/\text{Pa}) = -3768/(T/\text{K}) + 11.54$; $\Delta H_{vap} = -72.2 \text{ kJ} \cdot \text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)
- 0.0202 (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)
- 0.0966 (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56 \text{ J/mol K}$, Mader & Pankow 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 5.55 (gas stripping-GC, Southworth 1979)
- 3.981 (gas stripping-GC, Mackay et al. 1979; Mackay & Shiu 1981; Mackay et al. 1982)
- 3.65 (gas stripping-GC, Mackay & Shiu 1981; Mackay et al. 1982)
- 2.38 (wetted-wall column-GC, Fendinger & Glotfelty 1990; quoted, Shiu & Mackay 1997; Shiu et al. 1999)
- 3.97 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
- 4.68* (gas stripping-GC, measured range 5.9–34.7°C, Alaei et al. 1996)
 $\ln K_{AW} = 6.0314 - 3524.18/(T/\text{K})$; temp range 5.9–34.7°C (gas stripping-GC, Alaei et al. 1996)
- 3.61 (gas stripping-GC, Shiu & Mackay 1997)
- 2.90 (gas stripping-HPLC/fluor., De Maagd et al. 1998)
- 4.29* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)
 $\ln K_{AW} = -5689.2/(T/\text{K}) + 12.75$, $\Delta H = 47.3 \text{ kJ} \cdot \text{mol}^{-1}$; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
- $\log (H/(\text{Pa m}^3/\text{mol})) = 8.14 - 2120/(T/\text{K})$ (Passivirta et al. 1999)
- 3.85 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 2.417 - 1530/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$ at 25°C or as indicated:

- 4.46 (Hansch & Fujita 1964; Leo et al. 1971; Hansch et al. 1973; Hansch & Leo 1979)
- 4.66 (calculated-molecular connectivity indices MCI, Kier et al. 1971)
- 4.67 (calculated-fragment const., Rekker 1977)
- 4.57 (shake flask-UV, concn ratio, Karickhoff et al. 1979)
- 4.45 (HPLC- k' correlation, McDuffie 1981)
- 4.63 (RP-TLC- k' correlation, Bruggeman et al. 1982)
- 4.53 (HPLC- k' correlation, Hammers et al. 1982)
- 4.52; 4.31 (shake flask; HPLC correlation, Eadsforth & Moser 1983)
- 4.46 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
- 4.28 (HPLC- k' correlation, Haky & Young 1984)
- 4.39 (RP-HPLC-RT correlation, Chin et al. 1986)
- 4.50 (HPLC-RT correlation, Wang et al. 1986)
- 4.56 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
- 4.52 \pm 0.15 (recommended, Sangster 1989, 1993)
- 4.374 \pm 0.034, 4.562 \pm 0.006 (shake flask/slow stirring-GC/HPLC, interlaboratory studies, Brooke et al. 1990)
- 4.30 (centrifugal partition chromatography, Berthod et al. 1992)
- 4.46 (shake flask-UV spectroscopy, pH 7.4, Alcron et al. 1993)
- 4.46 (recommended, Hansch et al. 1995)
- 4.53, 4.83 (26°C, 4°C, quoted, Piatt et al. 1996)
- 4.48 \pm 0.19, 4.54 \pm 0.61 (HPLC- k' correlation: ODS column, Diol column, Helweg et al. 1997)
- 4.57, 4.49–4.64 (shake flask/slow stirring-HPLC/fluor., mean value, De Maagd et al. 1998)
- 4.60 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
- 4.50; 4.65, 4.52 (shake flask-SPME solid-phase micro-extraction; quoted lit. values, Paschke et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equation:

- 7.45 (calculated, Finizio et al. 1997)
- 7.57*; 7.41 (generator column-GC; calculated-concn ratio C_o/C_A , measured range 0–40°C, Harner & Bidleman 1998)
- $\log K_{OA} = -5.62 + 3942/(T/K)$; temp range 0–40°C, $\Delta H_{OA} = 63.3$ kJ/mol (generator column-GC, Harner & Bidleman 1998)
- 7.52 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)
- 7.88 (solid-phase microextraction SPME-GC, Treves et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 3.42 (fathead minnow, Carlson et al. 1978)
- 2.51 (*Daphnia pulex*, Southworth et al. 1978)
- 2.57 (kinetic estimation, Southworth et al. 1978)
- 3.80 (mixed microbial population, Steen & Karickhoff 1981)
- 4.28 (*P. hoyi*, Eadie et al. 1982)
- 3.67 (microorganisms-water, Mabey et al. 1982)
- 4.38, 4.03, 4.57 (average, *Selenastum capricornutum*-dosed singly, dosed simultaneously, Casserly et al. 1983)
- 3.25 (*Chlorella fusca*; Geyer et al. 1984)
- 2.51 (fish, Govers et al. 1984)
- 2.97, 3.25, 3.25 (activated sludge, algae, fish, Freitag et al. 1985)
- 4.18; 4.28 (*P. hoyi* of Lake Michigan interstitial waters; of high sediment study site, Landrum et al. 1985)
- 2.51 (*Daphnia magna*, Newsted & Giesy 1987)
- 3.21 (10–20°C, *h. limbata*, rate constant ratio k_1/k_2 , Landrum & Poore 1988)
- 4.45; 3.77; 3.43 (4°C, *P. hoyi*; *S. heringianus*; *Mysis relicta*, quoted, Landrum & Poore 1988)
- 0.756, 1.487 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 4.36 (natural sediment, average of sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
- 4.08 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)
- 4.60 (fluorescence quenching interaction with AB humic acid, Gauthier et al. 1986)
- 4.28 (sediment from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
- 4.00 (Aldrich and Fluka humic acids, Chin et al. 1989)
- 6.12 (sediments average, Kayal & Connell 1990)
- 4.22, 4.28 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo 1990b)
- 4.42 (sandy surface soil, batch equilibrium-sorption isotherm, Wood et al. 1990)
- 4.07 (Quarry dark sand, batch equilibrium-sorption isotherm, Magee et al. 1991)
- 4.64 (DOM derived from soil, fluorescence quenching method, Magee et al. 1991)
- 4.42, 4.30 (marine porewater organic colloids; marine sediment, Fort Point Channel FPC 25–29 cm, Chin & Gschwend 1992)
- 4.17; 4.18, 4.17 (sediment: concn ratio C_{sed}/C_w ; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
- 4.50 (Rotterdam Harbor sediment 4.6% OC, batch sorption equilibrium, Hegeman et al. 1995)
- 4.37 (Speyer soil 1.08% OC, batch sorption equilibrium, Ou et al. 1995)
- 6.07, 7.03, 6.39; 4.12 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island; quoted lit., McGroddy & Farrington 1995)
- 5.77 (marine sediments: Fort Point Channel FPC 25–29 cm, McGroddy & Farrington 1995)
- 4.28, 4.12, 4.23 (RP-HPLC- k' correlation on different stationary phases, Szabo et al. 1995)
- 4.09; 4.32 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 4.18 (range 4.13–4.20); 3.56 (range 3.54–3.56) (4°C, low organic carbon sediment $f_{OC} = 0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
- 4.13 (range 4.06–4.19); 3.48 (range 3.47–3.48) (26°C, low organic carbon sediment $f_{OC} = 0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
- 4.65; 4.81 ± 0.16 (humic acid, HPLC- k' correlation; quoted lit., Nielsen et al. 1997)
- 2.42–2.56 (5 soils, 20°C, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
- 4.27, 4.27, 4.12, 4.27, 4.10; mean 4.12 ± 0.088 (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)
- 4.38, 4.45, 4.53, 4.33, 4.42, 4.62, 4.64 ± 0.087 (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chou et al. 1998)
- 4.48 (4.46–4.50), 4.22 (4.20–4.23) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
- 3.67; 3.29, 4.04, 3.27, 4.37, 4.21 (calculated- K_{OW} ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 4.31–6.02 (range, calculated from sequential desorption of 11 urban soils; Krauss & Wilcke 2001)
- 5.34; 5.23, 4.82, 4.98 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
- 4.39 - algae, 4.66 - degraded algae, 3.33 - cellulose, 4.72 - collagen, 4.50 - cuticle, 4.18 - lignin, 4.67 - humic acid, 4.56 - oxidized humic acid, 4.64 - Green River kerogen, 4.88 - Pula kerogen (aliphatic-rich sedimentary organic matter, batch experiments, Salloum et al. 2002)
- 4.28 (Askov soil - a Danish agricultural soil, Sverdrup et al. 2000)
- 4.03, 4.08 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)
- 4.34 (average values for sediment $OC \geq 0.5\%$, Delle Site 2001)
- 4.70 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)
- 4.66–4.90 (sediment/water, initial-final values of 5–100 d contact time, gas-purge technique-HPLC/fluor., ten Hulscher et al. 2003)
- 5.29–5.92, 5.98 (NIST SRM diesel particulate matter: flocculation-based batch equilibrium method with 59-d equilibration time, air-bridge equilibrium with 123-d equilibration time, Nguyen et al. 2004)

- 4.30–5.3, 5.2–5.5 (sediments of 5 lakes with OC ranges from 0.12–21.03%, solute concn at 1 mg/L, at 1 ng/L, sorption isotherms, Cornelissen et al. 2004)
- 4.80, 4.80, 4.50, 4.84 (sediment free of BC “black carbon”: Lake Varparanta OC 0.12%, Lake Kuorinka OC 1.39%, Lake Höytiäinen OC 3.3%, Lake Ketelmeer OC 5.51%, equilibrium sorption isotherm, Cornelissen et al. 2004)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: half-lives from solution: 97, 108 min (exptl., calculated, Mackay et al. 1983).

Photolysis: calculated $t_{1/2} = 8.4$ h for direct sunlight photolysis at 40°N latitude of midday in midsummer, near surface water and $t_{1/2} = 59$ d (inland water) and $t_{1/2} = 69$ d for inland water with sediment partitioning in a 5-m deep inland water body (Zepp & Schlotzhauer 1979)

$t_{1/2} = 3$ h, atmospheric and aqueous half-life, based on measured aqueous photolysis quantum yields and calculated for midday summer sunlight at 40°N latitude and $t_{1/2} = 25$ h after adjusting for approximate winter sunlight intensity (Howard et al. 1991);

half-lives on different atmospheric particulate substrates (appr. 25 $\mu\text{g/g}$ on substrate): $t_{1/2} = 150$ h on silica gel, $t_{1/2} = 45$ h on alumina and $t_{1/2} = 49$ h on fly ash (Behymer & Hites 1985);

$t_{1/2} = 59$ d under sunlight (Mill & Mabey 1985);

$k = 0.11 \text{ h}^{-1}$ with $t_{1/2} = 6.3$ h in distilled water (Fukuda et al. 1988);

photodegradation $k = 6.53 \times 10^{-3} \text{ min}^{-1}$ and $t_{1/2} = 1.78$ h in methanol-water (2:3, v/v) solution with an initial concn of 5.0 ppm under high pressure mercury lamp or sunlight (Wang et al. 1991)

$k(\text{expt}) = 0.00653 \text{ min}^{-1}$ pseudo-first-order direct photolysis rate constant with the calculated $t_{1/2} = 1.78$ h and the predicted $k = 0.00165 \text{ min}^{-1}$ calculated by QSPR, in aqueous solution when irradiated with a 500-W medium pressure mercury lamp (Chen et al. 1996);

direct photolysis $t_{1/2} = 4.62$ h (observed), $t_{1/2} = 3.89$ h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001);

photochemical degradation under atmospheric conditions: $k = (4.49 \pm 0.68) \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = (4.29 \pm 0.57) \text{ h}$ in diesel particulate matter, $k = (2.11 \pm 0.04) \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = (9.1 \pm 0.19) \text{ h}$ in diesel particulate matter/soil mixture, and $t_{1/2} = 17 - 4.97$ h in various soil components using a 900-W photo-irradiator as light source; $k = (3.17 \pm 0.06) \times 10^{-6} \text{ s}^{-1}$ and $t_{1/2} = (60.63 \pm 1.33) \text{ h}$ in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation $k = 0.09 \times 10^{-4} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (aquatic fate rate) $= 0.01 \text{ L M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 8 \times 10^6 \text{ d}$ (Callahan et al. 1979)

k (calc) $< 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k < 36 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k = (1.33 - 1.57) \times 10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ over the pH range 1–7 for the reaction with O_3 in water at 25°C, $t_{1/2} = 0.44 \text{ s}$ in presence of 10^{-4} M ozone at pH 7 (Butković et al. 1983)

$k_{\text{OH}} = 3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 1 \text{ K}$, $k_{\text{OH}} = 2.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $319 \pm 1 \text{ K}$ (relative rate method, Biermann et al. 1985)

$k_{\text{OH}}^* = 3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Atkinson 1989)

$k_{\text{OH}} = 25.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}}^* = 27 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 346–386 K with a calculated atmospheric lifetime of 11 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: 100% degradation within 7 d for a domestic sewage of an average of three static-flask screening test (Tabak et al. 1981);

$t_{1/2}(\text{aerobic}) = 384\text{--}4800 \text{ h}$, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$k = 0.0447 \text{ d}^{-1}$ with $t_{1/2} = 16 \text{ d}$ for Kidman sandy loam and $k = 0.0196 \text{ d}^{-1}$ with $t_{1/2} = 35 \text{ d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990);

$t_{1/2}(\text{anaerobic}) = 1536\text{--}19200 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 4$ d in inorganic solution and $t_{1/2} = 11$ d in Kendaia soil (Manilal & Alexander 1991)

removal rate of 1.10 and 0.12 mg (g of volatile suspended solid d)⁻¹, degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers respectively under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

first-order $k = 0.033$ to 0.139 L mg⁻¹ d⁻¹ for a marine PAH-degrading enrichment without sediment, the degradation rate was 2.1 to 3.5 times faster with sediment present (Poeton et al. 1999)

Biotransformation: for bacteria, 1.6×10^{-7} mL cell⁻¹ h⁻¹ (Paris et al. 1980; quoted, Mabey et al. 1982)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 203$ h⁻¹; $k_2 = 0.543$ h⁻¹ (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 2.31$ h⁻¹; $\log k_2 = -0.27$ h⁻¹ (*Daphnia pulex*, as per the correlation of Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 129.0$ mL g⁻¹ h⁻¹; $k_2 = 0.0046$ h⁻¹ (4°C, *p. hoyi*, Landrum 1988; quoted, Landrum & Poore 1988)

$k_1 = 52.5$ h⁻¹; $k_2 = 0.032$ h⁻¹ (10–20°C, *H. limbata*, Landrum & Poore 1988)

$k_1 = 94.0$ h⁻¹; $k_2 = 0.016$ h⁻¹ (4°C, *S. heringianus*, quoted, Landrum & Poore 1988)

$k_1 = 32.0$ h⁻¹; $k_2 = 0.012$ h⁻¹ (4°C, *Mysis relicta*, quoted, Landrum & Poore 1988)

$k_1 = 8.8$ mg g⁻¹ h⁻¹; $k_2 = 0.045$ h⁻¹ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 6$ h with a steady-state concn of tropospheric ozone of 2×10^{-9} M in clean air (Butković et al. 1983)

$t_{1/2} = 2.01$ – 20.1 h, based on photooxidation half-life in air (Howard et al. 1991);

calculated atmospheric lifetime of 11 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: computed near-surface of a water body, $t_{1/2} = 8.4$ h for direct photochemical transformation at latitude 40°N, midday, midsummer with $t_{1/2} = 59$ d (no sediment-water partitioning), $t_{1/2} = 69$ d (with sediment-water partitioning) on direct photolysis in a 5-m deep inland water body (Zepp & Schlotzhauer 1979);

$t_{1/2} = 0.44$ s in presence of 10^{-4} M ozone at pH 7 (Butković et al. 1983);

calculated $t_{1/2} = 59$ d under sunlight for summer at 40°N latitude (Mill & Mabey 1985);

$t_{1/2} = 3$ – 25 h, based on aqueous photolysis half-life (Howard et al. 1991);

photolysis $t_{1/2} = 1.78$ h in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2} = 768$ – 9600 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: reduction $t_{1/2}(\text{est.}) = 1196$ h, $t_{1/2}(\text{exptl}) = 825$ h for chemical available phenanthrene and $t_{1/2} = 151$ h for bioavailable phenanthrene for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C. The average uptake clearance from sediment was (0.041 ± 0.023) g of dry sediment·g⁻¹ of organism·h⁻¹, and the rate constants to become biologically unavailable was (0.0055 ± 0.003) h⁻¹ resulting a bioavailable $t_{1/2} = 126$ h (Landrum 1989); desorption $t_{1/2} = 8.6$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} = 2.5$ – 26 d (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 9.7$ d for 5 mg/kg treatment and $t_{1/2} = 14$ d for 50 mg/kg (Bulman et al. 1987);

biodegradation $k = 0.0447$ d⁻¹ with $t_{1/2} = 16$ d in Kidman sandy loam soil and $k = 0.0196$ d⁻¹ with $t_{1/2} = 35$ d in McLaurin sandy loam soil (Park et al. 1990);

biodegradation $t_{1/2} = 11$ d in Kendaia soil (Manilal & Alexander 1991);

$t_{1/2} = 384$ – 4800 h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988);

$t_{1/2} = 0.4$ – 26 wk, 5.7 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: depuration $t_{1/2} = 40.9$ h in *S. heringianus* (Frank et al. 1986);

elimination $t_{1/2} = 9$ d from rainbow trout, $t_{1/2} = 8.4$ d from clam *Mya arenaria*, $t_{1/2} = 1.9$ d from mussel *Mytilus edulis*; $t_{1/2} = 7$ d from polychaete *Abarenicola pacifica*, $t_{1/2} = 3.4$ d from Oyster, $t_{1/2} = 0.9$ d from shrimp, $t_{1/2} = 4.8$ d from polychaete *Nereis virens*, $t_{1/2} = 6.1$ d from clam *Mercenaria mercenaria* (Meador et al. 1995).

TABLE 4.1.1.23.1

Reported aqueous solubilities of phenanthrene at various temperatures

1.

Wauchope & Getzen 1972				Schwarz 1977		May et al. 1978a	
shake flask-UV				shake flask-fluorescence		generator column-HPLC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
	experimental		smoothed				
24.6	1.12	0	0.39	8.4	0.501	8.5	0.423
24.6	1.11	24.8	1.16	11.1	0.5507	10.0	0.468
29.9	1.49	25	1.18	14.0	0.640	12.5	0.512
29.9	1.49	29.9	1.49	17.5	0.784	15.0	0.601
30.3	1.47	30.3	1.52	20.2	0.881	21.0	0.816
30.3	1.48	38.4	2.27	23.3	1.085	24.3	0.995
38.4	2.44, 2.45	40.1	2.47	25.0	1.151	29.9	1.277
40.1	2.27, 2.28	47.5	3.63	29.3	1.372		
40.1	2.25	50	4.14	34.6	1.627	temp dependence eq. 2	
47.5	3.87, 3.88	50.1	4.16	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 36.32$		S	μg/kg
47.5	3.87	50.2	4.19			a	0.0025
50.1	4.30, 4.38	54.7	5.34			b	0.8059
50.1	4.32	59.2	6.85			c	5.413
50.2	4.08, 4.04	60.5	7.30			d	324
50.2	4.11	65.1	9.60				
54.7	5.66, 5.64	70.7	13.3			May et al. 1978b	
54.7	5.63	71.9	14.2			generator column-HPLC	
59.2	7.17, 7.19	73.4	15.6			t/°C	S/g·m ⁻³
59.2	7.21	75	17.2			25	1.002
60.5	7.20, 7.60					29	1.220
65.1	9.80	temp dependence eq. 1				temp dependence eq. 2	
65.1	9.70	ln x	mole fraction			S	μg/kg
65.1	9.80	ΔH_{fus}	16.28 ± 0.08			a	0.0025
70.7	12.4	$10^2 \cdot b$	3.74 ± 0.13			b	0.8059
70.7	12.6	c	27.9 ± 0.4			c	5.413
70.7	12.4					d	324
71.9	18.8						
73.4	21.5						

$$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 16.28$$

$$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 34.81$$

for temp range 5–30°C

Empirical temperature dependence equations:

$$\text{Wauchope \& Getzen (1972): } R \cdot \ln x = -[H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K) \quad (1)$$

$$\text{May et al. (1978): } S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t_{1/2} + c \cdot t + d \quad (2)$$

TABLE 4.1.1.23.1 (Continued)

2.

May 1980		May et al. 1983		Whitehouse 1984		Shaw 1989	
generator column-HPLC		generator column-HPLC		generator column-HPLC/UV		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4.0	0.361	4.0	0.361	4.6	0.358	0	0.40
8.5	0.423	8.5	0.423	8.8	0.437	10	0.50
10	0.468	10.0	0.468	12.9	0.556	20	0.85
12.5	0.512	12.5	0.512	17.0	0.720	25	1.10
15	0.601	15.5	0.602	21.1	0.880	30	1.40
20	0.787	20.0	0.788	25.3	1.10	40	2.50
21	0.816	21.0	0.817			50	4.10
24.3	0.955	24.3	0.956			50	7.20
29.9	1.227	29.9	1.188			70	13.0
						75	17.0

temp dependence eq. 2

S	μg/kg
a	0.0025
b	0.8059
c	5.412
d	324

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 34.81$
for temp range 5–30°C

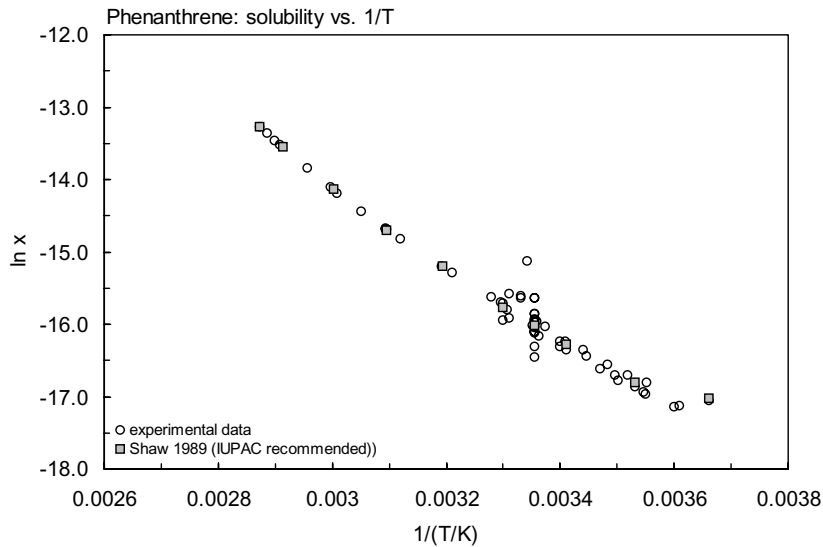


FIGURE 4.1.1.23.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for phenanthrene.

TABLE 4.1.1.23.2

Reported vapor pressures of phenanthrene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Nelson & Senseman 1922		Mortimer & Murphy 1923		Stull 1947		Bradley & Cleasby 1953	
isoteniscope-Hg manometer		isoteniscope-Hg manometer		summary of literature data		effusion	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
230	7773	203.6	3626	118.2	133.3	36.7	0.0853
235	9079	233.8	8999	154.3	666.6	39.85	0.1187
240	10532	246.0	12572	173.0	1333	42.0	0.160
245	12146	271.5	24265	193.7	2666	46.7	0.2466
250	13919	271.5	24398	215.8	5333	48.8	0.2973
255	15892	293.1	39957	229.0	7999	48.8	0.3000
260	18065	293.2	39970	249.0	13332	39.15	0.1080
265	20492	293.2	39983	277.1	26664	42.1	0.1480
270	23145	306.4	53222	308.0	53329	44.62	0.1933
275	26091	324.5	53289	340.2	101325	46.7	0.2426
280	18331	324.9	77954			49.65	0.3213
285	32891	325.4	78487	mp/ $^{\circ}\text{C}$	99.5		
290	36810	337.1	79007			eq. 2	P/mmHg
300	45823	337.1	98792			A	10.388
310	56529	345.1	115244			B	4519
320	69169	245.7	116110				
330	83913	346.8	117844				
340	100925						

2.

Hoyer & Peperle 1958		Osborn & Douslin 1975		Macknick & Prausnitz 1979		de Kruif 1980	
effusion		inclined-piston manometry		gas saturation-GC		effusion	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
data presented in		100.0	30.4	51.60	0.465	38.96	0.1
eq. 1	P/mmHg	105.0	41.20	57.70	0.813	45.29	0.2
A	16.0	110.0	54.66	61.85	1.321	49.11	0.3
B	5998	115.0	73.59	67.35	2.120	51.88	0.4
for temp range 0–60 $^{\circ}\text{C}$		120.0	95.99	71.80	3.093	54.06	0.5
		125.0	124.79	78.90	5.653	55.86	0.6
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.90$		130.0	161.05	83.40	8.892	57.40	0.7
		135.0	207.18	90.30	14.52	58.75	0.8
		140.0	264.91			9.95	0.9
		145.0	335.30	eq. 1a	P/mmHg	61.02	1.0
		150.0	420.76	A	26.648	25.0	0.18
				B	10.484		
		triple pt. tp/K	372.385			$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 90.5$	

TABLE 4.1.1.23.2 (Continued)

Hoyer & Peperle 1958		Osborn & Douslin 1975		Macknick & Prausnitz 1979		de Kruif 1980	
effusion		inclined-piston manometry		gas saturation-GC		effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
<div><div>$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) =$ at 398.15 K 68.58 at tp 70.79</div><div>$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 87.24$ at tp</div><div>$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 16.44$</div></div>							
3.							
Sonnefeld et al. 1983		Sato et al. 1986		Oja & Suuberg 1998			
generator column-HPLC		gas saturation-electrobalance		Knudsen effusion			
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa		
10.35	0.00219	322.9	0.340	30.34	0.0357		
10.35	0.00222	324.6	0.420	37.22	0.0909		
10.35	0.00211	328.5	0.655	40.77	0.140		
10.35	0.00238	333.0	1.05	44.79	0.227		
18.85	0.00738	335.2	1.34	40.1	0.323		
18.85	0.00731	337.8	1.73	59.78	0.998		
18.85	0.00749	339.5	2.03				
29.5	0.0262	343.2	2.98	eq. 1a	P/Pa		
29.5	0.0271	346.0	3.75	A	11.423		
29.5	0.0268	347.8	4.42	B	33.387		
38.65	0.0899					$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.0$	
38.65	0.0917	eq. 3a	P/Pa				
3865	0.0889	A	20.3950				
38.65	0.0849	B	3931.20				
38.80	0.0863	C	−139.743				
38.80	0.0844						
38.88	0.0902	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 96.5$					
38.90	0.0902						
38.90	0.0922						
38.90	0.0906						
25.0	0.0161						
eq. 1	P/Pa						
A	14.852						
B	4962.77						
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.0$							

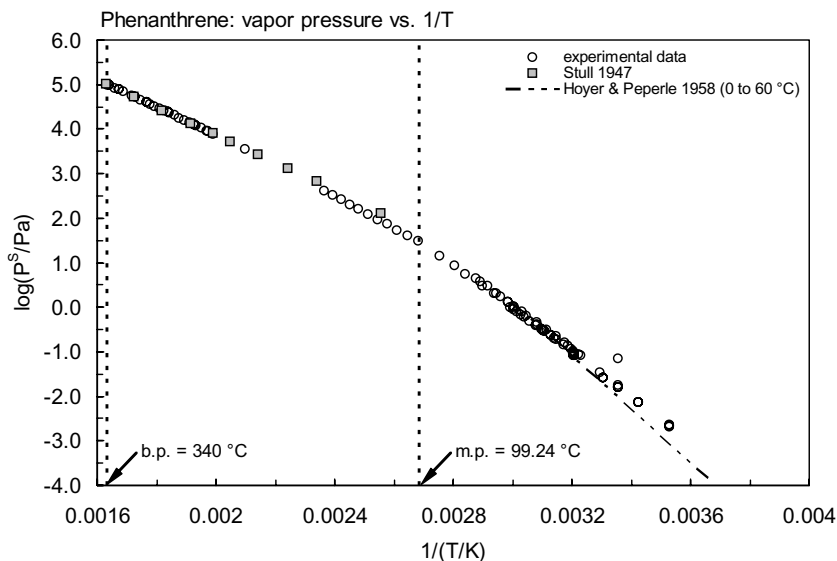


FIGURE 4.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for phenanthrene.

TABLE 4.1.1.23.3
 Reported Henry's law constants and octanol-air partition coefficients of phenanthrene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)	
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)	
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)				
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)	
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)				
Henry's law constant					$\log K_{OA}$	
Alaee et al. 1996		Bamford et al. 1999			Harner & Bidleman 1998	
gas stripping-GC		gas stripping-GC/MS			generator column-GC/FID	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	H/(Pa m ³ /mol)	t/°C	$\log K_{OA}$
				average		
5.9	1.81	4.1	0.88, 1.00	0.94	0	8.808
10.4	2.99	11.0	1.53, 1.67	1.60	10	8.267
15.0	3.06	18.0	2.55, 2.70	2.65	20	7.898
20.2	3.66	25.0	4.08, 4.51	4.29	30	7.418
25.7	4.73	31.0	5.97, 6.82	6.38	40	6.926
30.2	5.54				25(exptl)	7.57
34.7	7.90				25(calc)	7.41
$\ln K_{AW} = A - B/(T/K)$		$\ln K_{AW} = A - B/(T/K)$			$\log K_{OA} = A + B/(T/K)$	
A	6.0313	A	14.1293		A	-5.62
B	3524.2	B	5689.2		B	3942
enthalpy of volatilization:		enthalpy, entropy change:			enthalpy of phase change	
$\Delta H_{vol}/(\text{kJ}\cdot\text{mol}^{-1}) = 29.3$		$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 47.3 \pm 1.2$			$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 75.5$	
at 20°C		$\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 118$				
		at 25°C				

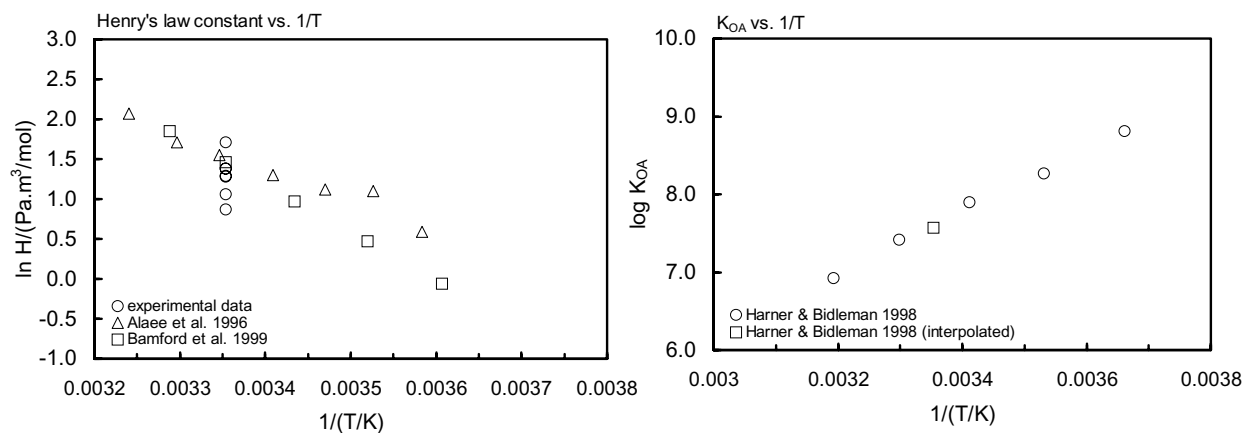
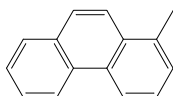


FIGURE 4.1.1.23.3 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for phenanthrene.

4.1.1.24 1-Methylphenanthrene



Common Name: 1-Methylphenanthrene

Synonym:

Chemical Name: 1-methylphenanthrene

CAS Registry No: 832-69-6

Molecular Formula: $C_{15}H_{12}$

Molecular Weight: 192.256

Melting Point ($^{\circ}C$):

123 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

354 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

188.0 (Ruelle & Kesselring 1997)

221.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.109 (mp at $123^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated *, are compiled at the end of this section):

0.255* ($24.1^{\circ}C$, generator column-HPLC/UV, measured range 6.6 – $29.9^{\circ}C$, May et al. 1978a, 1983)

0.269 (generator column-HPLC, May et al. 1978b)

$S/(\mu g/kg) = 55.42 + 6.8016 \cdot (t/^{\circ}C) - 0.1301 \cdot (t/^{\circ}C)^2 + 0.0080 \cdot (t/^{\circ}C)^3$; temp range 6.6 – $29.9^{\circ}C$ (generator column-HPLC/UV, May et al. 1978)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equation):

0.0186; 0.0160 (supercooled liquid P_L , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -3987/(T/K) + 11.64$; $\Delta H_{vap} = -76.3$ kJ \cdot mol $^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5.0* (gas stripping-GC, measured range 4.1 – $31^{\circ}C$, Bamford et al. 1999)

$\ln K_{AW} = -4257.88/(T/K) + 8.0587$, $\Delta H = 35.4$ kJ mol $^{-1}$; measured range 4.1 – $31^{\circ}C$ (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.08 (HPLC-RT correlation, Wang et al. 1986)

5.08 (recommended, Sangster 1989, 1994)

5.08 (recommended, Hansch et al. 1995)

5.10–5.20; 5.15 (quoted lit. range; lit. mean, Meador et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodegradation of 5 ppm initial concentration in methanol-water (3:7, v/v) by high pressure mercury lamp or sunlight with a rate constant $k = 1.84 \times 10^{-3}$ min $^{-1}$ and $t_{1/2} = 6.27$ h (Wang et al. 1991); the

pseudo-first-order direct photolysis $k(\text{exptl}) = 0.00184 \text{ min}^{-1}$ with the calculated $t_{1/2} = 6.27 \text{ h}$ and the predicted $k = 0.0026 \text{ min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);

direct photolysis $t_{1/2} = 3.10 \text{ h}$ (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: direct photolysis $t_{1/2} = 3.10 \text{ h}$ (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis $t_{1/2} = 6.27 \text{ h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 6.7 \text{ d}$ from Oyster, 6.0 d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.24.1

Reported aqueous solubilities and Henry's law constant of 1-methylphenanthrene at various temperature and the empirical temperature dependence equations

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

Aqueous solubility						Henry's law constant	
May et al. 1978a		May et al. 1978b		May 1980, 1983		Bamford et al. 1999	
generator column-HPLC		generator column-HPLC		generator column-HPLC		gas stripping-GC/MS	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)
6.6	0.0952	25.0	0.269	6.6	0.0952	4.1	1.42, 1.75
8.9	0.114			8.9	0.114		av. 1.58
14.0	0.147	temp dependence eq. 1		14.0	0.147	11.0	2.20, 2.53
19.2	0.193	S	μg/kg	19.2	0.193		av. 2.36
24.1	0.255	a	0.0080	24.1	0.255	18.0	3.26, 3.69
26.9	0.304	b	0.1301	26.9	0.304		av. 3.47
29.9	0.355	c	6.8016	29.9	0.355	25.0	4.62, 5.42
		d	55.42				av. 5.00
data of May et al. 1978a				data of May 1980 fitted to		31.0	6.09, 7.52
temp dependence eq. 1		ΔH _{sol} /(kJ mol ⁻¹) = 30.08		temp dependence eq. 1			av. 6.77
S	μg/kg	measured between 5–30°C		S	μg/kg	ln K _{AW} = A – B/(T/K)	
a	0.0080			a	0.0074	A	8.0587
b	0.1301			b	–0.0858	B	4257.88
c	6.8016			c	5.785		
d	55.42			d	62.9		
						enthalpy, entropy change:	
						ΔH/(kJ·mol ⁻¹) = 35.4 ± 1.9	
						ΔS/(J·K ⁻¹ mol ⁻¹) = 67	
						at 25°C	

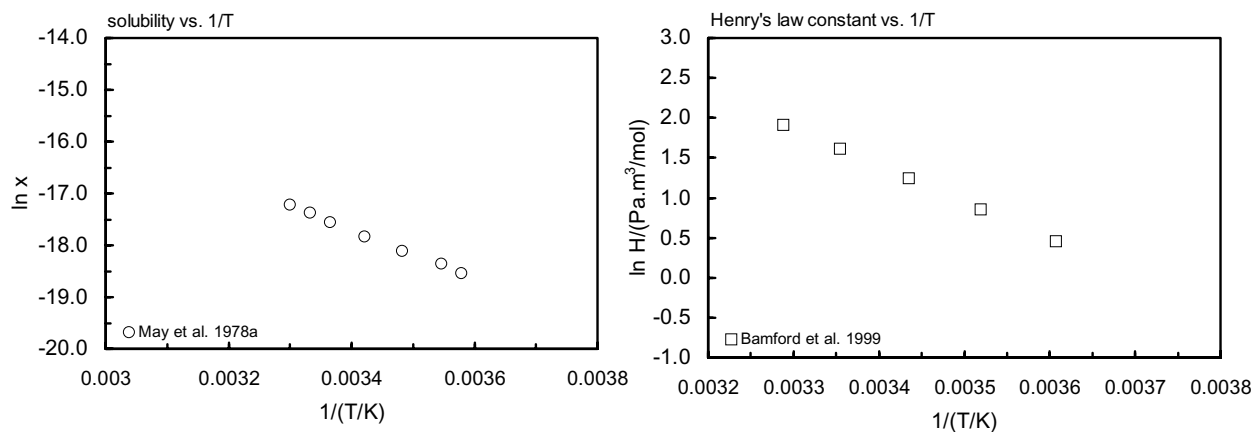
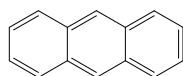


FIGURE 4.1.1.24.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1-methylphenanthrene.

4.1.1.25 Anthracene



Common Name: Anthracene

Synonym: paranaphthalene, green oil, tetra olive NZG

Chemical Name: anthracene

CAS Registry No: 120-12-7

Molecular Formula: $C_{14}H_{10}$

Molecular Weight: 178.229

Melting Point ($^{\circ}C$):

215.76 (Lide 2003)

Boiling Point ($^{\circ}C$):

339.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.25 ($27^{\circ}C$, Dean 1985)

1.28 ($25^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

139 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

196.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.83 (Parks & Huffman 1931)

28.87 (Tsonopoulos & Prausnitz 1971; Ruelle & Kesselring 1997)

29.37 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

58.99 (Tsonopoulos & Prausnitz 1971; Wauchope & Getzen 1972; Ubbelohde 1978)

58.58 (Casellato et al. 1973)

55.65 (De Kruif 1980)

60.08, 44.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0134 (mp at $215.76^{\circ}C$)

0.0101 (calculated, $\Delta S_{fus} = 58.6 J/mol K$, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.075 ($27^{\circ}C$, shake flask-nephelometry, Davis et al. 1942)

0.075 (shake flask-UV, Klevens 1950)

0.075 (Pierotti et al. 1959; Weimer & Prausnitz 1965)

0.112 (shake flask, binding to bovine serum albumin-UV, Sahyun 1966)

0.080 (shake flask-UV/fluorescence, Barone et al. 1967)

0.043 ($20^{\circ}C$, shake flask-UV, Eisenbrand & Baumann 1970)

0.040 (shake flask-UV, Eisenbrand & Baumann 1970)

0.171, 0.0392 ($20^{\circ}C$, HPLC-relative retention correlation, different stationary or mobile phases, Locke 1974)

0.075* (extrapolated value, shake flask-UV, measured range $25-74.7^{\circ}C$, Wauchope & Getzen 1972)

$R \cdot \ln x = -6930/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 19.3 + 0.0181 \cdot (T/K)$, temp range $35.4-73.4^{\circ}C$ (shake flask-UV measurements, Wauchope & Getzen 1972)

0.030 (fluorescence/UV, Schwarz & Wasik 1976)

0.073 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0446 (Rossi 1977; Neff 1979)

0.041* (shake flask-UV, measured range $8.6-31.3^{\circ}C$, Schwarz 1977)

0.074 (Lu et al. 1978)

0.0446* (generator column-HPLC/UV, measured range $5.2-29.3^{\circ}C$, May et al. 1978)

0.0434* ($24.6^{\circ}C$, generator column-HPLC, measured range $5.2-28.7^{\circ}C$, May 1980)

$S/(\mu\text{g/kg}) = 8.21 + 0.8861 \cdot (t/^\circ\text{C}) + 0.0097 \cdot (t/^\circ\text{C})^2 + 0.0013 \cdot (t/^\circ\text{C})^3$; temp range 5.2–29.3°C (generator column-HPLC/UV, May et al. 1978)

- 0.033 (20°C, generator column-fluorescence, Hashimoto et al. 1982)
 0.0434* (24.6°C, generator column-HPLC, measured range 5.6–29.3°C, May et al. 1983)
 0.030, 0.051 (generator column-HPLC/UV, Swann et al. 1983)
 0.04257* (generator column-spectrofluorimetry, measured range 10–30°C, Velapoldi et al. 1983)
 0.0446 (generator column-HPLC/UV, Wasik et al. 1983)
 0.066 (average lit. value, Pearlman et al. 1984)
 0.0698 (generator column-HPLC/fluorescence, Walters & Luthy 1984)
 0.0442* (generator column-HPLC/UV, measured range 4.6–25.3°C, Whitehouse 1984)
 0.0446 (vapor saturation-UV, Akiyoshi et al. 1987)
 0.0443, 0.034 (generator column-HPLC/UV, Billington et al. 1988)
 0.041 (20°C, shake flask/UV, ring test, Kishi & Hashimoto 1989)
 0.062* (recommended, IUPAC Solubility Data Series, Shaw 1989)
 0.070 (23°C, shake flask-HPLC/UV/fluorescence, Pinal et al. 1991)
 0.058 (generator column-HPLC, Vadas et al. 1991)
 0.0488 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
 0.043 (shake flask-HPLC, Haines & Sandler 1996)
 0.0796; 0.138, 0.0743 (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
 0.093 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
 0.070 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)
 $\log [S_L/(\text{mol/L})] = 1.679 - 1509/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\ln x = -1.43611 - 5307.35/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
 0.0434* (24.61°C, generator column-HPLC/fluoro., Reza et al. 2002)
 $\ln x = (0.50 \pm 0.45) + [(-5876 \pm 135)/(T/K)]$; temp range 282.09–323.07 K (Reza et al. 2002)
 0.0438* (generator column-HPLC/UV, measured range 0–50°C, Dohányosová et al. 2003)
 $\ln x = -33.7547 + 14.5018/\tau + C \ln \tau$, $\tau = (T/K)/298.15$ K; temp range 0–50°C (generator column-HPLC/UV, temp range 0–50°C, Dohányosová et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 5680* (220°C, isoteniscope-Hg, measured range 220–342°C, Nelson & Senseman 1922)
 6399* (223.3°C, isoteniscope-Hg manometer, measured range 223.3–340.5°C, Mortimer & Murphy 1923)
 $\log (P_s/\text{mmHg}) = 10.972 - 4595/(T/K)$; temp range 100–210°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)
 $\log (P_L/\text{mmHg}) = 7.910 - 3093/(T/K)$; temp range 223.2–340.5°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)
 133.3* (145.0°C, summary of literature data, temp range 145.0–342.0°C, Stull 1947)
 0.001014 (static method-Rodebush gauge, Sears & Hopke 1949)
 $\log (P/\text{mmHg}) = 12.0072 - 5102.6/(T/K)$; temp range 378–398 K (Rodebush gauge, Sears & Hopke 1949)
 3.60×10^{-3} (effusion method, Inokuchi et al. 1952; quoted, Bidleman 1984)
 8.31×10^{-4} * (effusion method, Bradley & Cleasby 1953)
 $\log (P/\text{cmHg}) = 11.638 - 5320/(T/K)$; temp range 65.7–80.4°C (Antoine eq., Bradley & Cleasby 1953)
 1.04×10^{-3} (fluorescence spectroscopy, Stevens 1953)
 $\log (P/\text{mmHg}) = 12.002 - 5102/(T/K)$; temp range 396–421 K (fluorescence, Stevens 1953)
 $\log (P/\text{mmHg}) = 11.15 - 5401/(T/K)$; temp range 30–100°C, (Knudsen effusion method, Hoyer & Peperle 1958)
 8.62×10^{-4} (effusion method, Kelley & Rice 1964)
 $\log (P/\text{mmHg}) = 12.068 - 5145/(T/K)$; temp range 69–86°C (effusion method, Kelley & Rice 1964)
 3.87×10^{-7} (Wakayama & Inokuchi 1967)
 0.0024* (effusion method-interpolated, measured range 290.1–358 K, Wiedemann & Vaughan 1969, Wiedemann 1972)

- $\log (P/\text{mmHg}) = 10.0216 - 4397.60/(T/K)$; temp range 290.1–358 K (Knudsen method, Wiedemann & Vaughan 1969, Wiedemann 1972)
- $\log (P/\text{mmHg}) = 7.67401 - 2819.63/(247.02 + t/^{\circ}\text{C})$; temp range: 175.5–380°C (liquid state, Antoine eq., Zwolinski & Wilhoit 1971)
- $\log (P/\text{mmHg}) = [-0.2185 \times 16823.6/(T/K)] + 8.70760$; temp range 100–600°C (Antoine eq., Weast 1972–73) 1.113×10^{-3} * (Knudsen effusion weight-loss method, extrapolated Malaspina et al. 1973)
- $\log (P/\text{torr}) = 12.616 - 5277/(T/K)$; temp range 352.7–432.3 K (Knudsen method, Malaspina et al. 1973) 1.47×10^{-5} (effusion method, Murray et al. 1974)
- 0.026 (20°C, Radding et al. 1976)
- 9.04×10^{-4} (effusion method, Taylor & Crooks 1976)
- 5.59×10^{-3} (gas saturation, Power et al. 1977)
- 1.41×10^{-3} * (gas saturation, extrapolated-Clapeyron eq., measured range 85.25–119.95°C, Macknick & Prausnitz 1979)
- $\log (P/\text{mmHg}) = 26.805 - 11402/(T/K)$; temp range 85.25–119.95°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
- 7.50×10^{-4} * (effusion methods, extrapolated, measured range 64.44–87.74°C, De Kruif 1980)
- 4.90×10^{-4} (calculated-TSA, Amidon & Anik 1981)
- 1.83×10^{-3} * (gas saturation, extrapolated-Antoine eq., measured range 50–85°C, Grayson & Fosbraey 1982)
- 1.44×10^{-3} * (gas saturation, extrapolated-Antoine eq. measured range 80–125°C, Bender et al. 1983)
- $\ln (P/\text{Pa}) = 31.620 - 11378/(T/K)$; temp range 353.6–398.6 K (Antoine eq., Bender et al. 1983)
- 8.0×10^{-4} * (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)
- $\log (P/\text{Pa}) = 12.977 - 4791.87/(T/K)$; temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)
- 8.0×10^{-4} (gas saturation-HPLC, Wasik et al. 1983)
- 0.10, 0.0638 (P_{GC} by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
- 0.0865 (supercooled liquid P_{L} , converted from literature P_{S} with ΔS_{fus} Bidleman 1984)
- $\log (P_{\text{L}}/\text{kPa}) = 6.53182 - 2550.737/(221.756 + t/^{\circ}\text{C})$; temp range 223.2–340.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P_{\text{L}}/\text{kPa}) = 6.66266 - 2659.55/(230.119 + t/^{\circ}\text{C})$; temp range 220–310°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P/\text{mmHg}) = 8.91 - 3761/(T/K)$; temp range: 100–160°C (Antoine eq., Dean 1985, 1992)
- $\log (P/\text{mmHg}) = 7.67401 - 2819.63/(247.02 + t/^{\circ}\text{C})$; temp range: 176–380°C (Antoine eq., Dean 1985, 1992)
- 1.06×10^{-3} * (gas saturation-GC, Rordorf 1985)
- 8.05×10^{-4} * (extrapolated-Clausius-Clapeyron eq. on gas saturation data, Hansen & Eckert 1986)
- $\log (P/\text{mPa}) = 17.88 - 5359/(T/K)$; temp range 313–363 K (Clausius-Clapeyron eq., Hansen & Eckert 1986)
- 1.14×10^{-3} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log (P_{\text{S}}/\text{kPa}) = 10.58991 - 4903.3/(-1.58 + T/K)$; temp range 299–439 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_{\text{S}}/\text{kPa}) = 11.76139 - 5315.532/(T/K)$; temp range 313–363 K, (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_{\text{S}}/\text{kPa}) = 10.75544 - 4947.751/(T/K)$; temp range 363–393 K (solid, Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log (P_{\text{L}}/\text{kPa}) = 7.47799 - 3612.44/(-44.906 + T/K)$; temp range 504–615 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)
- 5.73×10^{-4} ; 5.60×10^{-3} (literature mean solid P_{S} , supercooled liquid P_{L} , Bidleman & Foreman 1987)
- 0.086, 0.0940 (supercooled P_{L} , converted from literature P_{S} with different ΔS_{fus} values, Hinckley et al. 1990)
- 0.100, 0.0689 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
- $\log P_{\text{L}}/\text{Pa} = 11.18 - 3642/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
- $\log (P/\text{mmHg}) = -120.0992 + 4.478/(T/K) + 52.574 \cdot \log (T/K) - 4.7697 \times 10^{-2} \cdot (T/K) + 1.5020 \times 10^{-5} \cdot (T/K)^2$; temp range 489–873 K (vapor pressure eq., Yaws 1994)
- 0.0162; 7.64×10^{-4} , 0.0617 (liquid P_{L} by GC-RT correlation; quoted P_{S} , converted to P_{L} , Donovan 1996)
- 0.0661 (supercooled liquid P_{L} , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
- 0.000144–0.00313; 0.000804–0.00511; 0.000683–0.00484 (quoted exptl. values measured by: effusion, gas saturation; manometry, Delle Site 1997)
- 0.0049–0.00125; 0.000925–0.00129 (quoted lit. values by: calculation; from GC-RT relation, Delle Site 1997)

8.69×10^{-4} * (Knudsen effusion, extrapolated-Antoine eq. derived from exptl. data, temp range 30–60°C, Oja & Suuberg 1998)
 $\log(P/\text{Pa}) = 33.281 - 12024/(T/\text{K})$; temp range 318–363 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)
 9.01×10^{-2} ; 9.08×10^{-4} (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)
 $\log(P_S/\text{Pa}) = 11.66 - 4380/(T/\text{K})$ (solid, Passivirta et al. 1999)
 $\log(P_L/\text{Pa}) = 8.39 - 2872/(T/\text{K})$ (supercooled liquid value, Passivirta et al. 1999)
 $\log(P/\text{Pa}) = 12.977 - 4791.89/(T/\text{K})$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
0.0724; 0.0442 (supercooled liquid P_L , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
 $\log(P_L/\text{Pa}) = -3780/(T/\text{K}) + 11.54$; $\Delta H_{\text{vap}} = -72.4 \text{ kJ}\cdot\text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)
0.0014 (solid P_S , gas saturation-GC/MS, Mader & Pankow 2003)
0.0922 (supercooled liquid P_L , calculated from P_S assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$, Mader & Pankow 2003)
 $\ln(P/\text{Pa}) = 34.261 - 12339/(T/\text{K})$; temp range 313–363 K (regression eq. of Hansen & Eckert 1986 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (34.199 \pm 0.641) - (12332 \pm 229)/(T/\text{K})$; temp range 348–368 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6.59 (gas stripping-GC, Southworth 1977, 1979)
7.19 (gas stripping-GC, Mackay & Shiu 1981)
1.96 (wetted-wall column/GC, Fendinger & Glotfelty 1990)
3.30 (gas stripping-GC, Friesen et al. 1993)
8.68 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
4.94* (gas stripping-GC, measured range 4.1–31°C, Alaei et al. 1996)
 $\ln K_{\text{AW}} = 4.6774 - 3235.5/(T/\text{K})$; temp range: 5.4–35.3°C (gas stripping-GC, Alaei et al. 1996)
5.64* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)
 $\ln K_{\text{AW}} = -5629.06/(T/\text{K}) + 12.75$, $\Delta H = 46.8 \text{ kJ mol}^{-1}$, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
 $\log[H/(\text{Pa m}^3/\text{mol})] = 6.91 - 1363/(T/\text{K})$, (Passivirta et al. 1999)
4.58 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 2.065 - 1404/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.45 (Hansch & Fujita 1964; Leo et al. 1971; Hansch & Leo 1979)
4.67 (calculated-fragment const., Rekker 1977)
4.45 (calculated from Leo 1975, Southworth et al. 1978)
4.54 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)
3.45 (HPLC-RT correlation, Veith 1979a)
4.34 (Kenaga & Goring 1980)
4.49 (HPLC- k' correlation, McDuffie 1981)
4.38 (HPLC- k' correlation, Hanai et al. 1981)
4.63 (RP-TLC- k' correlation, Bruggeman et al. 1982)
4.20 (HPLC- k' correlation, D'Amboise 1982)
4.45 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
4.45 (RP-HPLC-RT correlation, Rapaport et al. 1984)
4.45 (shake flask-GC, Haky & Leja 1986)
4.51 (HPLC-RT correlation, Eadsforth 1986)
4.63 (HPLC-RT correlation, Wang et al. 1986)
4.80 (HPLC-RT correlation, De Kock & Lord 1987)
 4.50 ± 0.15 (recommended, Sangster 1989, 1993)
4.57 (TLC-RT correlation, De Voogt et al. 1990)
4.45 (recommended, Hansch et al. 1995)
 4.53 ± 0.19 , 4.55 ± 0.61 (HPLC- k' correlation: ODS column, Diol column, Helweg et al. 1997)

- 4.68 (range 4.55–4.79) (shake flask-HPLC/fluo., De Maagd et al. 1998)
 5.34 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 7.30 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
 7.34 (calculated, Finizio et al. 1997)
 7.55 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 3.08, 2.68 (*Daphnia pimephales*, Southworth 1977)
 2.88 (*Daphnia pulex*, Herbes & Risi 1978)
 2.96 (*Daphnia pulex*, Southworth et al. 1978)
 3.08 (kinetic estimation, Southworth et al. 1978)
 3.89 (algae, Geyer et al. 1981)
 4.22 (*P. hoyi*, Eadie et al. 1982)
 3.67 (microorganisms-water, Mabey et al. 1982)
 2.83 (bluegill sunfish, Spacie et al. 1983)
 3.83 (activated, sludge, Freitag et al. 1984)
 3.89 (algae, Geyer et al. 1984)
 2.21 (goldfish, Ogata et al. 1984)
 2.96, 3.89, 3.83 (fish, algae, activated sludge, Freitag et al. 1985)
 2.99 (*Daphnia magna*, Newsted & Giesy 1987)
 0.820, 1.373 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.42 (natural sediment, average of sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
 3.74 (22°C, suspended particulates, Herbes et al. 1980)
 4.204 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)
 4.20 (soil, shake flask-UV, Karickhoff 1981)
 3.95, 4.46 (Aldrich humic acid 9.4 mg/L DOC, RP-HPLC separation, equilibrium dialysis, Landrum et al. 1984)
 3.95, 4.73 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with 9.6 mg/L DOC: Landrum et al. 1984)
 4.87, 5.70 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 mg/L DOC, Landrum et al. 1984)
 3.81, 4.87, 4.62, 4.20 (humic materials in natural water: Huron River 6.1% DOC spring, Huron river 6.7% DOC winter, Grand River 10.7% DOC spring, Lake Michigan 5.5% DOC spring, Lake Erie 9.6% DOC spring, RP-HPLC separation method, Landrum et al. 1984)
 4.20 (soil, shake flask-LSC, Nkedi-Kizza 1985)
 4.93 (fluorescence quenching interaction with AB humic acid, Gauthier et al. 1986)
 4.38 (HPLC- k' correlation, Hodson & Williams 1988)
 4.21 \pm 0.11 (Aldrich and Fluka humic acids, observed; Chin et al. 1989)
 4.11 (soil-fine sand 0.2% OC, dynamic soil column studies, Enfield et al. 1989)
 5.76 (sediments average, Kayal & Connell 1990)
 4.41 (RP-HPLC correlation, Pussemier et al. 1990)
 4.53, 4.42 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)
 4.34, 4.38, 4.32 (RP-HPLC- k' correlation on different stationary phases, Szabo et al. 1995)
 4.65 (humic acid, HPLC- k' correlation; Nielsen et al. 1997)
 4.62 (4.60–4.64) (sediment from Lake Oostvaardersplassen, shake flask-HPLC/UV, de Maagd et al. 1998)
 4.40; 4.30 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
 4.36–5.97; 4.20–6.90 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
 5.31; 5.33, 5.12, 4.92 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
 4.34; 4.26; 3.95–5.70 (calculated- K_{OW} ; calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)

- 4.375 at pH 4, 4.42 at pH 7, 4.39 at pH 10 in 0.001 M NaCl; 4.415 at pH 4, 4.37 at pH 7, 4.30 at pH 10 in 0.01 M NaCl; 4.50 at pH 4, 4.24 at pH 7, 4.27 at pH 10 in 0.1 M NaCl; 4.38 at pH 4, 4.40 at pH 7, 4.12 at pH 10 in 1 mM Ca^{2+} in 0.1 M total ionic strength solutions (shake flask/fluorescence, humic acid; Schlautman & Morgan 1993a)
- 4.28 at pH 4, 4.18 at pH 7, 4.24 at pH 10 in 0.001 M NaCl; 4.285 at pH 4, 4.15 at pH 7, 4.22 at pH 10 in 0.01 M NaCl; 4.23 at pH 4, 4.12 at pH 7, 4.20 at pH 10 in 0.1 M NaCl; 4.21 at pH 4, 4.19 at pH 7, 4.24 at pH 10 in 1 mM Ca^{2+} in 0.1 M total ionic strength solutions (shake flask/fluorescence, fulvic acid; Schlautman & Morgan 1993a)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization:** removal rate constants from the water column at 25°C in midsummer sunlight were: $k = 0.002 \text{ h}^{-1}$ in deep, slow, somewhat turbid water; $k = 0.001 \text{ h}^{-1}$ in deep, slow muddy water; $k = 0.002 \text{ h}^{-1}$ in deep slow, clear water; $k = 0.042 \text{ h}^{-1}$ in shallow, fast, clear water; and $k = 0.179 \text{ h}^{-1}$ in very shallow, fast, clear water (Southworth 1977);
- aquatic $t_{1/2} = 18\text{--}300 \text{ h}$ (Callahan et al. 1979);
- calculated $t_{1/2} = 62 \text{ h}$ for a river 1-m deep with water velocity of 0.5 m/s and wind velocity of 1 m/s (Southworth 1979; quoted, Herbes et al. 1980; Hallett & Brecher 1984).
- Photolysis:** removal rate constants from the water at 25°C in midsummer sunlight were: $k = 0.004 \text{ h}^{-1}$ in deep, slow somewhat turbid water; $k < 0.001 \text{ h}^{-1}$ in deep, slow, muddy water; $k = 0.018 \text{ h}^{-1}$ in deep, slow, clear water; $k = 0.086 \text{ h}^{-1}$ in shallow, fast, clear water; and $k = 0.238 \text{ h}^{-1}$ in very shallow, fast, clear water (Southworth 1977)
- 24-h photolytic $t_{1/2} \sim 1.6 \text{ h}$ in summer and $t_{1/2} = 4.8 \text{ h}$ in winter at 35°N latitude (Southworth 1977)
- direct sunlight $k = 0.15 \text{ h}^{-1}$ in winter at 35°N latitude (Callahan et al. 1979)
- $t_{1/2}(\text{calc}) = 0.75 \text{ h}$ near surface water for direct sunlight photolysis at 40°N latitude of midday in midsummer (quoted, Herbes et al. 1980; Harris 1982)
- $t_{1/2} = 4.5 \text{ d}$ in inland water, and $t_{1/2} = 5.2 \text{ d}$ in inland water with sediment partitioning and $t_{1/2} = 0.75 \text{ h}$ for direct photochemical transformation near water surface (Zepp & Schlottzauer 1979)
- atmospheric and aqueous photolysis $t_{1/2} = 0.58 \text{ h}$, based on measured aqueous photolysis rate constant for midday summer sunlight at 35°N latitude (Southworth 1979; quoted, Howard et al. 1991) and adjusted for approximate winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
- half-lives on different atmospheric particulate substrates (appr. 25 $\mu\text{g/g}$ on substrate): $t_{1/2} = 2.9 \text{ h}$ on silica gel, $t_{1/2} = 0.5 \text{ h}$ on alumina and $t_{1/2} = 48 \text{ h}$ on flyash (Behymer & Hites 1985)
- $t_{1/2} = 4.5 \text{ d}$ for summer at 40°N latitude under sunlight in surface water (Mill & Mabey 1985)
- $k = 0.66 \text{ h}^{-1}$ in distilled water with $t_{1/2} = 1.0 \text{ h}$ (Fukuda et al. 1988)
- photodegradation $k = 0.023 \text{ min}^{-1}$ and $t_{1/2} = 0.50 \text{ h}$ for initial concentration of 5 ppm in methanol-water (1:1, v/v) solution by high pressure mercury lamp or sunlight (Wang et al. 1991)
- pseudo-first-order direct photolysis rate constants, $k(\text{exptl}) = 0.023 \text{ min}^{-1}$ with the calculated $t_{1/2} = 0.50 \text{ h}$, and the predicted $k = 0.030 \text{ min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
- $k = 0.0503\text{--}0.0521 \text{ min}^{-1}$ in natural water system by UV and sunlight (Yu et al. 1999)
- direct photolysis $t_{1/2}(\text{calc}) = 3.10 \text{ h}$, predicted by QSPR, in atmospheric aerosol (Chen et al. 2001)
- Photodegradation $k = 4.7 \times 10^{-4} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)
- Oxidation:** rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
- photooxidation $t_{1/2} = 1111\text{--}38500 \text{ h}$, based on measured rate constant for reaction with hydroxyl radical in water (Radding et al. 1976; quoted, Howard et al. 1991)
- $k(\text{aquatic})$ fate rate of 50 $\text{L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 1600 \text{ d}$ (Callahan et al. 1979)
- $k(\text{calc}) = 5.0 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet O_2 and $2.2 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)
- $k(\text{aq.}) = 3.3 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 0.6 \text{ h}$ under natural sunlight conditions (NRCC 1983)
- $k_{\text{OH}} = 110 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $325 \pm 1 \text{ K}$ (relative rate technique for propene, (Biermann et al. 1985; Atkinson 1989)
- photooxidation $t_{1/2} = 0.501\text{--}5.01 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987)
- $k_{\text{OH}}(\text{calc}) = 203 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k = 3.5 \times 10^{-5} \text{ s}^{-1}$, indirect total photoreaction rate constant in surface waters (Mill 1999)

$k_{\text{OH}}^* = 190 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 306–366 K with a calculated atmospheric lifetime of 1.5 h based on gas-phase OH reaction (Brubaker & Hites 1998)

Hydrolysis: $k < 0.001 \text{ h}^{-1}$ at 25°C (Southworth 1977); not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$k = 0.061 \text{ h}^{-1}$ for microbial degradation in Third Creek water incubated 18 h at 25°C; removal rate constants from water column at 25°C in midsummer sunlight were: $k = 0.060 \text{ h}^{-1}$ in deep, slow, somewhat turbid water; $k = 0.030 \text{ h}^{-1}$ in deep, slow, muddy water; $k = 0.061 \text{ h}^{-1}$ in deep, slow, clear water; $k = 0.061 \text{ h}^{-1}$ in shallow, fast, clear water; and $k = 0.061 \text{ h}^{-1}$ in very shallow, fast, clear water (Southworth 1977)

$k = 0.035 \text{ h}^{-1}$ for microbial degradation (Herbes et al. 1980; quoted, Hallett & Brecher 1984)

significant degradation in 7 d with rapid adaptation for an average of three static-flask screening test (Tabak et al. 1981)

$k = 2.5 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 12 \text{ d}$ and $k = 2.5 \times 10^{-4} \text{ h}^{-1}$ with $t_{1/2} = 115 \text{ d}$ for mixed bacterial populations in oil-contaminated and pristine stream sediments (Herbes & Schwall 1978, NRCC 1983)

$t_{1/2}(\text{aq. aerobic}) = 1200\text{--}11040 \text{ h}$, based on aerobic soil die-away test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991)

$k = 0.0052 \text{ d}^{-1}$ with $t_{1/2} = 134 \text{ d}$ for Kidman sandy loam and $k = 0.0138 \text{ d}^{-1}$ with $t_{1/2} = 50 \text{ d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)

$t_{1/2}(\text{aq. anaerobic}) = 4800\text{--}44160 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: aquatic fate rate, $k < 0.0612 \text{ h}^{-1}$ with $t_{1/2} > 11.3 \text{ h}$ (Callahan et al. 1979); estimated rate constant for bacteria of $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$\log k_1 = 2.89 \text{ h}^{-1}$; $\log k_2 = 0.0043 \text{ h}^{-1}$ (*Daphnia pulex*, Herbes & Risi 1978)

$k_1 = 702 \text{ h}^{-1}$; $k_2 = 0.589 \text{ h}^{-1}$ (*Daphnia pulex*, Southworth et al. 1978)

$k_1 = (1.73 \times 10^{-3} - 36) \text{ h}^{-1}$; $k_2 = 0.040 \text{ h}^{-1}$ (average, bluegill sunfish, Spacie et al. 1983)

$\log k_1 = 2.85 \text{ h}^{-1}$; $\log k_2 = -0.23 \text{ h}^{-1}$ (*Daphnia pulex*, correlated to Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 1.46, 16.9 \text{ h}^{-1}$; $k_2 = (1.58\text{--}1.88) \times 10^{-3} \text{ h}^{-1}$ (rainbow trout, Linder et al. 1985)

$k_1 = 87.2 \text{ h}^{-1}$; $k_2 = 0.019 \text{ h}^{-1}$ (4°C, *S. heringianus*, Frank et al. 1986)

$k_1 = 131.1 \text{ mL g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0033 \text{ h}^{-1}$ (4°C, *P. hoyi*, Landrum 1988)

$\log k_2 = .2, -0.01 \text{ d}^{-1}$ (fish, calculated- K_{OW} , Thomann 1989)

$\log k_2 = -0.96 \text{ d}^{-1}$ (oyster, calculated- K_{OW} , Thomann 1989)

$k_1 = 1.8\text{--}2.3 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.045 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.58\text{--}1.7 \text{ h}$, based on photolysis half-life in water (Howard et al. 1991);

half-lives under simulated atmospheric conditions: $t_{1/2} = 0.20 \text{ h}$ for simulated sunlight, $t_{1/2} = 0.15 \text{ h}$ for simulated sunlight + ozone with concn of 0.2 ppm, $t_{1/2} = 1.23 \text{ h}$ for dark reaction ozone with concn of 0.2 ppm (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

calculated atmospheric lifetime of 1.5 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: half-lives for removal from water column at 25°C in midsummer sunlight were, $t_{1/2} = 10.5 \text{ h}$ for deep, slow, somewhat turbid water; $t_{1/2} = 21.6 \text{ h}$ for deep, slow, muddy water; $t_{1/2} = 8.5 \text{ h}$ for deep, slow, clear water; $t_{1/2} = 3.5 \text{ h}$ for shallow, fast, clear water; and $t_{1/2} = 1.4 \text{ h}$ for very shallow, fast, clear water (Southworth 1977, Herbes et al. 1980);

computed near-surface $t_{1/2} = 0.75 \text{ h}$ of a water body and for direct photochemical transformation at latitude 40°N, midday, midsummer and half-lives: $t_{1/2} = 4.5 \text{ d}$ for no sediment-water partitioning, $t_{1/2} = 5.2 \text{ d}$ with sediment-water partitioning and for direct photolysis in a 5-m deep inland water body (Zepp & Schlotzhauer 1979);

$t_{1/2} = 0.58\text{--}1.7 \text{ h}$, based on photolysis half-life in water (Howard et al. 1991);

$t_{1/2} = 4.5 \text{ d}$ at 40°N under summer sunlight (Mill & Mabey 1985);

photolysis $t_{1/2} = 0.50 \text{ h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);

indirect photoreaction $t_{1/2} = 5.5 \text{ h}$ in surface waters (Mill 1999);

photolysis $t_{1/2} = 13.3\text{--}13.80$ min at 15°C in natural water system by UV and sunlight illumination (Yu et al. 1999).

Groundwater: $t_{1/2} = 2400\text{--}22080$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: reduction $t_{1/2} = 600$ h for chemical available anthracene and $t_{1/2} = 77$ h for bioavailable anthracene for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C . The uptake clearance from sediment was $(0.024 \pm 0.002)\text{g}$ of dry sediment $\cdot \text{g}^{-1}$ of organism $\cdot \text{h}^{-1}$, and the rate constants to become biologically unavailable were $(0.009 \pm 0.002)\text{h}^{-1}$ corresponding to $t_{1/2} = 77$ h (Landrum 1989).

Soil: $t_{1/2} = 3.3\text{--}175$ d (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 17$ d for 5 mg/kg treatment and $t_{1/2} = 45$ d for 50 mg/kg treatment (Bulman et al. 1987);

degradation rate constant $k = 0.0052\text{ d}^{-1}$ with $t_{1/2} = 134$ d for Kidman sandy loam soil and $k = 0.138\text{ d}^{-1}$ with $t_{1/2} = 50$ d for McLauren sandy loam soil (Park et al. 1990);

$t_{1/2} = 1200\text{--}11040$ h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2} = 0.5\text{--}26$ wk, 7.9 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: $t_{1/2} = 17$ h in bluegill sunfish (Spacie et al. 1983);

with depuration $t_{1/2} = 37.75$ h in *s. heringianus* (Frank et al. 1986);

elimination $t_{1/2} = 7$ d from rainbow trout, $t_{1/2} = 1.9$ d from mussel *Mytilus edulis* (quoted, Meador et al. 1995).

TABLE 4.1.1.25.1

Reported aqueous solubilities of anthracene at various temperatures and the reported empirical temperature dependence equations

$$R \cdot \ln x = -[\Delta H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K) \quad (1)$$

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (2)$$

$$\ln x = A - B/(T/K) \quad (3)$$

$$\ln x = A + B/(T/K) + C \cdot \ln (T/K) \quad (4)$$

$$\ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_o, T_o = 298.15\text{ K} \quad (4a)$$

1.

Wauchope & Getzen 1972				Schwarz 1977		May et al. 1978a	
shake flask-UV				shake flask-fluorescence		generator column-HPLC	
$t/^\circ\text{C}$	$S/\text{g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g} \cdot \text{m}^{-3}$
	experimental		smoothed*				
35.4	0.125	0	0.022	8.60	0.0233	5.2	0.0127
35.4	0.122	25	0.075	11.1	0.0244	10.0	0.0175
35.4	0.119	35.4	0.123	12.2	0.0257	14.1	0.0222
39.3	0.152	39.3	0.159	14.0	0.0274	18.3	0.0291
39.3	0.151	44.7	0.214	15.5	0.0296	22.4	0.0372
39.3	0.148	47.5	0.249	19.2	0.0323	24.6	0.0434
44.7	0.208	50	0.286	20.3	0.0396	28.7	0.0557
44.7	0.210	50.1	0.288	23.3	0.0417		
44.7	0.206	54.7	0.372	25.0	0.0410		
47.5	0.279	59.2	0.481	26.2	0.0476	temp dependence eq. 2	
50.1	0.301	64.5	0.66	28.5	0.0579	S	$\mu\text{g/kg}$
50.1	0.297	65.1	0.68	31.3	0.0695	a	0.0013
50.1	0.302	69.8	0.90			b	-0.0097
54.7	0.391	70.7	0.95			c	0.8861
54.7	0.389	71.9	1.02	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 34.81$		d	8.21
54.7	0.402	74.7	1.21				
59.2	0.480	75.0	1.23				
59.2	0.488						
59.2	0.525						
64.5	0.72	temp dependence eq. 1					

TABLE 4.1.1.25.1 (Continued)

Wauchope & Getzen 1972				Schwarz 1977		May et al. 1978a	
shake flask-UV				shake flask-fluorescence		generator column-HPLC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
64.5	0.62, 0.64	ln x	mole fraction				
65.1	0.67, 0.64	ΔH_{fus}	29.0 ± 0.29				
69.8	0.92	$10^2 \cdot b$	1.81 ± 0.15				
70.7	0.90, 0.97	c	19.3 ± 0.5				
70.7	0.96						
71.9	0.91	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 29.0$					
74.7	1.19, 1.13						
74.7	1.26						

2.

May et al. 1978b		May 1980		May et al. 1983		Velapoldi et al. 1983	
generator column-HPLC		generator column-HPLC		generator column-HPLC		generator column-fluo.	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
25	0.0446	5.2	0.0127	5.20	0.0127	10	0.0177
29	0.0579	10.0	0.0175	10.0	0.0175	15	0.02282
		14.1	0.0222	14.1	0.0222	20	0.03061
temp dependence eq. 2		18.3	0.0281	18.3	0.0291	25	0.04257
S	μg/kg	22.4	0.0372	22.4	0.0372	30	0.06123
a	0.0013	24.6	0.0434	24.6	0.0434		
b	-0.0097	28.7	0.0557	28.7	0.0557		
c	0.8861			9.70	0.0162	eq. 4	x
d	8.21			16.6	0.0251	A	-1078.056
		temp dependence eq. 2		23.2	0.0378	B	41884.5
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 43.76$		S	μg/kg	29.3	0.0572	C	161.175
for temp range 5–30°C		a	0.0013				
		b	-0.0097			$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 51.3$	
		c	0.8886				
		d	8.21				

3.

Whitehouse 1984		Shaw 1989		Reza et al. 2002		Dohányosová et al. 2003	
generator column-HPLC/UV		IUPAC recommended		generator column-HPLC/fluo		generator column-HPLC/UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4.6	0.00961	0	0.022	8.94	0.0155	0.30	0.00963
8.8	0.0129	10	0.021	11.57	0.0183	5.0	0.0124
12.9	0.0177	20	0.034	13.39	0.0198	10	0.0169
17.0	0.0237	25	0.062*	15.88	0.0246	15	0.0227
21.1	0.0323	30	0.080*	22.54	0.0287	20	0.0320
25.3	0.0442	40	0.16*	24.61	0.0434	25	0.0438
		50	0.29*	27.10	0.0505	30	0.0584
		60	0.51*	28.20	0.0540	35	0.0784
		70	0.91*	29.12	0.0565	40	0.106
				30.53	0.0633	45	0.145

(Continued)

TABLE 4.1.1.25.1 (Continued)

Whitehouse 1984		Shaw 1989		Reza et al. 2002		Dohányosová et al. 2003	
generator column-HPLC/UV		IUPAC recommended		generator column-HPLC/fluor		generator column-HPLC/UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
		*tentative		34.87	0.0890	50	0.190
				39.91	0.1157		
				44.90	0.1569	eq. 4a	x
				49.20	0.2123	A	-33.7647
						B	14.5018
				eq. 3	x	C	32.7269
				A	0.050 ± 0.45		
				B	5876 ± 135		
				temp range 282–323 K			
						$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 45.2 \pm 0.3$	
						at 298.15 K.	
						mp/K	489
						$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 29.37$	

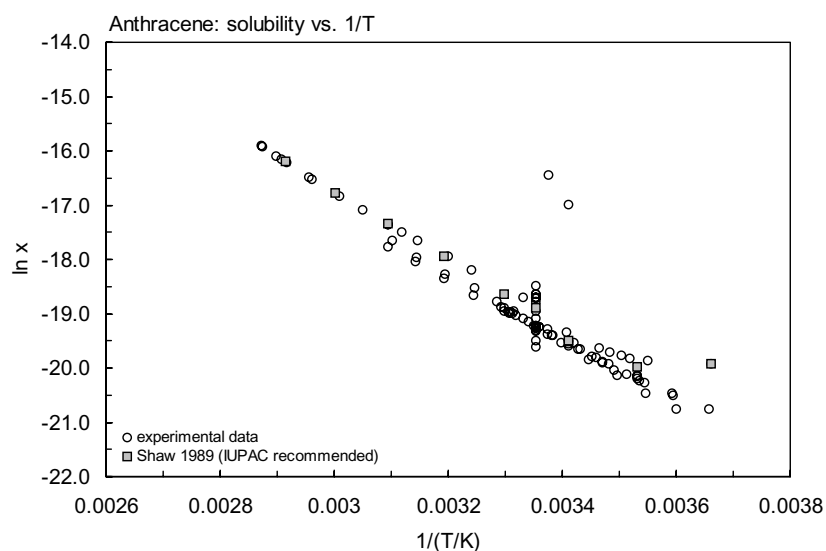
FIGURE 4.1.1.25.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for anthracene.

TABLE 4.1.1.25.2

Reported vapor pressures of anthracene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

1.

Nelson & Senseman 1922		Mortimer & Murphy 1923		Stull 1947		Sears & Hopke 1949	
isoteniscope-Hg manometer		isoteniscope-Hg manometer		summary of literature data		Rodebush gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
220	5680	223.3	6399	145.0	133.3	Data presented by	
225	6599	225.0	7333	173.5	666.6		
230	6306	244.4	11452	187.2	1333	eq. 1	P/mmHg
235	8813	244.6	11532	201.9	2666	A	12.002
240	10133	259.4	16972	217.5	5333	B	5102.0
245	11612	259.8	17105	231.8	7999	measured range 105–125°C	
250	13279	260.3	17359	250.0	13332	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 97.70$	
255	15132	282.0	29277	279.0	26664		
260	17212	282.1	29304	210.2	53329	25	.00103
265	19532	299.0	44050	342.0	101325	extrapolated	
270	22105	300.0	44170				
275	14971	312.8	57715	mp/°C	217.5		
280	28131	313.2	58155				
285	31624	313.4	58262				
290	35450	317.4	76980				
300	44263	327.9	77780				
310	54729	328.0	77860				
320	67048	340.6	98952				
330	81380	340.5	98950				
342	101325						
bp/°C	342	eq. 1	P/mmHg				
		A	7.910				
		B	3093				
		temp range 232–340°C					
		eq. 2	P/mmHg				
		A	10.972				
		B	4584				
		temp range 100–350°C					

2.

Bradley & Cleasby 1953		Kelley & Rice 1964		Malaspina et al. 1973		Power et al. 1977	
effusion		effusion		Knudsen effusion		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
65.7	0.115	data represented by		79.55	0.612	30	0.00937
69.91	0.167			88.25	1.373	30	0.00913
73.35	0.259	eq. 1	P/mmHg	98.05	3.506	50	0.0928

(Continued)

TABLE 4.1.1.25.2 (Continued)

Bradley & Cleasby 1953		Kelley & Rice 1964		Malaspina et al. 1973		Power et al. 1977	
effusion		effusion		Knudsen effusion		gas saturation	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
79.95	0.489	A	12.068	105.95	6.413	70	0.582
67.1	0.140	B	5145	113.75	12.17	70	0.5826
68.75	0.157	measured range 69–86°C		123.75	29.33	100	7.738
71.25	0.208	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 93.91$		135.25	61.06	100	7.771
73.2	0.223			142.35	106.32		
80.4	0.524	reported extrapolated data		149.75	189.31		
		95	1.667	159.15	483.95	eq. 2	P/mmHg
		100	2.546			A	36.40
eq. 1	P/mmHg	105	3.880			B	8634
A	11.638			eq. 1	P/mmHg	C	238.6
B	5320			A	12.616		
				B	5277		

3.

Macknick & Prausnitz 1979		de Kruif 1980		Grayson & Fosbraey 1982		Sonnefeld et al. 1983	
gas saturation-GC		teorsion-, weighing effusion		gas saturation-GC		gas saturation-HPLC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
85.25	0.892	64.44	0.10	20.0	0.00102	12.3	1.64×10^{-4}
90.15	1.36	71.18	0.20	50.1	0.035	12.3	1.57×10^{-4}
95.65	2.13	75.20	0.30	60.0	0.0849	12.3	1.60×10^{-4}
100.7	3.32	78.12	0.40	70.0	0.267	19.2	3.76×10^{-4}
104.7	4.59	80.41	0.50	75.0	0.359	19.2	3.83×10^{-4}
111.9	8.04	82.31	0.60	80.5	0.588	19.2	3.54×10^{-4}
116.4	11.41	83.93	0.70			19.2	3.72×10^{-4}
119.93	14.67	85.35	0.80			25.0	8.43×10^{-4}
		86.61	0.90	eq. 1	P/Pa	25.0	8.17×10^{-4}
		87.74	1.00	A	30.5	25.0	8.19×10^{-4}
eq. 1	P/mmHg			B	10968	25.0	3.30×10^{-4}
A	26.805	25.0	0.00875			30.1	1.46×10^{-3}
B	111402	extrapolated				30.1	1.54×10^{-3}
		$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 100.4$				30.1	1.51×10^{-3}
						34.93	2.59×10^{-3}
						34.93	2.63×10^{-3}
						34.93	2.69×10^{-3}
						eq. 1	P/Pa
						A	12.977
						B	4891.87

TABLE 4.1.1.25.2 (Continued)

4.

Bender et al. 1983		Rordorf 1985		Hansen & Eckert 1986		Oja & Suuberg 1998	
gas saturation		gas saturation-GC		gas saturation-IR		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
80.45	0.55	25	0.00106	40	0.0058	27.7	0.00114
82.05	0.67	50	0.023	45	0.0105	39.7	0.00575
85.35	0.864	75	0.322	50	0.0193	47.6	0.0162
90.5	1.418	100	3.17	55	0.039	54.6	0.0355
94.5	2.019	125	23.4	60	0.0675	60.1	0.062
100.8	3.426	150	136.2	65	0.0987	72.7	0.204
105.65	4.99			70	0.1688	74.1	0.258
110.4	7.17	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 98.75$		75	0.3056		
115.35	10.01			80	0.5252	eq. 1a	P/Pa
115.65	10.58	av. selected literature value		85	0.9247	A	33.281
110.857	15.30	25	0.00108	90	1.244	B	12024
125.45	21.30	50	0.0243				
		75	0.344				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 100.0$
eq. 1	P/Pa	100	3.38	eq. 1	P/mPa		
A	31.620	125	24.5	A	17.88		
B	1138	150	139.7	B	5359		
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 98.79$		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 102.6$			

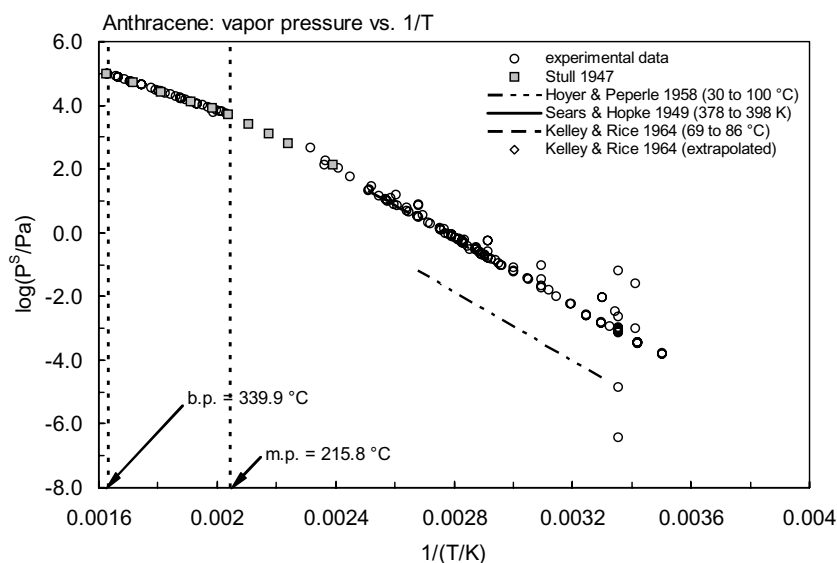


FIGURE 4.1.1.25.2 Logarithm of vapor pressure versus reciprocal temperature for anthracene.

TABLE 4.1.1.25.3
Reported Henry's law constants of anthracene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Alaee et al. 1996			Bamford et al. 1999		
gas stripping-GC			gas stripping-GC/MS		
t/°C	H/(Pa m³/mol)		t/°C	H/(Pa m³/mol)	H/(Pa m³/mol)
					average
5.4	2.76		4.1	1.14, 1.38	1.25
10.1	3.12		11.0	1.99, 2.26	2.12
14.8	3.44		18.0	3.31, 3.70	3.50
20.6	3.91		25.0	5.26, 6.06	5.64
25.0	4.94		31.0	7.60, 9.18	8.36
30.2	8.05				
34.3	8.94		eq. 1	K_{AW}	
			A	12.75	
eq. 1	K_{AW}		B	5629	
A	4.680				
B	3235.5				
enthalpy of volatilization: $\Delta H_{vol}/(\text{kJ}\cdot\text{mol}^{-1}) = 26.9$			enthalpy, entropy change: $\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 46.8 \pm 1.7$ $\Delta S/(\text{J}\cdot\text{K}^{-1} \text{mol}^{-1}) = 106$ at 25°C		

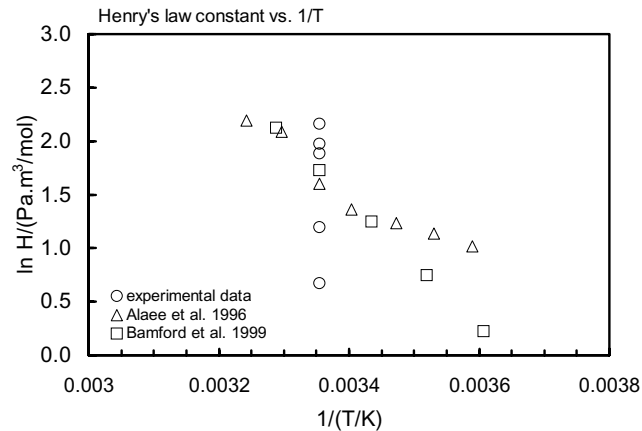
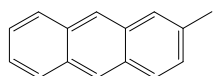


FIGURE 4.1.1.25.3 Logarithm of Henry's law constant versus reciprocal temperature for anthracene.

4.1.1.26 2-Methylantracene



Common Name: 2-Methylantracene

Synonym:

Chemical Name: 2-methylantracene

CAS Registry No: 613-12-7

Molecular Formula: $C_{15}H_{12}$

Molecular Weight: 192.256

Melting Point ($^{\circ}C$):

209 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

359 (sublimation, Bjørseth 1983)

Density (g/cm^3 at $20^{\circ}C$):

1.80 ($0^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

106 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

218.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0157 (mp at $209^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.039 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0219* (generator column-HPLC/UV, measured range 6.3 – $31.1^{\circ}C$, May et al. 1978a)

0.0213 (generator column-HPLC/UV, measured range 5 – $30^{\circ}C$, May et al. 1978b)

$S/(\mu g/kg) = 324.0 + 5.413 \cdot (t/^{\circ}) + 0.8059 \cdot (t/^{\circ}C)^2 + 0.0025 \cdot (t/^{\circ}C)^3$; temp range 5 – $30^{\circ}C$ (generator column-HPLC/UC, May et al. 1978b)

0.0191* ($23.1^{\circ}C$, generator column-HPLC/fluor., temp range 278.25 – $302.45 K$, May et al. 1983)

0.031 (average lit. value, Pearlman et al. 1984)

0.0225* (generator column-HPLC/UV, measured range 4.6 – $25.3^{\circ}C$, Whitehouse 1984)

0.03* (tentative value, IUPAC Solubility Data Series, Shaw 1989)

$\ln x = -1.841995 - 4616.86/(T/K)$, temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.0262* (generator column-HPLC/UV, measured range 0 – $50^{\circ}C$, Dohányosová et al. 2003)

$\ln x = -42.7975 + 22.9752/\tau + C \ln \tau$, $\tau = T/298.15 K$; temp range 0 – $50^{\circ}C$ (generator column-HPLC/UV, Dohányosová et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0207 (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -3976/(T/K) + 11.65$; $\Delta H_{vap} = -76.1 kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($Pa m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ and reported temperature dependence equations:

5.15 (calculated-fragment const., Yalkowsky & Valvani 1979,1980)

5.00 (shake flask-UV, Alcorn et al. 1993)

5.00 (recommended, Sangster 1993)

4.97; 4.70 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 1.093 + 1154.2/(T/K)$; temp range 5–55°C (temperature dependence HPLC- k' correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 2$ d from rainbow trout (quoted, Meador et al. 1995).

TABLE 4.1.1.26.1

Reported aqueous solubilities of 2-methylanthracene at various temperature and the empirical temperature dependence equations

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

$$\ln x = A + B/\tau + C \ln \tau \quad (2)$$

where $\tau = T/T_0$ and $T_0 = 298.15$ K

May et al. 1978a, May 1983		Whitehouse 1984		Shaw 1989b		Dohányosová et al. 2003	
generator column-HPLC		generator column-HPLC/UV		IUPAC "tentative" values		generator column-HPLC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
6.3	0.00706	4.6	—	5	0.006	0.30	0.00567
9.1	0.00848	8.8	0.00754	10	0.009	5.0	0.00738
10.8	0.00943	12.9	0.00969	20	0.016	20	0.0106
13.9	0.0111	17.0	0.0123	25	0.03	15	0.0142
18.3	0.0145	21.1	0.0161	30	0.03	20	0.0192
23.1	0.0191	25.3	0.0225			25	0.0262
27.0	0.0242					30	0.0352
31.1	0.0321					35	0.048
						40	0.0674
						45	0.0943
						50	0.125
temp dependence eq. 1						eq. 2	x
S	μg/kg					A	−42.7975
a	0.0011					B	22.9752
b	−0.0306					C	41.7206
c	0.8180						
d	2.78						
$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 39.08$						$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 46.15 \pm 0.3$	
measured between 5–30°C						0.3	
						at 298.15 K	
						mp/K	479
						$\Delta H_{fus}/(\text{kJ mol}^{-1}) = 24.06$	

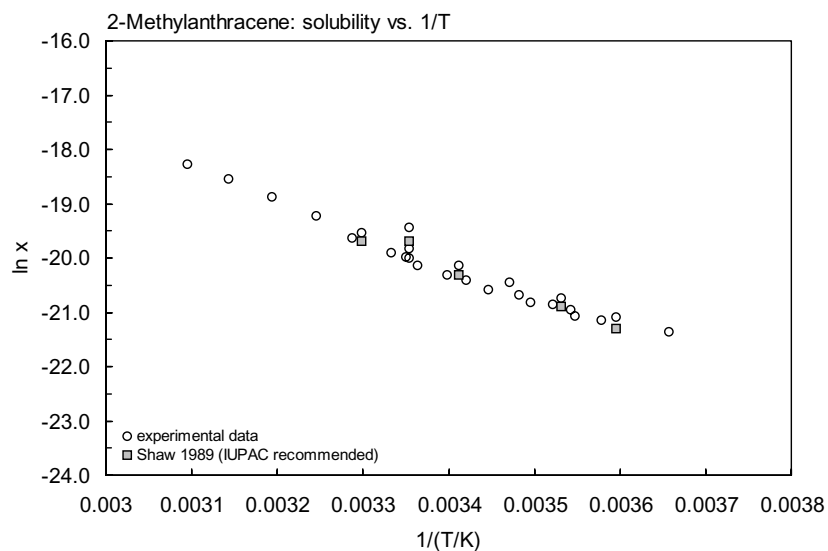
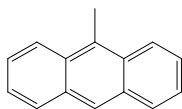


FIGURE 4.1.1.26.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-methylanthracene.

4.1.1.27 9-Methylanthracene



Common Name: 9-Methylanthracene

Synonym:

Chemical Name: 9-methylanthracene

CAS Registry No: 779-02-2

Molecular Formula: $C_{15}H_{12}$

Molecular Weight: 192.256

Melting Point ($^{\circ}C$):

81.5 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

196 (12 mm Hg, Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.065 ($99^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

181 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

218.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.279 (mp at $81.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.261 (shake flask-fluorescence, Mackay & Shiu 1977)

0.269 (average lit. value, Pearlman et al. 1984)

0.530 (generator column-HPLC, Vadas et al. 1991)

0.0376* (generator column-HPLC/UV, measured range 0 – $50^{\circ}C$, Dohányosová et al. 2003)

$\ln x = -76.9798 + 59.8386/\tau + C \ln \tau$, $\tau = T/298.15$ K, temp range 0 – $50^{\circ}C$ (generator column-HPLC/UV, Dohányosová et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00224 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 11.683 - 5168/(T/K)$; temp range 354 – 402 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.12 (calculated- π const., Southworth et al. 1978)

5.07 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)

5.15 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky & Valvani 1979,1980)

5.14 (average lit. value, Yalkowsky et al. 1983)

5.61 (HPLC-RT correlation; Burkhard et al. 1985)

5.10 (HPLC-RT correlation, Wang et al. 1986)

5.07 ± 0.20 (recommended, Sangster 1989, 1993)

5.07 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.66; 3.59 (*Daphnia pulex*; kinetic estimation, Southworth et al. 1978)

3.75	(calculated- K_{ow} , Mackay 1982)
3.94	(calculated-MCI χ , Sabljic 1987b)
3.683, 3.778	(calculated-MCI χ , calculated- K_{ow} , Lu et al. 1999)

Sorption Partition Coefficient, log K_{OC} :

4.81	(natural sediment, average of isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
4.50	(calculated-molecular connectivity indices χ , Sabljic 1984)
4.81	(calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

$t_{1/2}(\text{calc}) = 0.13$ h for direct photochemical transformation near water surface and $t_{1/2} = 0.78$ d for no sediment-water partitioning; and $t_{1/2} = 1.2$ d with sediment-water partitioning (Zepp & Schlotzhauer 1979)
 $t_{1/2} = 0.79$ d for summer at 40°N latitude under sunlight in surface water (Mill & Mabey 1985)
 photodegradation $k = 0.163 \text{ min}^{-1}$ and $t_{1/2} = 0.07$ h in methanol-water (2:3, v/v) solution for initial concentration of 5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
 the pseudo-first-order direct photolysis $k(\text{exptl}) = 0.0163 \text{ min}^{-1}$ with calculated $t_{1/2} = 0.07$ h and the predicted $k(\text{calc}) = 0.00343 \text{ min}^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

direct photolysis $t_{1/2} = 1.85$ h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Oxidation: $t_{1/2} = 10$ h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 561 \text{ h}^{-1}$; $k_2 = 0.144 \text{ h}^{-1}$ (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 2.75 \text{ h}^{-1}$; $\log k_2 = -0.84 \text{ h}^{-1}$ (*Daphnia pulex*, correlated as per Mackay & Highes 1984, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: direct photolysis $t_{1/2} = 1.85$ h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Surface water: computed $t_{1/2} = 0.13$ h at near-surface of a water body, for direct photochemical transformation, and $t_{1/2} = 0.79$ d for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning, $t_{1/2} = 1.2$ d with sediment-water partitioning to top cm bottom sediment; and $t_{1/2} = 10$ h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979);

$t_{1/2} = 0.79$ d for summer at 40°N latitude under sunlight (Mill & Mabey 1985);

photolysis $t_{1/2} = 0.07$ h in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 4$ d from rainbow trout (quoted, Meador et al. 1995).

TABLE 4.1.1.27.1

Reported aqueous solubilities of 9-methylanthracene at various temperature and the empirical temperature dependence equations

$$\ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_0 \text{ and } T_0 = 298.15 \text{ K} \quad (1)$$

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Generator column-HPLC

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0.30	0.113
5.0	0.137
20	0.174
15	0.228
20	0.286
25	0.376
30	0.508
35	0.699
40	0.953
45	1.270
50	1.770
eq. 1	mole fraction
A	-76.9798
B	59.8386
C	76.7066
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 41.8 \pm 0.2$	
at 298.15 K	
mp/K	348
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 16.95$	

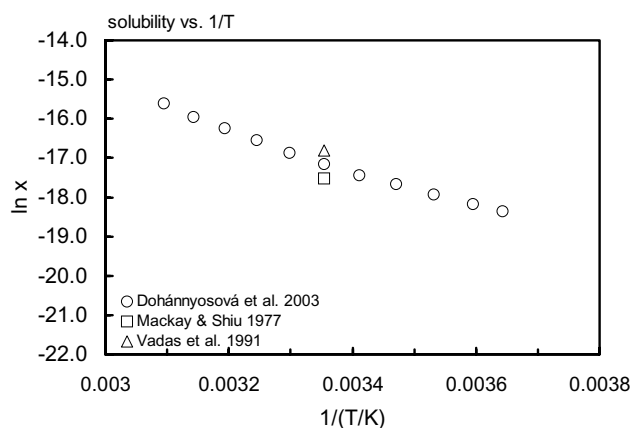
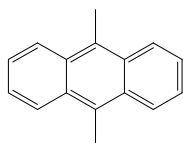


FIGURE 4.1.1.27.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 9-methylanthracene.

4.1.1.28 9,10-Dimethylantracene



Common Name: 9,10-Dimethylantracene

Synonym:

Chemical Name: 9,10-dimethylantracene

CAS Registry No: 781-43-1

Molecular Formula: $C_{16}H_{14}$

Molecular Weight: 206.282

Melting Point ($^{\circ}C$):

183.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

360 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

241.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0278 (at mp = $183.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.056 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0129* (generator column-HPLC/UV, measured range $0-50^{\circ}C$, Dohányosová et al. 2003)

$\ln x = -73.2594 + 52.6685/\tau + C \ln \tau$, $\tau = T/298.15$ K; temp range $0-50^{\circ}C$ (generator column-HPLC/UV, Dohányosová et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.53×10^{-4} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 11.266 - 5391/(T/K)$; temp range 381–434 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.69 (HPLC-RT correlation, Wang et al. 1986)

5.69 (recommended, Sangster 1989, 1993)

5.69 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photochemical transformation $t_{1/2}(\text{calc}) = 0.35$ h, computed near-surface water, latitude $40^{\circ}N$, midday, midsummer (Zepp & Schlotzhauer 1979)

photodegradation in methanol-water (2:3, v/v) solution for initial concentration of 5 ppm by high pressure mercury lamp or sunlight with a rate constant $k = 0.0633 \text{ min}^{-1}$ and $t_{1/2} = 0.18$ h (Wang et al. 1991)

pseudo-first-order direct photolysis k (exptl) = 0.0633 min^{-1} with the calculated $t_{1/2} = 0.18 \text{ h}$ and the predicted k (calc) = 0.0379 min^{-1} calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

direct photolysis $t_{1/2} = 1.17 \text{ h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Oxidation: $t_{1/2} = 1.5 \text{ h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N , midday, midsummer (Zepp & Schlotzhauer 1979)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: direct photolysis $t_{1/2} = 1.17 \text{ h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis $t_{1/2} = 0.35 \text{ h}$ near surface water, 40°N ; midday, midsummer and photosensitized oxygenation $t_{1/2} = 1.5 \text{ h}$ at near surface water, 40°N , midday, midsummer (Zepp & Schlotzhauer 1979).

photolysis $t_{1/2} = 0.18 \text{ h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 4.1.1.28.1

Reported aqueous solubilities of 9,10-dimethylanthracene at various temperature and the empirical temperature dependence equations

$$\ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_0 \text{ and } T_0 = 298.15 \text{ K} \quad (1)$$

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generator column-HPLC

$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0.30	0.000391
5.0	0.00382
20	0.00534
15	0.00698
20	0.00932
25	0.0129
30	0.0186
35	0.0252
40	0.0351
45	0.0501
50	0.0728
eq. 1	mole fraction
A	-73.2594
B	52.6685
C	71.9873

$$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 47.9 \pm 0.3$$

at 298.15 K

mp/K 455

$$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 23.46$$

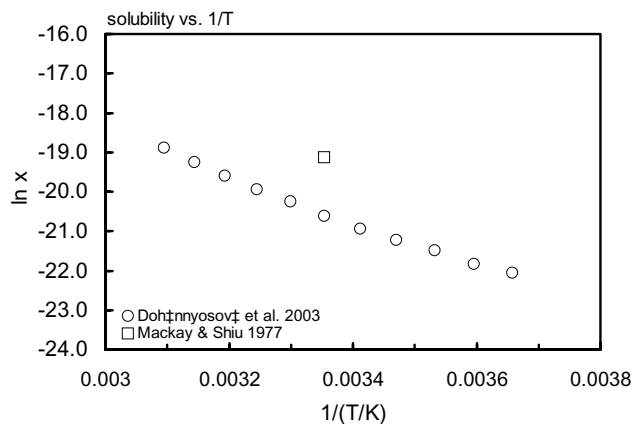
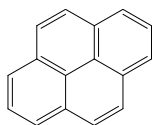


FIGURE 4.1.1.28.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 9, 10-dimethylantracene.

4.1.1.29 Pyrene



Common Name: Pyrene

Synonym: benzo[*def*]phenanthrene

Chemical Name: pyrene

CAS Registry No: 129-00-0

Molecular Formula: C₁₆H₁₀

Molecular Weight: 202.250

Melting Point (°C):

150.62 (Lide 2003)

Boiling Point (°C):

404 (Lide 2003)

Density (g/cm³ at 20°C):

1.271 (23°C, Weast 1982–83; Lide 2003)

Molar Volume (cm³/mol):

159.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

213.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.11 (Ruelle & Kesselring 1997)

0.29, 17.36; 17.65 (–152.35, 150.65°C; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

35.98 (Wauchope & Getzen 1972)

40.17 (Casellato et al. 1973)

54.8 (Hinckley et al. 1990)

40.97 (150.65°C, Chickos et al. 1999)

43.36, 43.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0585 (mp at 150.62°C)

0.128 (calculated, ΔS_{fus} = 40.3 J/mol K, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.165 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.175 (shake flask-UV, Klevens 1950)

0.148 (Pierotti et al. 1959)

1.56 (shake flask-UV/fluorescence, Barone et al. 1967)

0.105 (20°C, shake flask-UV, Eisenbrand & Baumann 1970)

0.148* (shake flask-UV, measured range 22.2–74.7°C, Wauchope & Getzen 1972)

$R \cdot \ln x = -3660/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 38.1 + 0.0478 \cdot (T/K)$; temp range 22.2–73.4°C (shake flask-UV measurements, Wauchope & Getzen 1972)

0.105, 0.133, 0.107, 0.069 (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)

0.171 (shake flask-fluorescence/UV, Schwarz & Wasik 1976)

0.135 (shake flask-fluorescence, Mackay & Shiu 1977)

0.132 (Rossi 1977; Neff 1979)

0.1295* (shake flask-fluorescence, measured range 12.2–31.3°C, Schwarz 1977)

0.132* (generator column-HPLC/UV, measured range 5–30°C, May et al. 1978b)

$S/(\mu\text{g/kg}) = 50.2 - 1.051 \cdot (t/^\circ\text{C}) + 0.2007 \cdot (t/^\circ\text{C})^2 - 0.0011 \cdot (t/^\circ\text{C})^3$; temp range 5–30°C (generator column-HPLC/UV, May et al. 1978b)

0.032 (shake flask-nephelometry, Hollifield 1979)

0.135 (shake flask-LSC, Means et al. 1979; 1980)

0.130 (shake flask-GC/UV, Rossi & Thomas 1981)

- 0.136* (25.5°C, generator column-HPLC/UV, measured range 277.85–303.05 K, May et al. 1983)
 0.129 (average lit. value, Pearlman et al. 1984)
 0.133 (generator column-HPLC/fluorescence, Walters & Luthy 1984)
 0.135 (RP-HPLC-RT correlation, Chin et al. 1986)
 0.118 (generator column-HPLC/UV, Billington et al. 1988)
 0.132* (recommended, IUPAC Solubility Data Series, Shaw 1989)
 0.150 (shake flask-LSC, Eadie et al. 1990)
 0.107 (generator column-HPLC, Vadas et al. 1991)
 0.132, 0.050 (solid S_s at 26°C); 2.61, 1.01 (supercooled liquid S_L at 4°C) (quoted, Piatt et al. 1996)
 0.131; 0.077, 0.422 (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
 0.150 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)
 $\log [S_L/(\text{mol/L})] = 0.316 - 895.4/(T/K)$; (supercooled liquid, Passivirta et al. 1999)
 $\ln x = -4.007476 - 4252.03/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
 0.1331* (25.55°C, generator column-HPLC/fluorescence, measured range 0.75–32.08°C, Reza et al. 2002)
 $\ln x = (-1.30 \pm 0.56) + (-5059 \pm 165)/(T/K)$; temp range 281.9–305.23 K (Reza et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.00339 (effusion method, Inokuchi et al. 1952)
 0.000882* (effusion method, extrapolated from Antoine eq., Bradley & Cleasby 1953)
 $\log (P/\text{cmHg}) = 10.270 - 4904/(T/K)$; temp range 71.75–85.25°C (Antoine eq., Bradley & Cleasby 1953)
 347* (200.4°C, temp range 200.4–394.7°C, Tsytkina 1955; quoted, Boublik et al. 1984)
 0.00033 (effusion method, Hoyer & Peperle 1958; quoted, Mabey et al. 1982; Tsai et al. 1991)
 $\log (P/\text{mmHg}) = 12.0 - 5248/(T/K)$, temp range 25–90°C, (Knudsen effusion method, Hoyer & Peperle 1958)
 0.2118* (348 K, Knudsen effusion, measured range 348–419 K, Malaspina et al. 1974)
 12.4* (125°C, inclined-piston gauge, measured range 125–185°C, Smith et al. 1980)
 0.00091 (effusion method, Pupp et al. 1974; quoted, Bidleman 1984)
 0.00027 (lit. average-interpolated, API 1979; quoted, Wasik et al. 1983)
 0.00088 (extrapolated from Antoine eq., Amidon & Anik 1981)
 0.00060* (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)
 $\log (P/\text{Pa}) = 12.748 - 4760.73/(T/K)$; temp range 10–50°C (solid, Antoine eq., Sonnefeld et al. 1983)
 0.0006 (generator column-HPLC/fluor./UV, Wasik et al. 1983)
 0.0113, 0.0049 (P_{GC} by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
 0.0158 (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)
 $\log (P_L/\text{kPa}) = 4.75092 - 1127.529/(16.02 + t/^\circ\text{C})$; temp range 200–394°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 0.00442 (Yamasaki et al. 1984)
 $\log (P_L/\text{mmHg}) = 5.6184 - 1122.0/(15.2 + t/^\circ\text{C})$; temp range 200–395°C (Antoine eq., Dean 1985, 1992)
 0.00033 (selected, Howard et al. 1986; quoted, Banerjee et al. 1990)
 0.00055 (interpolated Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_S/\text{kPa}) = 10.75452 - 5072.78/(T/K)$; temp range 298–401 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_S/\text{kPa}) = 11.35032 - 5286.784/(T/K)$; temp range 360–419 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.5106 - 1743.57/(-170.83 + T/K)$, temp range 513–668 K, (Antoine eq.-III, Stephenson & Malanowski 1987)
 0.000413, 0.00973 (lit. mean, supercooled liquid value P_L , Bidleman & Foreman 1987)
 0.000293* (pressure gauge, extrapolated-Antoine eq. derived exptl. data, temp 80–140°C, Sasse et al. 1988)
 $\log (P_S/\text{mmHg}) = 8.654859 - 2967.129/(182.314 + t/^\circ\text{C})$; temp range 80.11–139.97°C (solid, Antoine eq., pressure gauge, Sasse et al. 1988)
 $\log (P_L/\text{mmHg}) = 5.62672 - 1553.755/(112.964 + t/^\circ\text{C})$; temp range 139.93–194.16°C (liquid, Antoine eq., pressure gauge, Sasse et al. 1988)

0.010, 0.014 (quoted P_L , supercooled liquid P_L , GC-RT correlation, Hinckley 1989)
 0.0158, 0.0144 (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 0.0113, 0.00752 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log(P_L/Pa) = 11.92 - 4104/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
 $\log(P/mmHg) = 70.7671 - 6.9413 \times 10^3/(T/K) - 21.79 \cdot \log(T/K) + 6.0727 \times 10^{-3} \cdot (T/K) + 1.5767 \times 10^{-12} \cdot (T/K)^2$;
 temp range 424–926 K (vapor pressure eq., Yaws 1994)
 0.00446 (supercooled liquid P_L , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
 0.000334–0.00306; 0.000601; 0.000293 (quoted exptl.: effusion, gas saturation, manometry, Delle Site 1997)
 0.000173, 0.00088; 0.000247, 0.000572, 0.000713 (quoted lit., calculated; from GC-RT correlation, Delle Site 1997)
 0.00044* (Knudsen effusion, extrapolated-Antoine eq. derived from exptl. data, temp range 35–125°C, Oja & Suuberg 1998)
 $\log(P/Pa) = 33.856 - 12400/(T/K)$; temp range 308–398 K (Clausius-Clapeyron eq., Knudsen effusion, Oja & Suuberg 1998)
 1.51×10^{-2} ; 1.94×10^{-3} (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)
 $\log(P_S/Pa) = 11.60 - 4263/(T/K)$ (solid, Passivirta et al. 1999)
 $\log(P_L/Pa) = 9.49 - 3370/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 0.00073 ± 0.00033 (gas saturation-HPLC/fluorescence, de Seze et al. 2000)
 $\log(P/Pa) = 12.748 - 4760.73/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($Pa \text{ m}^3/\text{mol}$ 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.89 (gas stripping, Southworth 1979)
 1.10 (gas stripping, Mackay & Shiu 1981)
 1.21 (gas stripping-fluorescence, Shiu & Mackay 1997)
 2.0, 0.92 (gas stripping-HPLC/fluor., De Maagd et al. 1998)
 0.496 (wetted wall column-GC, Altschuh et al. 1999)
 1.71* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)
 $\ln K_{AW} = -5159.97/(T/K) + 10.103$, $\Delta H = 42.9 \text{ kJ mol}^{-1}$, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
 $\log[H/(Pa \text{ m}^3/\text{mol})] = 9.17 - 2475/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.90 (calculated- π const., Southworth et al. 1978)
 5.32 (calculated-fragment const., Callahan et al. 1979)
 4.88 (Hansch & Leo 1979)
 5.18 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)
 5.09 (shake flask-LSC, Means et al. 1979, 1980)
 5.22 (calculated- f const., Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)
 5.03 (HPLC- k' correlation, Hanai et al. 1981)
 5.05 (HPLC- k' correlation, McDuffie 1981)
 5.22 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 4.50 (HPLC- k' correlation, D'Amboise & Hanai 1982)
 4.88 (HPLC- k' correlation, Hammers et al. 1982)
 4.88 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
 4.96 (HPLC-RT correlation, Rapaport 1984)
 5.52 (HPLC-RT/MS correlation, Burkhard et al. 1985)
 4.80 (Hansch & Leo 1985)
 4.97 (RP-HPLC-RT correlation, Chin et al. 1986)
 4.95 (Leo 1986)
 5.00 ± 0.20 (recommended, Sangster 1989, 1993)
 4.88 (recommended, Hansch et al. 1995)
 5.08; 5.39 (26°C; 4°C, Piatt et al. 1996)
 4.84 ± 0.19 , 5.14 ± 0.62 (HPLC- k' correlation: ODS column; Diol column, Helweg et al. 1997)
 4.77 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
 4.79 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 8.60 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
- 8.61 (calculated, Finizio et al. 1997)
- 8.80*; 8.49 (generator column-GC; calculated- C_O/C_A , measured range 0–40°C, Harner & Bidleman 1998)
- $\log K_{OA} = -4.56 + 3985/(T/K)$; temp range 0–40°C (generator column-GC, Harner & Bidleman 1998)
- 8.75 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 3.43 (*Daphnia pulex*, Southworth et al. 1978)
- 4.38 (mixed microbial population, Steen & Karickhoff 1981)
- 4.65 (*P. hoyi*, Eadie et al. 1982)
- 4.56, 4.22, 4.75 (average, *Selenustrum capricornutum*-dosed singly, dosed simultaneously, Casserly et al. 1983)
- 2.66 (goldfish, shake flask-GC, concn. ratio, Ogata et al. 1984)
- 3.43 (*Daphnia pulex*, Mackay & Hughes 1984)
- 3.43 (*Daphnia magna*, Newsted & Giesy 1987)
- 3.65, 3.81, 2.35 (mussel, clam, shrimp, Gobas & Mackay 1989)
- 2.85, 2.70 (*Polychaete*, *Shrimo-hepatopancreas*, Gobas & Mackay 1989)
- 0.716, 1.124 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.92 (natural sediments, sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)
- 4.81 (average value of soil and sediment, shake flask-LSC, sorption isotherms, Means et al. 1979)
- 4.92 (Kenaga & Goring 1980)
- 4.80 (average value of 12 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1980)
- 4.78, 4.80 (soil/sediment: calculated- K_{OW} , regress of K_p versus substrate properties, Means et al. 1980)
- 4.826 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)
- 3.11, 3.46 (sediment suspensions, Karickhoff & Morris 1985)
- 5.23; 5.08 (fluorescence quenching interaction with AB humic acid; AB fulvic acid, Gauthier et al. 1986)
- 4.46–4.81; 4.94–5.51; 4.73–5.02 (marine humic acids; soil humic acids; soil fulvic acids, fluorescence quenching technique, Gauthier et al. 1987)
- 5.02 (dissolved humic materials, Aldrich humic acid, fluorescence quenching technique, Gauthier et al. 1987)
- 5.13 (sediment, batch equilibrium-GC, Vowles & Mantoura 1987)
- 4.88 (soil-fine sand 0.2% OC, dynamic soil column studies, Enfield et al. 1989)
- 5.65 (LSC, Eadie et al. 1990)
- 6.51 (sediments average, Kayal & Connell 1990)
- 4.83 (RP-HPLC-RT correlation, Pussemier et al. 1990)
- 4.82, 4.77 (RP-HPLC-RT correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)
- 6.50 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 5.05, 5.00, 4.88; 4.71 (marine porewater organic colloids: Fort Point Channel FPC 7–9 cm, FPC 15–17 cm, FPC 25–29 cm; Spectacle Island 14–16 cm, Chin & Gschwend 1992)
- 5.20, 5.18, 4.99; 5.23 (marine sediments: Fort Point Channel FPC 7–9 cm, FPC 15–17 cm, FPC 25–29 cm; Spectacle Island 14–16 cm, Chin & Gschwend 1992)
- 4.78; 4.78, 4.78 (sediment: concn ratio C_{sed}/C_w ; concn-based coeff., area-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
- 5.50, 6.61, 6.06 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island, McGroddy & Farrington 1995)
- 5.51, 5.34, 5.31; 7.43 (marine sediments: Fort Point Channel FPC 7–9 cm, FPC 15–17 cm, FPC 25–29 cm; Spectacle Island 14–16 cm, McGroddy & Farrington 1995)
- 4.64 (Aldrich humic acid, Ozretich et al. 1995)
- 4.80, 4.81, 4.72 (RP-HPLC- k' correlation on different stationary phases, Szabo et al. 1995)
- 4.81 (range 4.73–4.66); 4.22 (range 4.20–4.22) (4°C, low organic carbon sediment $f_{OC} = 0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)

- 4.62 (range 4.56–4.67); 4.0 (range 3.98–4.00) (26°C, low organic carbon sediment $f_{oc} = 0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
- 4.42–2.56 (5 soils, 20°C, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
- 4.99, 4.98, 4.96, 4.97, 4.97 (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chioiu et al. 1998)
- 5.14, 5.22, 5.23, 5.12, 5.04, 5.24, 5.45; mean 4.98 ± 0.009 (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Chioiu et al. 1998)
- 3.47, 4.60, 3.53, 4.78, 4.61; mean 5.18 ± 0.056 (HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 4.66, 4.78 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)
- 4.88, 4.90 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)
- 5.47–6.68; 4.60–6.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.90; 5.89, 5.60, 5.56 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
- 4.96; 4.70; 4.46–5.74 (calculated- K_{ow} ; calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)
- 4.50 at pH 4, 4.37 at pH 7, 4.33 at pH 10 in 0.001M NaCl; 4.35 at pH 4, 4.20 at pH 7, 4.245 at pH 10 in 0.01M NaCl; 4.35 at pH 4, 4.15 at pH 7, 4.15 at pH 10 in 0.1M NaCl; 4.33 at pH 4, 4.29 at pH 7, 4.15 at pH 10 in 1mM Ca^{2+} in 0.1M total ionic strength solutions (shake flask/fluorescence, humic acid; Schlautman & Morgan 1993a)
- 4.19 at pH 4, 3.89 at pH 7, 3.92 at pH 10 in 0.001M NaCl; 4.15 at pH 4, 3.88 at pH 7, 3.86 at pH 10 in 0.01M NaCl; 4.08 at pH 4, 3.81 at pH 7, 3.785 at pH 10 in 0.1M NaCl; 4.08 at pH 4, 3.90 at pH 7, 4.06 at pH 10 in 1mM Ca^{2+} in 0.1M total ionic strength solutions (shake flask/fluorescence, fulvic acid; Schlautman & Morgan 1993a)
- 5.52 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)
- 4.66 (Askov soil, a Danish agriculture soil, Sverdrup et al. 2002)
- 5.35–6.33 (field contaminated sediment, initial-final values of 5–100 d contact time, gas-purge technique-HPLC/fluorescence, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: sublimation rate constant of $1.1 \times 10^{-4} s^{-1}$ was measured as loss from glass surface at 24°C at an air flow rate of 3 L/min (Cope & Kalkwarf 1987)
- Photolysis: calculated $t_{1/2} = 4.2$ d for direct sunlight photolysis in midday of midsummer at 40°N for inland water, and $t_{1/2} = 5.9$ d for inland water with sediment partitioning (Zepp & Schlotzhauer 1979)
- $k = 1.014 h^{-1}$ (Zepp 1980)
- $t_{1/2} = 0.68$ h atmospheric and aqueous photolysis half-life, based on measured aqueous photolysis quantum yields calculated for midday summer sunlight at 40°N latitude (Zepp & Schlotzhauer 1979; quoted, Harris 1982; Howard et al. 1991) and $t_{1/2} = 2.04$ h after adjusting for approximate winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
- half-lives: $t_{1/2} = 21$ h on silica gel, $t_{1/2} = 31$ h on alumina and $t_{1/2} = 46$ h on fly ash on different atmospheric particulate substrates (approximate 25 $\mu g/g$ on substrate) (Behymer & Hites 1985);
- $t_{1/2} = 4.2$ d for summer sunlight photolysis in surface water (Mill & Mabey 1995)
- $k < 1.05 \times 10^{-4} m/s$ at 24°C with $[O_3] = 0.16$ ppm and light intensity of 1.3 kW/m^2 on glass surface of (Cope & Kalkwarf 1987)
- photodegradation $t_{1/2} = 1$ h in summer to days in winter by sunlight for adsorption on airborne particulates (Valerio et al. 1991);
- photolysis $t_{1/2} = 0.68$ h in water, based on direct photolysis in sunlight at midday, midsummer, latitude 40°N (Zepp 1991)
- $k(exptl) = 0.00362 min^{-1}$ for pseudo-first-order direct photolysis, with $t_{1/2} = 3.18$ h, and the predicted $k(calc) = 0.00382 min^{-1}$ by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
- $t_{1/2}(obs.) = 2.63$ h, $t_{1/2}(calc) = 2.56$ h by QSPR in atmospheric aerosol (Chen et al. 2001);
- $k = (2.08 \pm 0.13) \times 10^{-5} s^{-1}$ and $t_{1/2} = (9.24 \pm 0.53)h$ in diesel particulate matter, photochemical degradation under atmospheric conditions, $k = (1.88 \pm 0.16) \times 10^{-5} s^{-1}$ and $t_{1/2} = (10.22 \pm 0.95)h$ in diesel particulate matter/soil mixture, and $t_{1/2} = 0.80$ to 1.59 h in various soil components using a 900-W photo-irradiator as light source; $k = (2.61 \pm 0.53) \times 10^{-7} s^{-1}$ and $t_{1/2} = (737.55 \pm 124.49)h$ in diesel particulate matter using a 300 W light source (Matsuzawa et al. 2001)

Photodegradation $k = 3.9 \times 10^{-4} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $2.2 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k = (3.4\text{--}5.3) \times 10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ over pH range 1–7, with $t_{1/2} = 0.18 \text{ s}$ in presence of 10^{-4} M ozone at pH 7 for the reaction with O_3 in water at 25°C (Butković et al. 1983)

$k_{\text{OH}} = 5.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{\text{N}_2\text{O}_5} \approx -5.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with N_2O_5 at $296 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1990)

photooxidation $t_{1/2} = 0.802\text{--}8.02 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: significant degradation within 7 d for a domestic sewage 28-d test for an average of three static-flask screening (Tabak et al. 1981)

$t_{1/2}(\text{aq. aerobic}) = 5040\text{--}45600 \text{ h}$, based on aerobic soil die-away test data at $10\text{--}30^\circ\text{C}$ (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991)

$k = 0.29 \text{ h}^{-1}$ in atmosphere (Dragoscu & Friedlander 1989; quoted, Tsai et al. 1991)

$k = 0.0027 \text{ d}^{-1}$ with $t_{1/2} = 260 \text{ d}$ for Kidman sandy loam and $k = 0.0035 \text{ d}^{-1}$ with $t_{1/2} = 199 \text{ d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)

$t_{1/2}(\text{anaerobic}) = 20160\text{--}182400 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated to be $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 1126 \text{ h}^{-1}$; $k_2 = 0.343 \text{ h}^{-1}$ (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 3.05 \text{ h}^{-1}$; $\log k_2 = -0.46 \text{ h}^{-1}$ (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 113.0 \text{ h}^{-1}$; $k_2 = 0.017 \text{ h}^{-1}$ (4°C , *S. heringianus*, Frank et al. 1986)

$k_2 = 0.017 \text{ h}^{-1}$ (*S. heringianus*, Frank et al. 1986)

$k_1 = 199.2 \text{ mL g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0012 \text{ h}^{-1}$ (4°C , *P. hoyi*, Landrum 1988)

$k_1 = 3.4\text{--}5.3 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.022 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.68\text{--}2.04 \text{ h}$, based on estimated sunlight photolysis half-life in water (Zepp & Stotzhauer 1979; Lyman et al. 1982; quoted, Howard et al. 1991);

half-lives under simulated atmospheric conditions: $t_{1/2} = 4.20 \text{ h}$ under simulated sunlight, $t_{1/2} = 2.75 \text{ h}$ under simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 15.72 \text{ h}$ under dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

$t_{1/2} = 2.5 \text{ h}$ with a steady-state concn of tropospheric ozone of $2 \times 10^{-9} \text{ M}$ in clean air (Butković et al. 1983); photooxidation $t_{1/2} = 0.802\text{--}8.02 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: computed near-surface $t_{1/2} = 0.58 \text{ h}$ for direct photochemical transformation at latitude 40°N , midday, midsummer, $t_{1/2} = 4.2 \text{ h}$ for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning and $t_{1/2} = 5.9 \text{ d}$ with sediment-water partitioning (Zepp & Schlotzhauer 1979);

$t_{1/2} = 0.68\text{--}2.04 \text{ h}$, based on estimated sunlight photolysis half-life in water (Lyman et al. 1982; quoted, Howard et al. 1991);

$t_{1/2} = 1.8 \text{ s}$ in presence of 10^{-4} M ozone at pH 7 (Butković et al. 1983);

$t_{1/2} = 4.2 \text{ d}$ for summer at 40°N latitude under sunlight (Mill & Mabey 1985);

$t_{1/2} = 0.68 \text{ h}$, based on direct photolysis in sunlight at midday, mid-summer and 40°N latitude (quoted, Zepp 1991); photolysis $t_{1/2} = 3.18 \text{ h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2} = 10080\text{--}91200 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: reduction $t_{1/2} = 547 \text{ h}$ for chemical available pyrene and $t_{1/2} = 298 \text{ h}$ for bioavailable pyrene for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C . The uptake clearance from sediment, $k = (0.019\text{--}0.015) \text{ g of dry sediment} \cdot \text{g}^{-1} \text{ of organism} \cdot \text{h}^{-1}$, and the rate constants to become biologically unavailable were $k = 0.0019$

h^{-1} for 10-d aged sediment corresponding to a $t_{1/2} = 365$ d and $k = 0.0030$ h^{-1} for nonaged sediment corresponding to a $t_{1/2} = 231$ h (Landrum 1989).

Soil: $t_{1/2} = 3\text{--}35$ h (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 58$ d for 5 mg/kg treatment and $t_{1/2} = 48$ d for 50 mg/kg treatment (Bulman et al. 1987);

$t_{1/2} = 5040\text{--}45600$ h, based on aerobic soil die-away test data at $10\text{--}30^{\circ}\text{C}$ (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988);

degradation rate constant, $k = 0.0027$ d^{-1} with $t_{1/2} = 260$ d for Kidman sandy loam soil and $k = 0.0035$ d^{-1} with $t_{1/2} = 199$ d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 500$ d in soil (Jury et al. 1990);

$t_{1/2} = 0.4$ to more than 90 wk, 8.5 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: depuration $t_{1/2} = 40.8$ h in *s. heringianus* (Frank et al. 1986);

elimination $t_{1/2} = 4.1\text{--}5.5$ d from mussel *Mytilus edulis*; $t_{1/2} = 10.3$ d from clam *Mya arenaria*, $t_{1/2} = 14.4$ d from polychaete *Abarenicola pacifica*, $t_{1/2} = 6.7$ d from Oyster, $t_{1/2} = 0.80$ d from shrimp, $t_{1/2} = 3.6$ d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.29.1

Reported aqueous solubilities of pyrene at various temperatures

1.

Wauchope & Getzen 1972				Schwarz 1977		May et al. 1978a	
shake flask-UV				shake flask-fluorescence		generator column-HPLC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
experimental		smoothed					
22.2	0.129	0	0.049	12.2	0.055	25	0.132
22.2	0.128	22.2	0.130	15.5	0.069	29	0.162
22.2	0.124	25	0.148	17.4	0.079		
34.5	0.228	34.5	0.235	20.3	0.092	temp dependence eq. 2	
34.5	0.235	44.7	0.399	23.0	0.117	S	μg/kg
44.7	0.397	50	0.532	23.3	0.118	a	−0.0011
44.7	0.395	50.1	0.534	25.0	0.129	b	0.2007
44.7	0.405	55.6	0.730	26.2	0.144	c	−1.051
50.1	0.558	56.0	0.74	26.7	0.145	d	50.2
50.1	0.576	60.7	0.97	28.5	0.164		
50.1	0.556	65.2	1.27	31.3	0.188	ΔH _{sol} /(kJ mol ⁻¹) = 35.44	
55.6	0.75	71.9	1.90			for temp range 5–30°C	
55.6	0.75	74.7	2.26	ΔH _{sol} /(kJ mol ⁻¹) = 47.70			
55.6	0.77	75.0	2.31				
56.0	0.74						
60.7	0.96	temp dependence eq. 1					
60.7	0.95	ln x	mole fraction				
60.7	0.90	ΔH _{fus}	15.3 ± 0.084				
65.2	1.27	10 ² ·b	4.78 ± 0.09				
65.2	1.29	c	38.1 ± 0.3				
71.9	1.83						
71.9	1.86						
71.9	1.89						
74.7	2.21						
ΔH _{fus} /(kJ mol ⁻¹) = 15.3							

Empirical temperature dependence equations:

Wauchope & Getzen (1972): $R \cdot \ln x = -[H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K)$ (1)

May et al. (1978): $-S/(\mu\text{g}/\text{kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d$ (2)

TABLE 4.1.1.29.1 (Continued)

2.

May 1980		May et al. 1983		Shaw 1989		Reza et al. 2002	
generator column-HPLC		generator column-HPLC		IUPAC recommended		generator column-HPLC/fluor	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4.7	0.0492	4.7	0.0492	0	0.050	8.54	0.0474
9.5	0.0585	9.5	0.0586	20	0.090	10.39	0.0566
14.3	0.0720	14.3	0.0721	25	0.132	13.5	0.0635
18.7	0.0933	18.7	0.0934	30	0.175	14.46	0.0694
21.2	0.109	21.2	0.1091	40	0.30	15.7	0.0804
25.5	0.136	25.5	0.1361	50	0.50	18.05	0.0871
29.9	0.170	29.9	0.1701	60	0.90	21.53	0.1087
				70	1.70	25.55	0.1331
				75	2.30	27.36	0.1505
temp dependence eq. 2						29.66	0.1686
S	μg/kg					21.28	0.1931
a	-0.0011						
b	0.2007						
c	-1.051						
d	50.2						
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 35.44$						$\ln x = A - B/T(\text{K})$	
for temp range 5–30°C						A	
						B	
						temp range 282–305 K	

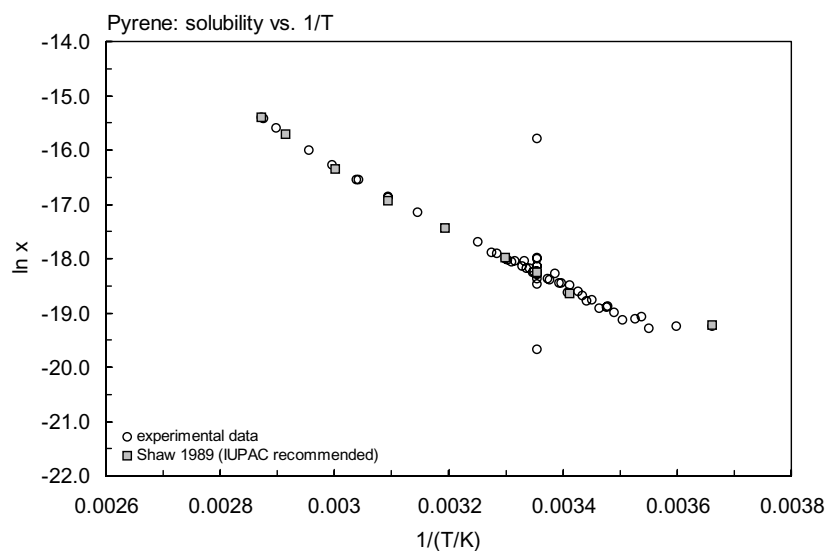
FIGURE 4.1.1.29.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for pyrene.

TABLE 4.1.1.29.2

Reported vapor pressures of pyrene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Bradley & Cleasby 1953		Tsyapkina 1955		Hoyer & Peperle 1958		Malaspina et al. 1974	
effusion		in Boublik et al. 1984		effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
68.9	0.1147	200.4	347	data presented by		348	0.2118
74.15	0.1880	220.8	920	eq. 1	P/mmHg	361	0.508
78.1	0.263	242.7	2440	A	12.00	364	0.717
78.1	0.274	256.4	4373	B	5348	369	1.034
81.7	0.2746	270.0	6493	temp range 25–90°C		377	2.016
82.65	0.3893	277.0	7999	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 100.5$		384	3.871
85.0	0.4093	288.7	10866			393	7.934
71.75	0.1440	293.0	12599			402	15.20
75.85	0.2226	306.0	17932			411	31.01
82.7	0.2880	316.0	22665			419	55.42
82.25	0.4053	394.7	101324				
85.0	0.5066			for solid pyrene:			
		bp/°C	394.707			eq. 1	P/atm
eq. 1	P/mmHg					A	8.848
A	10.270					B	5091
B	4904						
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 93.90$				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 101.04$ at 298.15 K			

2.

Smith et al. 1980		Sonnefeld et al. 1983		Sasse et al. 1988		Oja & Suuberg 1998	
inclined-piston gauge		gas saturation-HPLC		electronic manometry		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
solid				solid			
125	12.4	10.5	9.20×10^{-5}	80.11	0.30	46.95	0.00863
130	17.5	10.5	9.21×10^{-5}	90.10	0.764	56.99	0.0243
135	24.7	10.5	9.53×10^{-5}	100.11	1.853	37.98	0.0209
140	34.7	20.9	3.35×10^{-4}	110.14	4.360	68.03	0.0852
145	48.0	20.9	3.35×10^{-4}	120.08	9.213	72.99	0.164
149	62.1	20.9	3.39×10^{-4}	120.10	9.40	83.99	0.428
150	66.1	30.0	1.10×10^{-4}	129.99	19.20	93.02	0.945
liquid		30.0	1.09×10^{-4}	134.98	26.80		
125	17.1*	30.0	1.03×10^{-4}	139.97	37.07	eq. 1a	P/Pa
130	22.5*	39.34	3.31×10^{-3}	liquid		A	33.856
135	29.9*	39.34	3.47×10^{-3}	139.93	40.80	B	12400
140	39.5*	39.34	3.25×10^{-3}	144.90	53.06		
145	51.3*	39.45	3.41×10^{-3}	149.82	68.66	$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 103.10$	

TABLE 4.1.1.29.2 (Continued)

2.

Smith et al. 1980		Sonnefeld et al. 1983		Sasse et al. 1988		Oja & Suuberg 1998	
inclined-piston gauge		gas saturation-HPLC		electronic manometry		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
149	63.3*	39.45	3.20×10^{-3}	159.75	112.5		
150	66.7*	25.0	6.0×10^{-4}	169.61	178.8		
152	78.3			179.45	279.4		
155	86.5	eq. 2	P/Pa	189.25	405.7		
160	110.7	A	12.748	194.16	490.1		
165	141.6	B	4760.73				
170	178.9	temp range 10–50°C		for solid			
175	224.6			eq. 2	P/mmHg		
180	280.4	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 91.20$		A	8.654859		
185	345.3	B		2967.129			
				C	182,314		
				temp range: 80.1–139.97°C			
				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 97.70$			
*supercooled liquid values							
reported vapor pressure eq.							
see foot note		eq. 2		P/mmHg			
				A	5.62672		
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 103.9$		B		1553.755			
				C	112.964		
				temp range: 139.97–194°C			

note: $\ln(P_L/P_S) = 268.6187 - 699.31/(T/K) - 45.6846 \ln(T/K) + 0.057217(T/K)$; in which P_L and P_S are the vapor pressure of supercooled liquid and crystal phase, respectively, at temperature T.

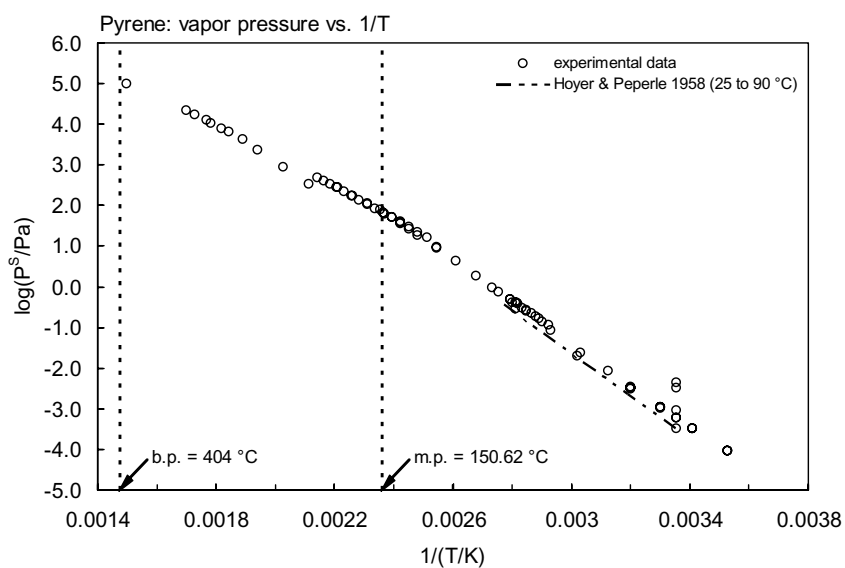


FIGURE 4.1.1.29.2 Logarithm of vapor pressure versus reciprocal temperature for pyrene.

TABLE 4.1.1.29.3

Reported Henry's law constants and octanol-air partition coefficients of pyrene at various temperatures and temperature dependence equations

Henry's law constant			log K _{OA}	
Bamford et al. 1999			Harner & Bidleman 1998	
gas stripping-GC/MS			generator column-GC/FID	
t/°C	H/(Pa m ³ /mol)	H/(Pa m ³ /mol)	t/°C	log K _{OA}
		average		
4.1	0.37, 0.49	0.43	0	9.966
11.0	0.63, 0.76	0.69	10	9.528
18.0	1.02, 1.19	1.10	20	9.155
25.0	1.54, 1.89	1.71	30	8.647
31.0	2.15, 2.80	2.45	40	8.121
			25(exptl)	8.80
			25(calc)	8.49
ln K _{AW} = A - B/(T/K)				
A	10.1034		log K _{OA} = A + B/(T/K)	
B	5160		A	-4.56
			B	3985
enthalpy, entropy change:				
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 42.9 \pm 2.3$				
$\Delta S/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = 84$				
at 25°C				
enthalpy of phase change				
$\Delta H_{\text{OA}}/(\text{kJ}\cdot\text{mol}^{-1}) = 76.3$				

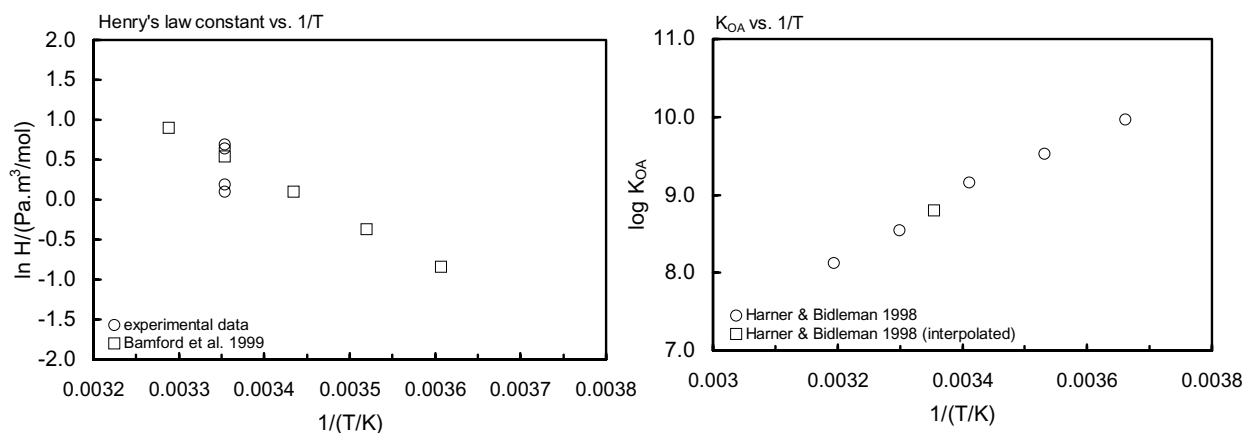
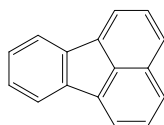


FIGURE 4.1.1.29.3 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for pyrene.

4.1.1.30 Fluoranthene



Common Name: Fluoranthene

Synonym: idryl, 1,2-benzacenaphthene, benzo[*j,k*]fluorene, benz[*a*]acenaphthylene, fluoranthrene

Chemical Name: 1,2-benzacenaphthene

CAS Registry No: 206-44-0

Molecular Formula: C₁₆H₁₀

Molecular Weight: 202.250

Melting Point (°C):

110.19 (Lide 2003)

Boiling Point (°C):

384 (Lide 2003)

Density (g/cm³ at 20°C):

1.252 (0°C, Weast 1982–83, Dean 1985; Lide 2003)

Molar Volume (cm³/mol):

162 (calculated-density, liquid molar volume, Lande & Banerjee 1981)

217.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.87 (Ruelle & Kesselring 1997)

18.74 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

49.37 (Casellato et al. 1973; quoted, Yalkowsky 1981)

47.70 (differential scanning calorimetry, Hinckley et al. 1990)

48.89, 36.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

49.6 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.146 (mp at 110.19°C)

0.191 (calculated, $\Delta S_{\text{fus}} = 49.6$ J/mol K, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.240 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.265 (shake flask-UV, Klevens 1950)

0.240 (20°C, shake flask-UV, Eisenbrand & Baumann 1970)

0.236 (fluorescence/UV, Schwarz & Wasik 1976)

0.260 (shake flask-fluorescence, Mackay & Shiu 1977)

0.206 (Rossi 1977; Neff 1979)

0.206* (generator column-HPLC/UV, measured range 8.1–29.9°C, May et al. 1978a,b)

$S/(\mu\text{g/kg}) = 50.4 + 4.322 \cdot (t/^\circ\text{C}) - 0.1047 \cdot (t/^\circ\text{C})^2 + 0.0072 \cdot (t/^\circ\text{C})^3$; temp range 5–30°C (generator column-HPLC/UC, May et al. 1978b)

0.120 (shake flask-nephelometry, Hollifield 1979)

0.218 (OECD 1979/1980; quoted, He et al. 1995)

0.275, 0.373 (15, 25°C, generator column/elution method, average values of 6–7 laboratories, OECD 1981)

0.200 (20°C, quoted, Schmidt-Bleek et al. 1982)

0.190 (20°C, generator column-fluorescence, Hashimoto et al. 1982)

0.203* (24.6°C, generator column-HPLC, measured range 281.25–303.05 K, May et al. 1983)

0.243 (average lit. value, Pearlman et al. 1984)

0.199 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

1.43 (RP-HPLC-RT correlation, Chin et al. 1986)

0.283 (vapor saturation-UV, Akiyoshi et al. 1987)

0.240 (recommended, Shaw 1989)

0.222 (generator column-HPLC/fluorescence, Kishi & Hashimoto 1989)

0.373 (average value of Japan, OECD tests, Kishi & Hashimoto 1989)
 0.166 (shake flask-fluorescence, Kishi & Hashimoto 1989)
 0.265 (shake flask-HPLC/UV/fluorescence, Pinal et al. 1991)
 0.177 (generator column-HPLC, Vadas et al. 1991)
 0.248 (generator column-HPLC/UV, Yu & Xu 1993)
 0.207 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
 0.2289 ± 0.0008 (shake flask-SPME (solid-phase micro-extraction)-GC, Paschke et al. 1999)
 $\log [S_L/(\text{mol/L})] = 0.779 - 987.5/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\ln x = -1.796327 - 4772.17/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

653* (197.0°C, temp range 197.0–384.2°C, Tsyphina 1955; quoted, Boublik et al. 1984)
 6.67×10^{-4} (effusion method, Hoyer & Peperle 1958)
 $\log (P/\text{mmHg}) = 12.67 - 5357/(T/K)$; temp range 25–85°C (Knudsen effusion method, Hoyer & Peperle 1958)
 0.00123* (gas saturation-HPLC/fluor. or UV, Sonnefeld et al. 1983)
 $\log (P/\text{Pa}) = 11.901 - 4416.56/(T/K)$; temp range 10–50°C (Antoine eq., gas saturation, Sonnefeld et al. 1983)
 0.00124 (generator column-HPLC/fluor., Wasik et al. 1983)
 1.79 (supercooled liquid P_L , extrapolated from Antoine eq., Boublik et al. 1984)
 0.0154, 0.0067 (P_{GC} by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
 0.00861 (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)
 0.000125 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 5.45017 - 1717.489/(114.025 + t/^\circ\text{C})$; temp range 197–384.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 1.65×10^{-4} (extrapolated, Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 6.373 - 1756/(118 + t/^\circ\text{C})$; temp range 197–384°C (Antoine eq., Dean 1985, 1992)
 0.00105 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_S/\text{kPa}) = 11.96071 - 5348.06/(T/K)$; temp range 298–383 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.67549 - 2957.01/(-24.15 + T/K)$; temp range 503–658 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 0.00068, 0.0056 (lit. solid P_S , supercooled liquid P_L , Bidleman & Foreman 1987)
 0.992 (WERL Treatability database, quoted, Ryan et al. 1988)
 0.00861, 0.00635 (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 0.0155, 0.00955 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log (P_L/\text{Pa}) = 11.35 - 4040/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
 $\log (P/\text{mmHg}) = 70.6802 - 6.484 \times 10^3/(T/K) - 22.241 \cdot \log (T/K) + 7.2184 \times 10^{-3} \cdot (T/K) - 6.3035 \times 10^{-13} \cdot (T/K)^2$;
 temp range 383–905 K (vapor pressure eq., Yaws 1994)
 0.00692 (supercooled liquid P_L , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
 0.00168, 0.000672; 0.00124 (quoted exptl. values, effusion; gas saturation, Delle Site 1997)
 0.00218, 0.000939, 0.000889 (quoted lit. values, from GC-RT correlation, Delle Site 1997)
 7.48×10^{-3} ; 1.43×10^{-3} (supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 11.62 - 4310/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 9.03 - 3323/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P/\text{Pa}) = 11.901 - 4415.56/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 0.00598 (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)
 $\log (P_L/\text{Pa}) = -4141/(T/K) + 11.66$; $\Delta H_{vap.} = -79.3 \text{ kJ} \cdot \text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.65* (gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)
 1.10 (gas stripping-HPLC/fluorescence, De Maagd et al. 1998)
 1.96* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)
 $\ln K_{AW} = -4654.8/(T/K) + 8.42$, $\Delta H = 38.7 \text{ kJ} \cdot \text{mol}^{-1}$; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 8.23 - 2336/(T/K)$ (Passivirta et al. 1999)

- 1.96 (quoted from Bamford et al. 1999; Dachs & Eisenreich 2000)
 0.602 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 6.175 - 2868/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.22 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 4.47 (HPLC- k' correlation, Harnisch et al. 1983)
 4.84 (RP-HPLC-RT correlation, Chin et al. 1986)
 4.85 (HPLC-RT correlation, Wang et al. 1986)
 5.16 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 5.20 (recommended, Sangster 1989, 1993)
 5.17 (TLC-RT correlation, De Voogt et al. 1990)
 5.148 ± 0.077 , 5.155 ± 0.015 (shake flask/slow stirring-GC/HPLC, interlaboratory studies, Brooke et al. 1990)
 5.00 (shake flask-UV spec., Alcorn et al. 1993)
 5.16 (recommended, Hansch et al. 1995)
 5.23 (5.12–5.31) (shake flask/slow stirring-HPLC/fluorescence., De Maagd et al. 1998)
 5.16 (shake flask-SPME solid-phase micro-extraction; Paschke et al. 1999)
 0.602 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 5.485 - 2682/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.
 Additional data at other temperatures designated * are compiled at the end of this section:

- 8.60 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
 8.60 (calculated, Finizio et al. 1997)
 8.80*; 8.60 (generator column-GC; calculated- C_O/C_A , measured range 0–40°C, Harner & Bidleman 1998)
 $\log K_{OA} = -5.94 + 4417/(T/K)$; temp range 20–40°C (generator column-GC, Harner & Bidleman 1998)
 8.61 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 3.18 (calculated as per Kenaga & Goring 1979, Eadie et al. 1982)
 4.90 (*P. hoyi*, Eadie et al. 1982)
 4.08 (microorganisms-water, calculated from K_{OW} , Mabey et al. 1982)
 3.24 (*Daphnia magna*, Newsted & Giesy 1987)
 0.756, 1.079 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 6.38 (sediments average, Kayal & Connell 1990)
 4.74, 4.62 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)
 6.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 4.816; 4.81, 4.82 (sediment: concn ratio C_{sed}/C_W ; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
 4.51, 5.05, 4.16 (sediments from Brown's Lake, Hamlet City Lake, WES reference soil, shake flask-LSC, Brannon et al. 1995)
 6.56, 6.66, 6.08 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island, McGroddy & Farrington 1995)
 4.62 (calculated-MCI χ , Sabljic et al. 1995)
 5.25 (10°C), 5.22, 5.12 (20°C), 5.05 (35°C), 4.89, 4.96 (45°C) ($\log K_{DOC}$ - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
 5.40 (20°C, $\log K_{POC}$ - particulate organic material from lake, Lüers & ten Hulscher 1996)
 4.81, 4.65, 4.80, 4.82; 4.813; 4.727 (4 soils with different organic carbon content f_{OC} , adsorption equilibrium-shake flask-HPLC; calculated- K_{OW} ; calculated- S , He et al. 1996)
 5.32 (5.29–5.35), 4.89 (4.89–4.90) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
 4.62, 4.03; 3.40, 4.49, 3.55, 4.53, 4.56 (quoted lit., calculated- K_{OW} ; HPLC-screening method with different LC-columns, Szabo et al. 1999)

- 5.32–6.59; 4.60–6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
 5.83; 6.79, 5.53, 5.52 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
 4.91, 4.65 (average values for sediments, soils, organic carbon OC $\geq 0.5\%$, Delle Site 2001)
 4.62 (Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)
 5.21–6.60 (field contaminated sediment, initial-final values of 5–100 d contact time, gas-purge technique-HPLC/fluorescence, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photochemical transformation $t_{1/2}(\text{calc}) = 21$ h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis $t_{1/2} = 160$ d and 200 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)
 $t_{1/2} = 21$ h, atmospheric and aqueous photolysis half life, based on measured sunlight photolysis rate constant in water adjusted for midday summer sunlight at 40°N latitude and $t_{1/2} = 63$ h after adjusting for approximate winter sunlight intensity (Howard et al. 1991);
 $t_{1/2} = 160$ d under summer sunlight in surface water (Mill & Mabey 1985);
 half-lives on different atmospheric particulate substrates (appr. 25 $\mu\text{g/g}$ on substrate): $t_{1/2} = 74$ h on silica gel, $t_{1/2} = 23$ h on alumina and $t_{1/2} = 44$ h on fly ash (Behymer & Hites 1985);
 direct photolysis $t_{1/2}(\text{obs.}) = 3.61$ h, $t_{1/2}(\text{calc}) = 4.78$ h, by QSPR in atmospheric aerosol (Chen et al. 2001);
 $k = (1.76 \pm 0.13) \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = (10.93 \pm 0.75) \text{ h}$ in diesel particulate matter, photochemical degradation under atmospheric conditions, $k = (2.97 \pm 0.40) \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = (6.48 \pm 1.03) \text{ h}$ in diesel particulate matter/soil mixture, and $t_{1/2} = 1.6$ to 4.15 h in various soil components using a 900-W photo-irradiator as light source; $k = (8.69 \pm 0.29) \times 10^{-6} \text{ s}^{-1}$ and $t_{1/2} = (22.16 \pm 0.77) \text{ h}$ in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation $k = 5.0 \times 10^{-6} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant, k , and for gas-phase second-order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 , or as indicated *data at other temperatures and/or the Arrhenius expression see reference:

$k(\text{calc}) < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $< 360 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{\text{OH}} = 5.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{\text{N}_2\text{O}_5} \approx 1.8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with N_2O_5 at 296 ± 2 K (relative rate method, Atkinson et al. 1990)

photooxidation half-life of 2.02–20.2 h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{\text{OH}}^* = 11 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 306–366 K with a calculated atmospheric lifetime of 26 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aquatic $k = 2.2 \times 10^{-3} \mu\text{mol h}^{-1} \text{ mg}^{-1}$ with bacterial protein (Barnsley 1975; quoted, Callahan et al. 1979)

significant with gradual degradation for a domestic sewer test for an average three static-flask screening (Tabak et al. 1981)

$t_{1/2}(\text{aerobic}) = 3360\text{--}10560$ h, based on aerobic soil die-away test data at 10–30°C (Coover & Sims 1987; quoted, Howard et al. 1991)

$k = 0.19 \text{ h}^{-1}$ in atmosphere (Dragoescu & Friedlander 1989)

$k = 0.0018 \text{ d}^{-1}$ with $t_{1/2} = 377$ d for Kidman sandy loam and $k = 0.0026 \text{ d}^{-1}$ with $t_{1/2} = 268$ d for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)

$t_{1/2}(\text{anaerobic}) = 13440\text{--}42240$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

first order $k = 0.132$ to $0.162 \text{ L mg}^{-1} \text{ d}^{-1}$ for a marine PAH-degrading enrichment without sediment, the degradation rate was 2.1 to 5.3 times faster with sediment present (Poeton et al. 1999)

Biotransformation: estimated rate constant for bacteria, $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 4.1\text{--}6.1 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.026 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

$k_2 = 0.15 \text{ h}^{-1}$ in water with corresponding $t_{1/2} = 4.7 \text{ h}$ and $k_2 = 0.14 \text{ h}^{-1}$ in sediment with corresponding $t_{1/2} = 4.9 \text{ h}$ for copepods *S. knabeni* in 24-h experiments (Lotufo 1998)

$k_2 = 0.17 \text{ h}^{-1}$ in sediment with corresponding $t_{1/2} = 4.2 \text{ h}$ and $k_2 = 0.09 \text{ h}^{-1}$ in sediment with corresponding $t_{1/2} = 7.4 \text{ h}$ for copepods *Coullana* sp. in 24-h experiments (Lotufo 1998)

Half-Lives in the Environment:

Air: $t_{1/2} = 2.02\text{--}20.2 \text{ h}$, based on estimated sunlight photolysis half-life in water (Howard et al. 1991); calculated atmospheric lifetime of 26 h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: computed near-surface $t_{1/2} = 21 \text{ h}$ for photochemical transformation of a water body (latitude 40°N , midday, midsummer), $t_{1/2} = 160 \text{ d}$ for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning and $t_{1/2} = 200 \text{ d}$ with sediment-water partitioning (Zepp & Schlotzhauer 1979);

$t_{1/2} = 21\text{--}63 \text{ h}$, based on photolysis half-life in water (Howard et al. 1991);

$t_{1/2} = 160 \text{ d}$ for summer sunlight at 40°N latitude (Mill & Mabey 1985).

Groundwater: $t_{1/2} = 6720\text{--}21120 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption $t_{1/2} = 8.3 \text{ d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} = 44\text{--}182 \text{ d}$ (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 39 \text{ d}$ for 5 mg/kg treatment and 34 d for 50 mg/kg treatment (Bulman et al. 1987);

biodegradation rate constant $k = 0.0018 \text{ d}^{-1}$ with $t_{1/2} = 377 \text{ d}$ for Kidman sandy loam soil, and $k = 0.0026 \text{ d}^{-1}$ with $t_{1/2} = 268 \text{ d}$ for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 3360\text{--}10560 \text{ h}$, based on aerobic soil die-away test data at $10\text{--}30^\circ\text{C}$ (Howard et al. 1991);

$t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988);

$t_{1/2} = 17.961 \text{ wk}$, 7.8 yr (Luddington soil, Wild et al. 1991).

Biota: $t_{1/2} = 5 \text{ d}$ depuration half life by oysters (Lee et al. 1978);

elimination $t_{1/2} = 6 \text{ d}$ from rainbow trout, $t_{1/2} = 2.0\text{--}29.8 \text{ d}$ from mussel *Mytilus edulis*; $t_{1/2} = 8.4 \text{ d}$ from clam *Mya arenaria*, $t_{1/2} = 5.8 \text{ d}$ from polychaete *Abarenicola pacifica*, $t_{1/2} = 5.9 \text{ d}$ from Oyster, $t_{1/2} = 0.8 \text{ d}$ from shrimp (Meador et al. 1995)

depuration $t_{1/2} \sim 4.8 \text{ h}$ in sediment and water for copepod *S. knabeni*, $t_{1/2} = 4.2 \text{ h}$ in sediment and $t_{1/2} = 7.4 \text{ h}$ in water for copepod *Coullana* sp. (Lotufo 1998)

TABLE 4.1.1.30.1
Reported aqueous solubilities of fluoranthene at various temperatures
and reported temperature dependence equation

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

May 1980, 1983		May et al. 1978b	
generator column-HPLC		generator column-HPLC/fluo.	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
8.1	0.082	25	0.206
13.2	0.107	29	0.264
19.7	0.1483		
24.6	0.2027	temp dependence eq. 1	
29.9	0.2793	S	$\mu\text{g/kg}$
		a	0.0072
		b	-0.1047
		c	4.322
		d	50.4
temp dependence eq. 1			
given in May et al. 1980			
S	$\mu\text{g/kg}$		
a	0.0072		
b	-0.1047	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 39.83$	
c	4.322	measured between $5\text{--}30^\circ\text{C}$	
d	50.4		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 39.83$			
measured between $5\text{--}30^\circ\text{C}$			

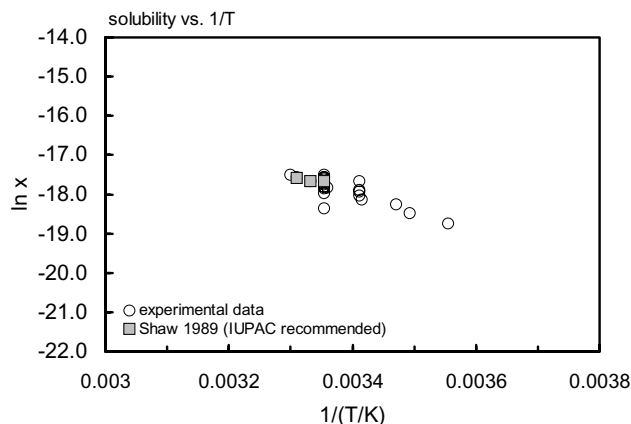


FIGURE 4.1.1.30.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for fluoranthene.

TABLE 4.1.1.30.2

Reported vapor pressures of fluoranthene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Tsypkina 1955		Hoyer & Peperle 1958		Sonnefeld et al. 1983	
		effusion		generator column-HPLC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
197.0	653	data presented in eq.		10.88	2.17×10^{-4}
209.0	1053	eq. 1	P/mmHg	10.88	2.05×10^{-4}
228.5	2586	A	12.67	10.88	2.15×10^{-4}
238.1	3786	B	5357	10.88	2.57×10^{-4}
247.7	5386	for temp range 25–85°C		20.25	7.07×10^{-4}
255.0	6586			20.25	7.39×10^{-4}
261.3	7919	$\Delta H_{\text{sub}}(\text{kJ/mol}) = 100$		20.25	7.25×10^{-4}
270.9	10319			20.25	7.63×10^{-4}
281.5	13386			29.79	2.03×10^{-3}
305.0	20318			29.79	1.99×10^{-3}
314.5	27384			29.80	2.17×10^{-3}
382.9	99058			29.80	2.20×10^{-3}
384.2	101325			38.9	5.81×10^{-3}
				38.9	5.67×10^{-3}
				38.9	5.58×10^{-3}
				38.9	5.77×10^{-3}
				38.9	5.46×10^{-3}
				38.9	5.45×10^{-3}
				25.0	1.23×10^{-3}
				eq. 2	P/Pa
				A	11.901
				B	4415.56
				temp range 10–50°C	

ref. Tsyapkina, O.YA. Zh. Prikl. Khim 28, 185 (1955).

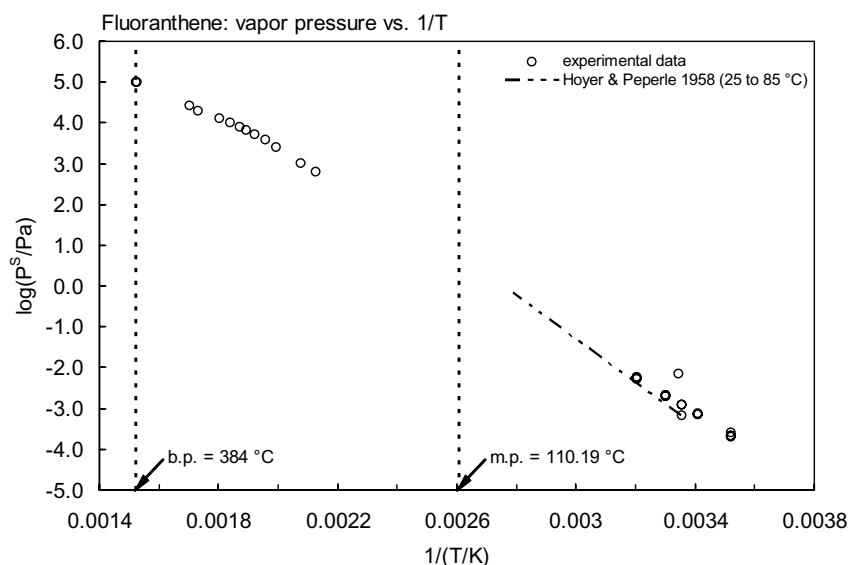


FIGURE 4.1.1.30.2 Logarithm of vapor pressure versus reciprocal temperature for fluoranthene.

TABLE 4.1.1.30.3

Reported Henry's law constants and octanol-air partition coefficients of fluoranthene at various temperatures and temperature dependence equations

Henry's law constant					log K_{OA}	
ten Hulscher et al. 1992		Bamford et al. 1999			Harner & Bidleman 1998	
gas stripping-HPLC/fluo.		gas stripping-GC/MS			generator column-GC/FID	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	H/(Pa m ³ /mol)	t/°C	log K_{OA}
				average		
10.0	0.26	4.1	0.37, 0.49	0.56	0	-
20.0	0.64	11.0	0.79, 0.95	0.87	10	-
35.0	1.63	18.0	1.21, 1.43	1.32	20	11.124
40.1	2.38	25.0	1.76, 2.18	1.96	30	8.652
45.0	5.84	31.0	2.36, 3.14	2.72	40	8.161
55.0	6.23				25(exptl)	8.88
					25(calc)	8.60
$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\ln K_{AW} = A - B/(T/K)$			$\log K_{OA} = A + B/(T/K)$	
$R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$		A			A	
$\Delta S/R$		B			B	
$\Delta H/R$		enthalpy, entropy change:			enthalpy of phase change	
		$\Delta H/(\text{kJ} \cdot \text{mol}^{-1}) = 38.7 \pm 2.5$			$\Delta H_{OA}/(\text{kJ mol}^{-1}) =$	
		$\Delta S/(\text{J} \cdot \text{K}^{-1} \text{ mol}^{-1}) = 70$				
		at 25°C				
enthalpy of volatilization:						
$\Delta H/(\text{kJ} \cdot \text{mol}^{-1}) = 57 \pm 5$						
entropy of volatilization, ΔS						
$T\Delta S/(\text{kJ} \cdot \text{K}^{-1} \text{ mol}^{-1}) = 54 \pm 5$						
at 20°C						

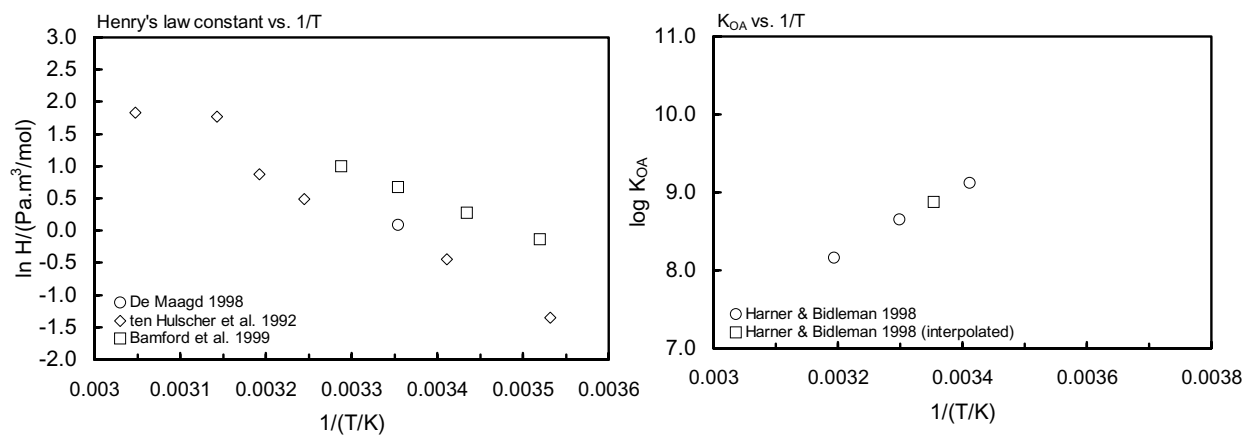
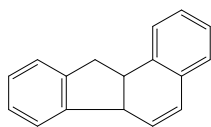


FIGURE 4.1.1.30.3 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for fluoranthene.

4.1.1.31 Benzo[a]fluorene

Common Name: Benzo[a]fluorene

Synonym: 1,2-benzofluorene, 11*H*-benzo[a]fluorene, chrysofluorene

Chemical Name: benzo[a]fluorene, 1,2-benzofluorene

CAS Registry No: 238-84-6

Molecular Formula: C₁₇H₁₂

Molecular Weight: 216.227

Melting Point (°C):

189.5 (Lide 2003)

Boiling Point (°C):

405 (Lide 2003)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

200.9 (Ruelle & Kesselring 1997)

239.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, Δ*H*_{fus} (kJ/mol):

3.8, 18.4; 22.2 (126.75, 189.65°C; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, Δ*S*_{fus} (J/mol K):

39.76 (exptl., Chickos et al. 1999)

49.26, 50.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming Δ*S*_{fus} = 56 J/mol K), *F*: 0.0243 (mp at 189.5°C)

Water Solubility (g/m³ or mg/L at 25°C):

0.045 (shake flask-fluorescence, Mackay & Shiu 1977)

0.045 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):

0.00136 (supercooled liquid *P*_L, calibrated GC-RT correlation, Lei et al. 2002)

log (*P*_L/Pa) = -4373/(*T*/K) + 11.80; Δ*H*_{vap} = -83.7 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

2.70* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)

ln *K*_{AW} = -4113.54/(*T*/K) + 6.976, Δ*H* = 34.2 kJ mol⁻¹, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, log *K*_{OW}:

5.68 (HPLC-RT correlation, Wang et al. 1986)

5.40 (recommended, Sangster 1989, 1993)

6.5387 (calculated-UNIFAC group contribution, Chen et al. 1993)

5.68 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log *K*_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log *K*_{OC}:

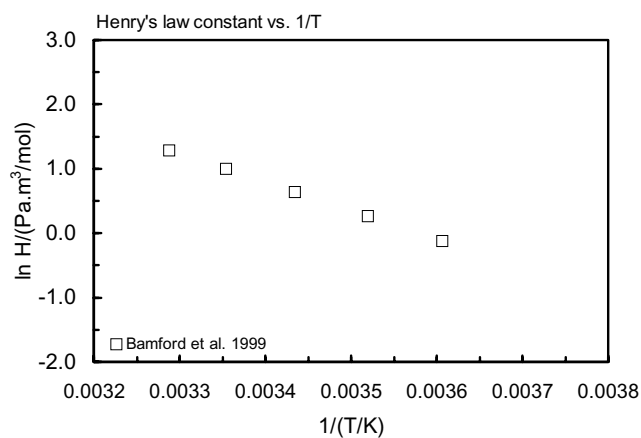
Environmental Fate Rate Constants, *k*, or Half-Lives, *t*_{1/2}:

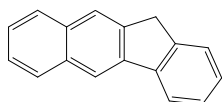
Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 10.5$ d from Oyster, $t_{1/2} = 4.2$ d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.31.1**Reported Henry's law constants of benzo[a]fluorene at various temperatures**

Bamford et al. 1999		
gas stripping-GC/MS		
$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$	$H/(\text{Pa m}^3/\text{mol})$
		average
4.1	0.67, 1.16	0.88
11.0	1.08, 1.57	1.30
18.0	1.61., 2.23	1.89
25.0	2.19, 3.33	2.70
31.0	2.74, 4.78	3.62
$\ln K_{\text{AW}} = A - B/(T/\text{K})$		
A	6.9762	
B	4113.5	
enthalpy, entropy change:		
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 34.2 \pm 4.9$		
$\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 58$		
at 25°C		

**FIGURE 4.1.1.31.1** Logarithm of Henry's law constant versus reciprocal temperature for benzo[a]fluorene.

4.1.1.32 Benzo[*b*]fluorene

Common Name: Benzo[*b*]fluorene

Synonym: 2,3-benzofluorene, 11H-benzo[*b*]fluorene, isonaphthofluorene

Chemical Name: benzo[*b*]fluorene

CAS Registry No: 243-17-4

Molecular Formula: C₁₇H₁₂

Molecular Weight: 216.227

Melting Point (°C):

212 (Lide 2003)

Boiling Point (°C):

401 (Lide 2003)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

200.9 (Ruelle & Kesselring 1997)

239.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.4 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

47.78, 50.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0146 (mp at 212°C)

Water Solubility (g/m³ or mg/L at 25°C):

0.0020 (shake flask-fluorescence, Mackay & Shiu 1977)

0.002 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7.37 × 10⁻⁶* (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 71–125°C, Oja & Suuberg 1998)

log (P/Pa) = 36.325 – 14354/(T/K); temp range 344–398 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

0.00107 (supercooled liquid P_L, calibrated GC-RT correlation, Lei et al. 2002)

log (P_L/Pa) = –4423/(T/K) + 11.86; ΔH_{vap} = –84.7 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:

5.77 (HPLC-RT correlation, Wang et al. 1986)

5.75 (recommended, Sangster 1989, 1994)

5.77 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:

Half-Lives in the Environment:

Biota: elimination t_{1/2} = 10.5 d from Oyster, t_{1/2} = 4.3 d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.32.1

Reported vapor pressures of benzo[b]fluorene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Oja & Suuberg 1998

Knudsen effusion

t/°C	P/Pa
70.92	0.00454
83.14	0.0188
97.55	0.0936
124.4	1.230
mp/K	484–486
eq. 1a	P/Pa
A	36.325
B	14354
for temp range 344–398 K	
$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 119.3$	

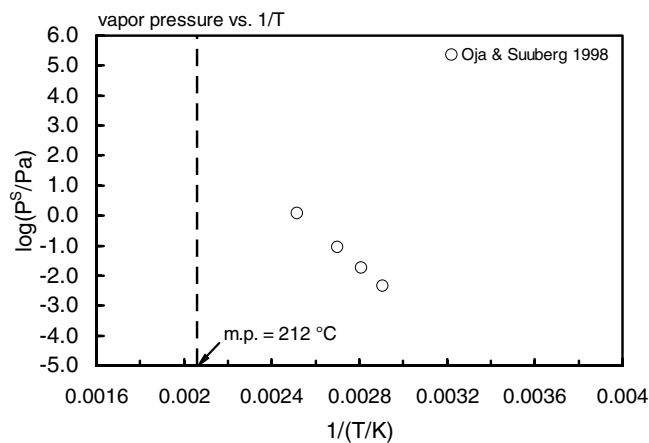
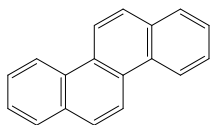


FIGURE 4.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for benzo[b]fluorene.

4.1.1.33 Chrysene



Common Name: Chrysene

Synonym: 1,2-benzophenanthrene, benzo(*a*)phenanthrene, 1,2,5,6-dibenzonaphthalene

Chemical Name: chrysene

CAS Registry No: 218-01-9

Molecular Formula: C₁₈H₁₂

Molecular Weight: 228.288

Melting Point (°C):

255.5 (Lide 2003)

Boiling Point (°C):

448 (Weast 1975; Lide 2003)

Density (g/cm³ at 20°C):

1.274 (Weast 1982–83; Lide 2003)

Molar Volume (cm³/mol):

179.2 (20°C, calculated-density)

250.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} cal/mol:

26.153 (Ruelle & Kesselring 1997)

3.22, 26.15; 29.37 (239.05, 28.25°C, total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

49.37 (Casellato et al. 1973)

62.34 (Ubbelohde 1978)

49.21 (Chickos et al. 1999)

55.5, 44.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00548 (mp at 255.5°C)

0.00976 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0015 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.006 (shake flask-UV, Klevens 1950)

0.0015 (Weimer & Prausnitz 1965)

0.0041, 0.0014 (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)

0.002 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0018 (Rossi 1977; Neff 1979; quoted, Eadie et al. 1982)

0.0018* (generator column-HPLC/UV, measured range 6.5–29°C May et al. 1978a,b)

S/(μg/kg) = 0.609 + 0.0144·(t/°C) + 0.0024·(t/°C)²; temp range 5–30°C (generator column-HPLC/UV, May et al. 1978)

0.017 (shake flask-nephelometry, Hollifield 1979)

0.00189* (25.3°C, generator column-HPLC, measured range 279.65–301.85 K, May et al. 1983)

0.0018* (average lit. value, Pearlman et al. 1984)

0.00327 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

0.00102, 0.0012 (generator column-HPLC/UV, Billington et al. 1988)

0.0019 (recommended, Shaw 1989)

0.0016 (generator column-HPLC, Vadas et al. 1991)

0.0015 (generator column-HPLC/fluorescence, De Maagd et al. 1998)

log [S_L/(mol/L)] = −0.323 − 1369/(T/K) (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 5.7×10^{-7} * (effusion method, extrapolated, De Kruif 1980)
- 8.4×10^{-7} (effusion method, Hoyer & Peperle 1958; quoted, Mabey et al. 1982)
- $\log(P/\text{mmHg}) = 13.07 - 6340/(T/K)$; temp range 80–145°C (Knudsen effusion method, Hoyer & Peperle 1958)
- 6.08×10^{-7} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_s/\text{kPa}) = 11.445 - 6160/(T/K)$; temp range 358–463 K (Antoine eq., Stephenson & Malanowski 1987)
- $\log(P/\text{mmHg}) = -50.1566 - 3.4381 \times 10^3/(T/K) + 25.178 \cdot \log(T/K) - 2.462 \times 10^{-2} \cdot (T/K) + 7.1044 \times 10^{-6} \cdot (T/K)^2$;
temp range 531–979 K (vapor pressure eq., Yaws 1994)
- 2.29×10^{-4} (supercooled liquid P_L , calculated from Yamasaki et al. 1984, quoted, Finizio et al. 1997)
- 5.70×10^{-7} ; 5.84×10^{-5} (quoted solid P_s from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)
- $\log(P_s/\text{Pa}) = 12.24 - 5507/(T/K)$ (solid, Passivirta et al. 1999)
- $\log(P_L/\text{Pa}) = 9.66 - 4139/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
- $\log(P/\text{Pa}) = 14.848 - 6189/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 1.70×10^{-4} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)
- $\log(P_L/\text{Pa}) = -4679/(T/K) + 11.92$; $\Delta H_{\text{vap}} = -89.6 \text{ kJ} \cdot \text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)
- 2.11×10^{-6} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)
- 4.03×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$, Mader & Pankow 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.107 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
- 0.53* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)
- $\ln K_{\text{AW}} = -12136.2/(T/K) + 32.235$, $\Delta H = 100.9 \text{ kJ} \cdot \text{mol}^{-1}$, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
- $\log(H/(\text{Pa m}^3/\text{mol})) = 9.98 - 2770/(T/K)$ (Passivirta et al. 1999)
- 0.53 (quoted, Dachs & Eisenreich 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 5.79 (HPLC- k' correlation, Hanai et al. 1981)
- 5.91 (RP-TLC- k' correlation, Bruggeman et al. 1982)
- 5.73 (HPLC-RT correlation, Wang et al. 1986)
- 5.61 ± 0.40 (recommended, Sangster 1989)
- 5.84 (TLC retention time correlation, De Voogt et al. 1990)
- 5.50 (shake flask-UV, Alcorn et al. 1993)
- 5.86 (recommended, Sangster 1993)
- 5.73 (recommended, Hansch et al. 1995)
- 5.81 (range 6.63–5.94) (shake flask/slow stirring-HPLC/fluor., De Maagd et al. 1998)
- 5.78 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 10.40 (calculated- $K_{\text{OW}}/K_{\text{AW}}$, Wania & Mackay 1996)
- 10.44 (calculated, Finizio et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

- 4.31 (*P. hoyi*, Eadie et al. 1982)
- 4.72 (microorganisms-water, calculated from K_{OW} , Mabey et al. 1982)
- 3.785 (*Daphnia magna*, Newsted & Giesy 1987)
- 1.17, 0.792 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 6.27 (sediments average, Kayal & Connell 1990)
- 6.9 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 4.0 (predicted dissolved $\log K_{\text{OC}}$, Broman et al. 1991)

- 5.79 (5.74–5.83), 5.40 (5.35–5.50) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
- 5.52–7.38; 4.90–7.80 (for chrysene + triphenylene, range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.92; 6.12, 5.77, 6.14 (for chrysene + triphenylene, 20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: calculated $t_{1/2} = 4.4$ h of direct sunlight photolysis for 50% conversion at 40°N latitude of midday in midsummer: 4.4 h in near-surface water; (Herbes et al. 1980)

direct photochemical transformation $t_{1/2}(\text{calc}) = 4.4$ h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis $t_{1/2} = 13$ d and 68 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)

$t_{1/2} = 13$ d in 5-m deep inland water and $t_{1/2} = 68$ d in inland water with sediment partitioning (Zepp & Schlotzhauer 1979)

half-lives on different atmospheric particulate substrates (appr. 25 µg/g on substrate): $t_{1/2} = 100$ h on silica gel, $t_{1/2} = 78$ h on alumina and $t_{1/2} = 38$ h on fly ash (Behymer & Hites 1985)

first order daytime decay constants: $k = 0.0056 \text{ min}^{-1}$ for soot particles loading of 1000–2000 ng/mg and $k = 0.0090 \text{ min}^{-1}$ with 30–350 ng/mg loading (Kamens et al. 1988)

photodegradation $k = 7.07 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 1.63$ h in ethanol-water (1:1, v/v) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)

$k(\text{exptl}) = 0.00707 \text{ min}^{-1}$ with the calculated $t_{1/2} = 1.63$ h and the predicted $k = 0.0114 \text{ min}^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

$k = 1.01\text{--}1.30 \text{ min}^{-1}$ in natural water system by UV and sunlight (Yu et al. 1999)

$t_{1/2}(\text{obs}) = 1.58$ h, $t_{1/2}(\text{calc}) = 1.34$ h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

photochemical degradation $k = (1.60 \pm 0.08) \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = (11.99 \pm 0.53) \text{ h}$ in diesel particulate matter under atmospheric conditions; $k = (2.29 \pm 0.22) \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = (8.41 \pm 0.91) \text{ h}$ in diesel particulate matter/soil mixture, and $t_{1/2} = 1.69\text{--}8.82$ h in various soil components using a 900-W photo-irradiator as light source; $k = (4.76 \pm 0.40) \times 10^{-7} \text{ s}^{-1}$ and $t_{1/2} = (405.26 \pm 37.27) \text{ h}$ in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation $k = 9.0 \times 10^{-5} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: $t_{1/2} = 2.6$ h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

$k > 1 \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 0.802\text{--}8.02$ h in air, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: significant degradation with gradual adaptation within 7 d for a domestic sewer 28 d test for an average of three static-flask screening (Tabak et al. 1981)

aerobic $t_{1/2} = 8904\text{--}24000$ h, based on aerobic soil dieaway test data (Howard et al. 1991)

rate constants $k = 0.0019 \text{ d}^{-1}$ with $t_{1/2} = 371$ d for Kidman sandy loam and $k = 0.0018 \text{ d}^{-1}$ with $t_{1/2} = 387$ d for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)

anaerobic $t_{1/2} = 35616\text{--}96000$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated to be $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.35\text{--}0.71 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.15 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.802\text{--}8.02$ h, based on estimated photooxidation half-life in air (Howard et al. 1987);

$t_{1/2} = 1.3$ h for adsorption on wood soot particles in an outdoor Teflon chamber with an estimated rate constant $k = 0.0092 \text{ min}^{-1}$ at $1 \text{ cal cm}^{-2} \text{ min}^{-1}$, $10 \text{ g/m}^3 \text{ H}_2\text{O}$ and 20°C (Kamens et al. 1988).

Surface water: photolysis $t_{1/2} = 4.4$ h near surface water, $t_{1/2} = 13$ d and 68 d in 5-m deep water body without and with sediment-water partitioning in full summer day, 40°N ; photosensitized oxygenation $t_{1/2} = 2.6$ h at near surface water, 40°N , midday, midsummer (Zepp & Schlotzhauer 1979)

$t_{1/2} \sim 4.4\text{--}13$ h, based on photolysis half-life in water (Howard et al. 1991);

photolysis $t_{1/2} = 1.63$ h in aqueous solution when irradiated with a 500 W medium-pressure mercury lamp (Chen et al. 1996);

photolysis $t_{1/2} = 533\text{--}693$ min at 18°C in natural water system by UV and sunlight illumination (Yu et al. 1999).

Groundwater: $t_{1/2} = 17808\text{--}48000$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption $t_{1/2} = 31.9$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} > 5.5$ d (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 328$ d for 5 mg/kg treatment and $t_{1/2} = 224$ d for 50 mg/kg treatment (Bulman et al. 1987);

biodegradation rate constant $l = 0.0019 \text{ d}^{-1}$ with $t_{1/2} = 371$ d for Kidman sandy loam soil, and $k = 0.0018 \text{ h}^{-1}$ with $t_{1/2} = 387$ d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 8904\text{--}24000$ h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988).

Biota: elimination $t_{1/2} = 5.0\text{--}14.2$ d from mussel *Mytilus edulis*; $t_{1/2} = 15.1$ d from Oyster, $t_{1/2} = 4.3$ d from clam *Mercenaria mercenaria*, $t_{1/2} = 3.3$ d from clam *Macoma balthica* (quoted, Meador et al. 1995).

TABLE 4.1.1.33.1

Reported aqueous solubilities of chrysene at various temperatures and reported temperature dependence equations

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

May et al. 1978b		May 1980, May et al. 1983	
generator column-HPLC		generator column-HPLC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
25	0.0018	6.5	0.00071
29	0.0022	11.0	0.00080
		20.4	0.0014
		24.0	0.00168
		25.3	0.00189
		28.7	0.00221
temp dependence eq. 1		temp dependence eq. 1 given in May 1980	
S	$\mu\text{g/kg}$		
a	0	S	$\mu\text{g/kg}$
b	0.0024	a	0
c	-0.0144	b	0.0024
d	0.69	c	-0.0144
		d	0.69
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 41.25$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 41.25$	
measured between $5\text{--}30^\circ\text{C}$		measured between $5\text{--}30^\circ\text{C}$	

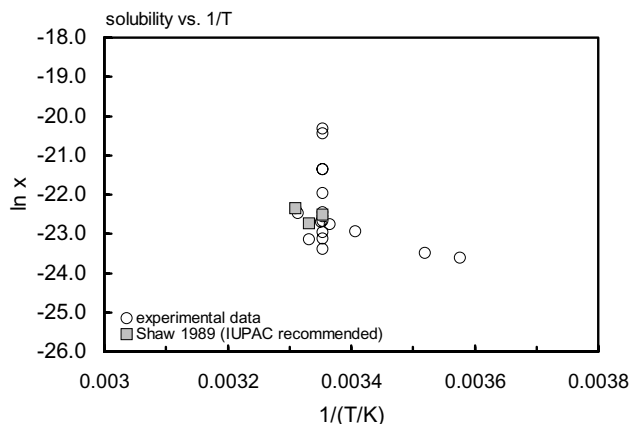


FIGURE 4.1.1.33.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for chrysene.

TABLE 4.1.1.33.2

Reported vapor pressures and Henry's law constants of chrysene at various temperatures and temperature dependence equations

Vapor pressure		Henry's law constant			
Hoyer & Peperle 1958		de Kruif 1980		Bamford et al. 1999	
effusion		torsion-, weighing effusion		gas stripping-GC/MS	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
				average	
data presented by equation		117.31	0.1	4.1	0.01, 0.03
log P/mmHg = A – B/(T/K)		124.84	0.2	11.0	0.05, 0.09
A	13.07	129.38	0.3	18.0	0.15, 0.25
B	6340	132.67	0.4	25.0	0.38, 0.73
temp range 80–145°C		135.26	0.5	31.0	0.78, 1.86
		137.39	0.6		
$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 118.8$		139.22	0.7	$\ln K_{\text{AW}} = A - B/(T/K)$	
		140.81	0.8	A	32.235
		142.23	0.9	B	12136
		143.51	1.0		
		25.0	5.7×10^{-7}	enthalpy, entropy change:	
		extrapolated)		$\Delta H/(\text{kJ} \cdot \text{mol}^{-1}) = 100.9 \pm 7.7$	
$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 118.5$				$\Delta S/(\text{J} \cdot \text{K}^{-1} \text{mol}^{-1}) = 268$	
				at 25°C	

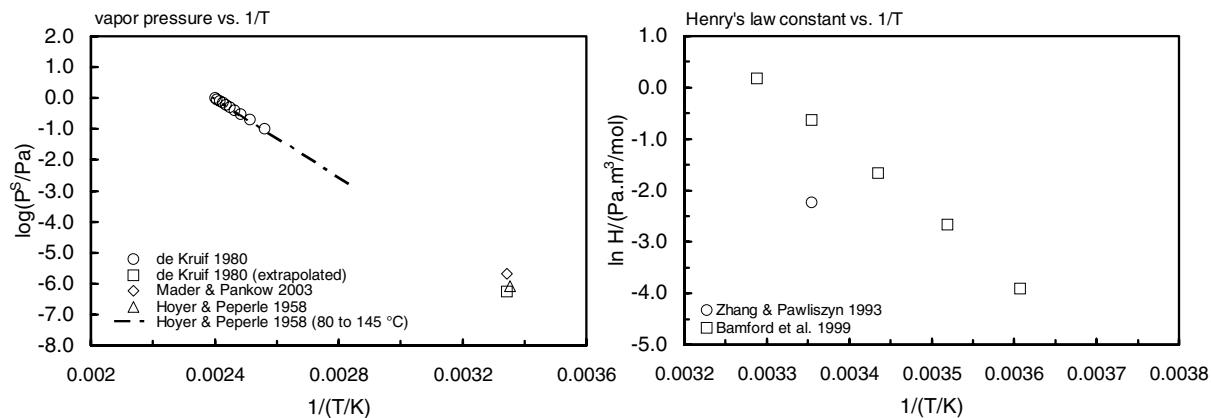
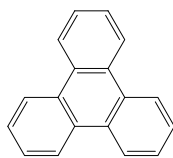


FIGURE 4.1.1.33.2 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for chrysene.

4.1.1.34 Triphenylene



Common Name: Triphenylene

Synonym: 9,10-benzophenanthrene, isochrysene, 1,2,3,4-dibenzonaphthalene

Chemical Name: triphenylene

CAS Registry No: 217-59-4

Molecular Formula: $C_{18}H_{12}$

Molecular Weight: 228.288

Melting Point ($^{\circ}C$):

197.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

425 (Weast 1982–83; Dean 1985; Pearlman et al. 1984; Budavari 1989; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.302 (Dean 1985; Budavari 1989)

Molar Volume (cm^3/mol):

211.8 (Ruelle & Kesselring 1997)

250.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.74 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

52.53, 44.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0202 (mp at $197.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0388 ($27^{\circ}C$, nephelometry, Davis et al. 1942)

0.043 (shake flask-UV, Klevens 1950)

0.043 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0049* ($20.5^{\circ}C$, generator column-HPLC, measured range 281.15–301.35 K, May et al. 1983)

0.041 (lit. mean, Pearlman et al. 1984)

0.0307 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

0.041 (vapor saturation-UV, Akiyoshi et al. 1987)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

$\log(P/mmHg) = 12.89 - 6154/(T/K)$; temp range: $65-125^{\circ}C$ (Knudsen effusion method, Hoyer & Peperle 1958)

2.30×10^{-6} * (effusion, De Kruif 1980)

3.85×10^{-7} (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 9.435 - 5620/(T/K)$; temp range: 363–468 K (Antoine eq.-I, Stephenson & Malanowski 1987)

1.17×10^{-2} (extrapolated-Antoine eq.-II, supercooled liquid P_L , Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.8974 - 3527/(T/K)$; temp range: 600–720 K (Antoine eq.-II, Stephenson & Malanowski 1987)

2.39×10^{-4} (supercooled liquid P_L , GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -4624/(T/K) + 11.89$; $\Delta H_{vap} = -88.5 kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($Pa m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ and the reported temperature dependence equations:

5.45 (shake flask-UV, Karickhoff et al. 1979)

5.49 (HPLC-RT correlation, Wang et al. 1986)

5.84 (TLC retention time correlation, De Voogt et al. 1990)

- 5.49 (recommended, Sangster 1993)
 5.49 (recommended, Hansch et al. 1995)
 5.15; 4.83 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)
 $\log K_{OW} = 1.313 + 1138.55/(T/K)$; temp range 5–55°C (temperature dependence HPLC-k' correlation, Lei et al. 2000)
 6.27 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 3.96 (*Daphnia magna*, Newsted & Giesy 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.90 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 4.0 (predicted dissolved $\log K_{OC}$, Broman et al. 1991)
 5.52–7.38; 4.90–7.80 (for chrysene + triphenylene, range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
 5.92; 6.12, 5.77, 6.14 (for chrysene + triphenylene, 20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

- Biota: elimination $t_{1/2} = 2$ d from rainbow trout, $t_{1/2} = 4.4$ d from clam *Mya arenaria*, $t_{1/2} = 8.0$ d from mussel *Mytilus edulis*, $t_{1/2} = 14.4$ d from polychaete *Abarenicola pacifica*, $t_{1/2} = 21.7$ d from Oyster, $t_{1/2} = 2.4$ d from shrimp (quoted, Meador et al. 1995).

TABLE 4.1.1.34.1

Reported aqueous solubilities and vapor pressures of triphenylene at various temperatures and reported temperature dependence equation

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

Aqueous solubility		Vapor pressure					
May 1980, May et al. 1983		Hoyer & Peperle 1958		de Kruif 1980			
generator column-HPLC		effusion		torsion, weighing effusion			
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa		
8.0	0.00299	data presented by		107.02	0.1		
12.0	0.00393	log P/mmHg = A – B/(T/K)		114.36	0.2		
14.8	0.00339	A	12.89	118.39	0.3		
20.5	0.00489	B	6154	134.52	0.4		
27.3	0.00765	temp range 65–125°C		122.0	0.5		
28.2	0.00811	ΔH _{subl} /(kJ mol ⁻¹) = 114.6		126.61	0.6		
temp dependence eq. 1 given in May 1980				128.38	0.7		
				129.94	0.8		
				131.32	0.9		
				132.56	1.0		
S	μg/kg			25.0	2.3 × 10 ⁻⁶		
a	–0.0002			extrapolated			
b	0.0250						
c	–0.4250						
d	4.89			ΔH _{subl} /(kJ mol ⁻¹) = 115.2			
ΔH _{sol} /(kJ mol ⁻¹) = 41.25 measured between 5–30°C							

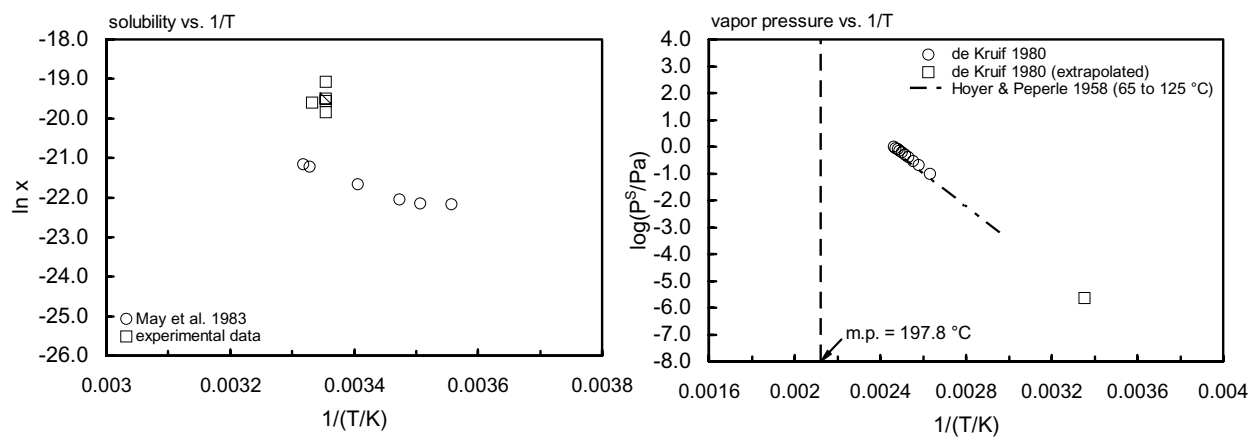
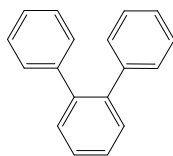


FIGURE 4.1.1.34.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for triphenylene.

4.1.1.35 *o*-Terphenyl

Common Name: *o*-Terphenyl

Synonym: 1,2-diphenyl benzene

Chemical Name:

CAS Registry No: 84-15-1

Molecular Formula: $C_{18}H_{14}$, 1,2- $(C_6H_5)_2C_6H_4$

Molecular Weight: 230.304

Melting Point ($^{\circ}C$):

56.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

332 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

225.4 ($93^{\circ}C$, Stephenson & Malanowski 1987)

273.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.2 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

52.3, 73.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.494 (mp at $56.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.24 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/kPa) = 6.29308 - [2160.24/(-106.38 + (T/K))]$; temp range 462–650 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -8.0641 - 4.0928 \times 10^3/(T/K) + 9.1076 \cdot \log(T/K) - 1.6326 \times 10^{-2} \cdot (T/K) + 6.0467 \times 10^{-6} \cdot (T/K)^2$; temp range 329–891 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air:

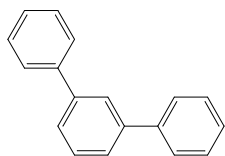
Surface water: a first order reduction process in river water with an estimated $t_{1/2} = 0.6$ d for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).

Ground water:

Sediment:

Soil:

Biota:

4.1.1.36 *m*-Terphenyl

Common Name: *m*-Terphenyl

Synonym: 1,3-diphenyl benzene

Chemical Name:

CAS Registry No: 92-06-8

Molecular Formula: $C_{18}H_{14}$, 1,3- $(C_6H_5)_2C_6H_4$

Molecular Weight: 230.304

Melting Point ($^{\circ}C$):

87 (Lide 2003)

Boiling Point ($^{\circ}C$):

363 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.199 (Lide 2003)

Molar Volume (cm^3/mol):

227 ($93^{\circ}C$, Stephenson & Malanowski 1987)

192.1 ($20^{\circ}C$, calculated-density)

273.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.59 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

62.76, 73.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.246 (mp at $87^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.51 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

0.0305* ($24.99^{\circ}C$, generator column-HPLC/fluorescence, Reza et al. 2002)

$\ln x = (-2.62 \pm 0.91) + (-5134 \pm 271)/(T/K)$; temp range 278–323.13 K (Reza et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/kPa) = 6.48808 - [2445.98/(-102.76 + (T/K))]$; temp range 462–691 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

$\log (P/mmHg) = -14.7175 - 4.3577 \times 10^3/(T/K) + 11.935 \cdot \log (T/K) - 1.8441 \times 10^{-2} \cdot (T/K) + 6.437 \times 10^{-6} \cdot (T/K)^2$; temp range 360–925 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air:

Surface water: a first order reduction process in river water with an estimated $t_{1/2} = 0.6$ d for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).

Ground water:
Sediment:
Soil:
Biota:

TABLE 4.1.1.36.1
Reported aqueous solubilities of *m*-terphenyl at various temperatures

Reza et al. 2002			
generator column-HPLC			
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
4.85	0.009	40.07	0.0741
7.64	0.0115	45.07	0.095
11.8	0.012	49.98	0.1159
14.98	0.0183	$\ln x = A - B/(T/\text{K})$	
19.95	0.0219	A	-2.62
24.99	0.0305	B	5134
30.0	0.0409	for temp range 287–323 K	
35.0	0.0535		

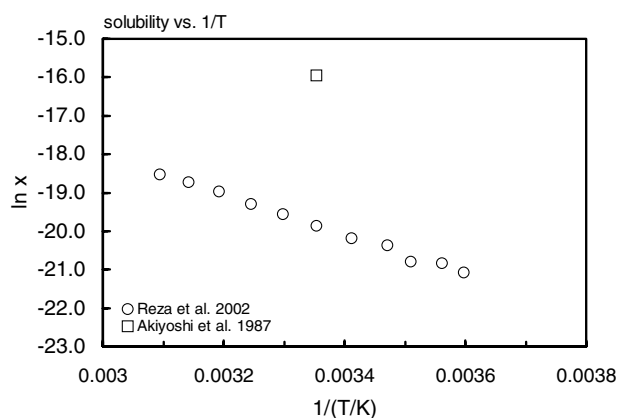
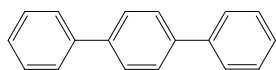


FIGURE 4.1.1.36.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *m*-terphenyl.

4.1.1.37 *p*-Terphenyl

Common Name: *p*-Terphenyl

Synonym: 1,4-diphenyl benzene

Chemical Name: *p*-terphenyl

CAS Registry No: 92-94-4

Molecular Formula: $C_{18}H_{14}$, 1,4- $(C_6H_5)_2C_6H_4$

Molecular Weight: 230.304

Melting Point ($^{\circ}C$):

213.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

376 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

262.0 (315.6 $^{\circ}C$, Stephenson & Malanowski 1987)

273.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

0.3, 35.3; 35.6 (−79.55, 213.85 $^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

74.1, 73.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.014 (mp at 213.9 $^{\circ}C$)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

1.80 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations):

4.86×10^{-6} (extrapolated from solid, Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.515 - 6210/(T/K)$; temp range 338–431 K (Antoine eq.-I, solid phase, Stephenson & Malanowski 1987)

1.78×10^{-5} (P_L extrapolated from liquid state, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.16107 - [2125.84/(-145.29 + (T/K))]$; temp range 499–700 K (Antoine eq.-II, liquid phase, Stephenson & Malanowski 1987)

$\log (P/mmHg) = -39.6342 - 3.2661 \times 10^3/(T/K) + 21.08 \cdot \log (T/K) - 2.2574 \times 10^{-2} \cdot (T/K) + 6.902 \times 10^{-6} \cdot (T/K)^2$; temp range 485–926 K (vapor pressure eq., Yaws 1994)

5.40×10^{-4} (supercooled liquid P_L , GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -4135/(T/K) + 10.60$; $\Delta H_{vap.} = -79.2$ kJ $\cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa $\cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.03, 5.88 (HPLC-RV correlation, Garst 1984)

6.03 ± 0.50 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air:

Surface water: a first order reduction process in river water with an estimated $t_{1/2} = 0.6$ d for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).

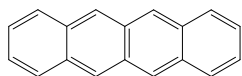
Ground water:

Sediment:

Soil:

Biota:

4.1.1.38 Naphthacene



Common Name: Naphthacene

Synonym: benz[*b*]anthracene, 2,3-benzanthracene, tetracene

Chemical Name: benz[*b*]anthracene

CAS Registry No: 92-24-0

Molecular Formula: C₁₈H₁₂

Molecular Weight: 228.288

Melting Point (°C):

357 (Lide 2003)

Boiling Point (°C):

450 (sublimation, Bjørseth 1983; Lide 2003)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

211.8 (Ruelle & Kesselring 1997)

250.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

38.64 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.000553 (mp at 357°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.0010 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.0015 (approximate, shake flask-UV, Klevens 1950)

0.0036 (shake flask-UV, Eisenbrand & Baumann 1970)

0.00057 (shake flask-fluorescence, Mackay & Shiu 1977)

0.044 (shake flask-nephelometry, Hollifield 1979)

0.00103 (lit. mean, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7.30×10^{-9} * (effusion method, De Kruif 1980)

3.70×10^{-8} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 11.505 - 6540/(T/\text{K})$; temp range 376–489 K (Antoine eq., Stephenson & Malanowski 1987)

2.31×10^{-8} * (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 113–199°C, Oja & Suuberg 1998)

$\log(P/\text{Pa}) = 33.594 - 15151/(T/\text{K})$; temp range 368–472 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:

5.90 (shake flask-UV, concn. ratio, Karickhoff et al., 1979)

6.02 (HPLC-*k'* correlation, McDuffie 1981)

5.76 (HPLC-RT correlation, Wang et al. 1986)

5.76. (recommended, Sangster 1989, 1993)

5.84 (TLC retention time correlation, De Voogt et al. 1990)

5.90 (shake flask-HPLC, De Voogt et al. 1990)

5.90 (recommended, Hansch et al 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, $\log K_{OC}$:

5.81 (sediment, batch equilibrium-sorption isotherms by GC/UV, Karickhoff et al. 1979)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photochemical transformation $t_{1/2} = 0.034$ h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis $t_{1/2} = 0.20$ d and 0.95 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)

photodegradation $k = 0.051 \text{ min}^{-1}$ and $t_{1/2} = 0.23$ h in ethanol-water (1:1, v/v) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)

pseudo-first-order direct photolysis $k(\text{exptl}) = 0.051 \text{ min}^{-1}$ with the calculated $k = 0.051 \text{ min}^{-1}$ and $t_{1/2} = 0.23$ h and the predicted $k(\text{calc}) = 0.0355 \text{ min}^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

direct photolysis $t_{1/2} = 0.92$ h predicted by QSPR in atmospheric aerosol (Chen et al. 2001).

Oxidation: $t_{1/2} = 2.6$ h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: direct photolysis $t_{1/2} = 0.92$ h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis $t_{1/2} = 0.034$ h near surface water, $t_{1/2} = 0.20$ d and 0.95 d in 5-m deep water body without and with sediment-water partitioning in full summer day, 40°N; photosensitized oxygenation $t_{1/2} = 2.6$ h at near surface water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979).

photolysis $t_{1/2} = 0.23$ h in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996).

TABLE 4.1.1.38.1

Reported vapor pressures of naphthacene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
de Kruif 1980		Oja & Suuberg 1998	
torsion-, weighing effusion		Knudsen effusion	
t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	P/Pa
147.35	0.1	113.4	0.00344
155.46	0.2	128.78	0.0199
160.35	0.3	139.56	0.0535
163.89	0.4	145.44	0.0496
166.67	0.5	160.69	0.322
168.97	0.6	172.88	0.584
170.94	0.7	198.99	4.81
172.65	0.8		
173.98	0.9	mp/K	630
175.65	1.0		

TABLE 4.1.1.38.1 (Continued)

de Kruif 1980		Oja & Suuberg 1998	
torsion-, weighing effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
25.0	9.7×10^{-9}	eq. 1a	P/Pa
	extrapolated	A	35.594
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 155.0$		for temp range 386–472 K	
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 126.1$	

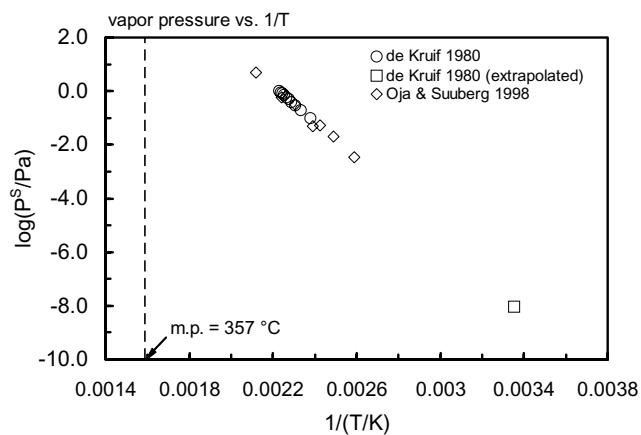
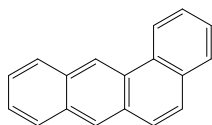


FIGURE 4.1.1.38.1 Logarithm of vapor pressure versus reciprocal temperature for naphthalene.

4.1.1.39 Benz[a]anthracene



Common Name: Benz[a]anthracene

Synonym: 1,2-benzanthracene, 2,3-benzophenanthrene, naphthanthracene, BaA, B(a) a, tetraphene

Chemical Name: 1,2-benzanthracene

CAS Registry No: 56-55-3

Molecular Formula: $C_{18}H_{12}$

Molecular Weight: 228.288

Melting Point ($^{\circ}C$):

160.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

438 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2544 (Mailhot & Peters 1988)

Molar Volume (cm^3/mol):

211.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

248.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.38 (Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

49.23, 44.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

49.2 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0468 (mp at $160.5^{\circ}C$)

0.040 (calculated, assuming $\Delta S_{fus} = 56 J/mol K$, Mackay et al. 1980)

0.0661 (calculated, $\Delta S_{fus} = 49.2 J/mol K$, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.011 ($27^{\circ}C$, shake flask-nephelometry, Davis & Parker 1942)

0.010 (shake flask-UV, Klevens 1950)

0.014 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0094, 0.0122 ($25, 29^{\circ}C$, generator column-HPLC/UV, May et al. 1978b)

$S/(\mu g/kg) = 1.74 + 0.1897 \cdot (t/^{\circ}C) + 0.0031 \cdot (t/^{\circ}C)^2 + 0.0003 \cdot (t/^{\circ}C)^3$, temp range $5-30^{\circ}C$ (generator column-HPLC/UV, May et al. 1978b, May 1980)

0.044 (shake flask-nephelometry, Hollifield 1979)

0.00837* (generator column-HPLC, measured range $6.9-29.7^{\circ}C$, May 1980)

0.0086* (generator column-HPLC, measured range $6.9-29.7^{\circ}C$, May et al. 1983)

0.00935* (generator column-fluo., measured range $10-30^{\circ}C$, Velapoldi et al. 1983)

0.011 (average lit. value, Pearlman et al. 1984)

0.0168 (generator column-HPLC/fluorescence, Walters & Luthy 1984)

0.00854 (generator column-HPLC/UV, measured range $3.7-25.0^{\circ}C$, Whitehouse 1984)

0.011 (recommended, IUPAC Solubility Data Series, Shaw 1989)

0.0146 (shake flask-HPLC, Haines & Sandler 1995)

0.0130 (generator column-HPLC/fluorescence, De Maagd et al. 1998)

$\log [S_L/(mol/L)] = -0.326 - 1119/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -3.060466 - 5354.51/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.93×10^{-6} ($20^{\circ}C$, Hoyer & Peperle 1958)

$\log (P/mmHg) = 13.68 - 6250/(T/K)$; temp range $60-120^{\circ}C$ (Knudsen effusion method, Hoyer & Peperle 1958)

2.17×10^{-5} (solid, extrapolated from Antoine eq., Kelley & Rice 1964; quoted, Bidleman 1984)
 $\log(P/\text{mmHg}) = 11.528 - 5461/(T/K)$; temp range: 104–127°C (effusion method, Kelley & Rice 1964)
 3.87×10^{-7} (effusion method, Wakayama & Inokuchi 1967)
 1.47×10^{-5} (solid, effusion method, extrapolated-Antoine eq., Murray et al. 1974)
 $\log(P/\text{mmHg}) = 10.045 - 5929/(T/K)$; temp range: 330–390 K (effusion method, Murray et al. 1974)
 6.67×10^{-7} (20°C, effusion, Pupp et al. 1974)
 $7.30 \times 10^{-6*}$ (effusion method, De Kruif 1980)
 $2.71 \times 10^{-5*}$ (gas saturation-HPLC/fluor./UV, Sonnefeld et al. 1983)
 $\log(P/\text{Pa}) = 9.684 - 4246.51/(T/K)$; temp range 10–50°C (solid, Antoine eq., Sonnefeld et al. 1983)
0.00107, 0.0003 (P_{GC} by GC-RT correlation, different GC columns, Bidleman 1984)
0.000543 (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)
 2.49×10^{-4} (Yamasaki et al. 1984)
 4.10×10^{-6} (selected, Howard et al. 1986)
 1.51×10^{-5} , 2.17×10^{-5} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_S/\text{kPa}) = 12.0507 - 5925/(T/K)$; temp range 330–390 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_S/\text{kPa}) = 10.653 - 5461/(T/K)$; temp range 377–400 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
 5.43×10^{-4} (supercooled P_L , converted from literature P_S , Hinckley et al. 1990)
0.00107, 3.23×10^{-4} (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log P_L/\text{Pa} = 12.63 - 4742/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
 2.51×10^{-4} (supercooled liquid P_L , calculated from Yamasaki et al. 1984, Finizio et al. 1997)
 $(4.11\text{--}281) \times 10^{-7}$; 2.76×10^{-5} (P_S , quoted exptl., effusion; gas saturation, Delle Site 1997)
 3.39×10^{-5} ; 5.29×10^{-5} , 1.48×10^{-5} , 2.57×10^{-5} (P_S , quoted lit., calculated; GC-RT correlation, Delle Site 1997)
 5.47×10^{-4} ; 3.59×10^{-5} (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 $\log(P_S/\text{Pa}) = 11.91 - 4858/(T/K)$ (solid, Passivirta et al. 1999)
 $\log(P_L/\text{Pa}) = 9.34 - 3760/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log(P/\text{Pa}) = 9.683 - 4246.51/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.813 (gas stripping-GC, Southworth 1979)
0.102 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
1.22* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)
 $\ln K_{AW} = -7986.53/(T/K) + 19.124$, $\Delta H = 66.4 \text{ kJ mol}^{-1}$, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
 $\log(H/(\text{Pa m}^3/\text{mol})) = 9.67 - 2641/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C and the reported temperature dependence equations:

5.61 (Radding et al. 1976)
5.66 (Leo 1986; quoted, Schüürmann & Klein 1988)
5.79 (HPLC-RT correlation, Wang et al. 1986)
5.91 (recommended, Sangster 1989, 1993)
5.84 (TLC retention time correlation, De Voogt et al. 1990)
5.79 (recommended, Hansch et al. 1995)
 5.54 ± 0.19 , 5.50 ± 0.64 (HPLC- k' correlation: ODS column; Diol column, Helweg et al. 1997)
5.91 (range 5.74–6.04) (shake flask/slow stirring-HPLC/fluorescence, De Maagd et al. 1998)
5.75 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)
5.33; 4.98 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)
 $\log K_{OW} = 1.238 + 1216.89/(T/K)$; temp range 5–55°C (temperature dependence HPLC- k' correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.50 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
9.54 (calculated, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 4.56 (Smith et al. 1978; Steen & Karickhoff 1981)
- 4.0 (*Daphnia pulex*, Southworth et al. 1978)
- 4.0 (fathead minnow, Veith et al. 1979)
- 4.56, 5.0 (bacteria, Baughman & Paris 1981)
- 4.39 (activated sludge, Freitag et al. 1984)
- 4.0 (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Howell & Connell 1986)
- 4.39, 3.50, 2.54 (activated sludge, algae, fish, Freitag et al. 1985)
- 4.01 (*Daphnia magna*, Newsted & Giesy 1987)
- 4.303, 4.266 (calculated-molecular connectivity indices, calculated- K_{ow} , Lu et al. 1999)

Sorption Partition Coefficient, log K_{oc} :

- 4.52 (22°C, suspended particulates, Herbes et al. 1980)
- 6.30 (sediments average, Kayal & Connell 1990)
- 7.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 5.62 (humic acid, HPLC- k' correlation; Nielsen et al. 1997)
- 5.77 (5.73–5.80), 5.47 (5.44–5.50) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
- 5.20 (soil, calculated-universal solvation model; Winget et al. 2000)
- 5.63–7.53; 4.50–6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.11; 6.33, 5.84, 6.18 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

- Volatilization: aquatic fate rate $k = 8 \times 10^3 \text{ h}^{-1}$ with $t_{1/2} \sim 90 \text{ h}$ (Callahan et al. 1979);
 - half-lives predicted by one compartment model: $t_{1/2} > 1000 \text{ h}$ in stream, eutrophic pond or lake and oligotrophic lake (Smith et al. 1978);
 - calculated $t_{1/2} = 500 \text{ h}$ for a river of 1-m deep with water velocity of 0.5 m/s and wind velocity of 1 m/s (Southworth 1979; quoted, Herbes et al. 1980; Hallett & Brecher 1984).
- Photolysis: aquatic fate rate $k \sim 6 \times 10^{-5} \text{ s}^{-1}$ with $t_{1/2} = 10\text{--}50 \text{ h}$ (Callahan et al. 1979)
 - $t_{1/2} = 20 \text{ h}$ in stream, $t_{1/2} = 50 \text{ h}$ in eutrophic pond or lake and $t_{1/2} = 10 \text{ h}$ in oligotrophic lake, predicated by one compartment model (Smith et al. 1978)
- direct photochemical transformation $t_{1/2}(\text{calc}) = 0.59 \text{ h}$, computed near-surface water, latitude 40°N, midday, midsummer and photolysis $t_{1/2} = 3.7 \text{ d}$ and 9.2 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)
 - $t_{1/2} = 0.58 \text{ h}$ in aquatics (quoted of EPA Report 600/7-78-074, Haque et al. 1980)
 - $t_{1/2} = 0.2 \text{ d}$ for early day in March (Mill et al. 1981);
 - $k = 1.93 \text{ h}^{-1}$ (Zepp 1980; quoted, Mill & Mabey 1985)
 - $k = 13.4 \times 10^{-5} \text{ s}^{-1}$ in early March with $t_{1/2} = 5 \text{ h}$ in pure water at 366 nm, in sunlight at 23–28°C and $k = 2.28 \times 10^{-5} \text{ s}^{-1}$ at 313 nm with 1% acetonitrile in filter-sterilized natural water (Mill et al. 1981);
 - $k = 1.39 \text{ h}^{-1}$ for summer midday at 40°N latitude (quoted, Mabey et al. 1982)
 - $t_{1/2} = 1\text{--}3 \text{ h}$, atmospheric and aqueous photolysis half-life, based on measured photolysis rate constant for midday March sunlight on a cloudy day (Smith et al. 1978; quoted, Harris 1982; Howard et al. 1991) and adjusted for approximate summer and winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
 - half-lives on different atmospheric particulate substrates (approx. 25 µg/g on substrate): $t_{1/2} = 4.0 \text{ h}$ on silica gel, $t_{1/2} = 2.0 \text{ h}$ on alumina and $t_{1/2} = 38 \text{ h}$ on fly ash (Behymer & Hites 1985)
 - first order daytime decay $k = 0.0125 \text{ min}^{-1}$ for soot particles loading of 1000–2000 ng/mg and $k = 0.0250 \text{ min}^{-1}$ for soot particles loading of 30–350 ng/mg (Kamens et al. 1988)
 - photodegradation $k = 0.0251 \text{ min}^{-1}$ with $t_{1/2} = 0.46 \text{ h}$ in ethanol-water (2:3, v/v) solution for initial concentration of 12.5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
 - pseudo-first-order direct photolysis $k(\text{exptl}) = 0.0251 \text{ min}^{-1}$ with the calculated $t_{1/2} = 0.46 \text{ h}$ and the predicted $k = 0.0245 \text{ min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

direct photolysis $t_{1/2}(\text{obs}) = 0.94 \text{ h}$, $t_{1/2}(\text{calc}) = 0.89 \text{ h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001)

Photodegradation $k = 5.0 \times 10^{-4} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: half-lives predicted by one compartment model: $t_{1/2} = 38 \text{ h}$ in stream, eutrophic pond or lake and oligotrophic lake based on peroxy radical concentration of 10^{-9} M (Smith et al. 1978)

aquatic fate rate $k = 5 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 38 \text{ h}$ (Callahan et al. 1979);

$t_{1/2} = 6400 \text{ h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N , midday, midsummer (Zepp & Schlotzhauer 1979)

$k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $2 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k = 3.3 \times 10^{-4} \text{ h}^{-1}$ with $t_{1/2} = 0.6 \text{ h}$ under natural sunlight conditions; $k(\text{aq.}) = 5.0 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ with $t_{1/2} = 1.6 \text{ d}$ for free-radical oxidation in air-saturated water (NRCC 1983)

photooxidation $t_{1/2} = 0.801\text{--}8.01 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991);

photooxidation $t_{1/2} = 77\text{--}3850 \text{ h}$ in water, based on measured rate constant for reaction with hydroxyl radical in water (Howard et al. 1991)

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: not observed during enrichment procedures (Smith et al. 1978)

no significant degradation in 7 d for an average of three static-flask screening test (Tabak et al. 1981)

$k = 3.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 208 \text{ h}$ for mixed bacterial populations in stream sediment (NRCC 1983)

$k = 1.0 \times 10^{-4} \text{ h}^{-1}$ with $t_{1/2} = 288 \text{ d}$; $k = 4.0 \times 10^{-6} \text{ h}^{-1}$ with $t_{1/2} = 20 \text{ yr}$ for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)

$k = 0.0026 \text{ d}^{-1}$ with $t_{1/2} = 261 \text{ d}$ for Kidman sandy loam and $k = 0.0043 \text{ d}^{-1}$ with $t_{1/2} = 162 \text{ d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)

$t_{1/2}(\text{aq. aerobic}) = 2448\text{--}16320 \text{ h}$, based on aerobic soil dieaway test data at $10\text{--}30^\circ\text{C}$ (Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 9792\text{--}65280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant estimated to be $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 669 \text{ h}^{-1}$; $k_2 = 0.144 \text{ h}^{-1}$ (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 2.83 \text{ h}^{-1}$; $\log k_2 = -0.84 \text{ h}^{-1}$ (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 138.6 \text{ mL g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0022 \text{ h}^{-1}$ (4°C , *P. hoyi*, Landrum 1988)

$k_1 = 0.72\text{--}1.4 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0096 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 1\text{--}3 \text{ h}$, based on estimated photolysis half-life in air (Howard et al. 1991);

$t_{1/2} = 4.20 \text{ h}$ under simulated sunlight, $t_{1/2} = 1.35 \text{ h}$ in simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 2.88 \text{ h}$ in dark reaction ozone (0.2 ppm), under simulated atmospheric conditions (Katz et al. 1979)

$t_{1/2} = 0.4 \text{ h}$ for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant $k = 0.0265 \text{ min}^{-1}$ at $1 \text{ cal cm}^{-2} \text{ min}^{-1}$, $10 \text{ g/m}^3 \text{ H}_2\text{O}$ and 20°C (Kamens et al. 1988).

Surface water: photolysis $t_{1/2} = 0.59 \text{ h}$ near surface water, $t_{1/2} = 3.7 \text{ d}$ and 9.2 d in 5-m deep water body without and with sediment-water partitioning in full summer day, 40°N ; photosensitized oxygenation $t_{1/2} = 2.6 \text{ h}$ at near surface water, 40°N , midday, midsummer (Zepp & Schlotzhauer 1979)

$t_{1/2} = 0.20 \text{ d}$ under summer sunlight (Mill & Mabey 1985);

$t_{1/2} = 1\text{--}3 \text{ h}$, based on estimated photolysis half-life in water, Howard et al. 1991);

photolysis $t_{1/2} = 0.46 \text{ h}$ (reported in units of minutes) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2} = 4896\text{--}32640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: The uptake clearance from sediment was $k = (0.005 \pm 0.001) \text{ g of dry sediment} \cdot \text{g}^{-1} \text{ of organism} \cdot \text{h}^{-1}$, and the elimination rate constants $k = (0.0014 \pm 0.0006) \text{ h}^{-1}$ for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C (Landrum 1989);

desorption $t_{1/2} = 11.1 \text{ d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} = 4\text{--}6250 \text{ d}$ (Sims & Overcash 1983; quoted, Bulman et al. 1987);

$t_{1/2} = 240$ d for 5 mg/kg treatment and 130 d for 50 mg/kg treatment (Bulman et al. 1987);
 biodegradation $k = 0.0026$ d⁻¹ with $t_{1/2} = 261$ d for Kidman sandy loam soil, and $k = 0.0043$ d⁻¹ with $t_{1/2} = 162$ d for McLaurin sandy loam soil (Park et al. 1990);
 $t_{1/2} \sim 2448$ – 16320 h, based on aerobic die-away test data at 10–30°C (Howard et al. 1991);
 $t_{1/2} > 50$ d (Ryan et al. 1988).

Biota: depuration $t_{1/2} = 9$ d by oysters (Lee et al. 1978);

elimination $t_{1/2} = 4.3$ – 17.8 d from mussel *Mytilus edulis*; $t_{1/2} = 7$ – 15.4 d from Oyster, $t_{1/2} = 8.0$ d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.39.1

Reported aqueous solubilities of benz[a]anthracene at various temperatures and reported temperature dependence equation

$$S/(\mu\text{g/kg}) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)$$

$$\ln x = A + B/(T/K) + C \cdot \ln(T/K) \quad (2)$$

May 1980		May et al. 1978b		May et al. 1983		Velapoldi et al. 1983	
generator column-HPLC		generator column-HPLC		generator column-HPLC		generator column-fluo.	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
6.9	0.00299	25	0.0094	6.9	0.00299	10	0.00342
10.7	0.00378	29	0.0122	10.7	0.00378	15	0.00475
14.3	0.00479			11.0	0.00361	20	0.00669
19.3	0.00633			14.7	0.00558	25	0.00935
23.1	0.00837	temp dependence eq. 1		18.1	0.00634	30	0.01297
29.7	0.0127	S	μg/kg	19.3	0.00801		
		a	0.0003	23.6	0.00838		
temp dependence eq. 1		b	−0.0031	25.0	0.00862	eq. 2	mole fraction
S	μg/kg	c	0.1897	29.5	0.0124	A	−83.75982
a	0.0003	d	1.74	29.7	0.0127	B	41884.5
b	−0.0031					C	161.175
c	0.1897	ΔH _{sol} /(kJ mol ⁻¹) = 44.81					
d	1.74	measured between 5–30°C					
ΔH _{sol} /(kJ mol ⁻¹) = 44.81						ΔH _{sol} /(kJ mol ⁻¹) = 49.0	
measured between 5–30°C						at 25°C	

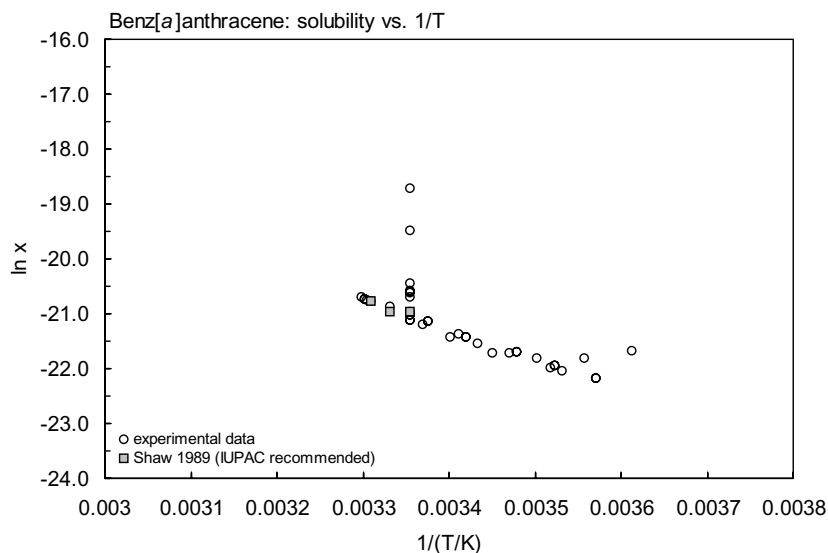


FIGURE 4.1.1.39.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for benz[a]anthracene.

TABLE 4.1.1.39.2

Reported vapor pressures of benz[a]anthracene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & \end{aligned}$$

Kelley & Rice 1964		Murray et al. 1972		de Kruif 1980		Sonnefeld et al. 1983	
effusion-electrobalance		Knudsen effusion		torsion-, effusion method		generator column-HPLC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
data represented by		data presented by graph and		98.07	0.1	13.81	8.05×10^{-5}
		eq. 2		105.21	0.2	13.81	6.06×10^{-5}
eq. 1	P/mmHg	A	10.045	109.51	0.3	13.81	1.13×10^{-5}
A	11.528	B	5925	112.62	0.4	25.1	2.66×10^{-5}
B	5461	temp range 330–390 K		115.06	0.5	25.1	2.56×10^{-5}
measured range 104–127°C				117.09	0.6	25.1	2.81×10^{-5}
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 104.56$				118.82	0.7	40.12	1.39×10^{-4}
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 113.5$		120.32	0.8	40.12	1.41×10^{-4}
mp/°C	160–161.5			121.66	0.9	40.12	1.36×10^{-4}
				122.87	1.0	40.75	1.31×10^{-4}
				25.0	7.3×10^{-6}	40.85	1.17×10^{-4}
				$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 113$		extrapolated	1.27×10^{-4}
						40.85	1.21×10^{-4}
						40.85	1.21×10^{-4}
						49.56	3.87×10^{-4}
Hoyer & Peperle 1958						49.56	3.85×10^{-4}
effusion method						49.56	3.88×10^{-4}
t/°C	P/Pa					49.56	3.88×10^{-4}
						34.93	2.69×10^{-4}
data presented by equation.						25.0	2.80×10^{-5}

(Continued)

TABLE 4.1.1.39.2 (Continued)

Kelley & Rice 1964		Murray et al. 1972		de Kruif 1980		Sonnefeld et al. 1983	
effusion-electrobalance		Knudsen effusion		torsion-, effusion method		generator column-HPLC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
eq. 1	P/mmHg					eq. 1	P/Pa
A	13.68					A	9.684
B	6250					B	4246.51
for temp range 60–120°C						$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 51.83$	
						for temp range 10–50°C	

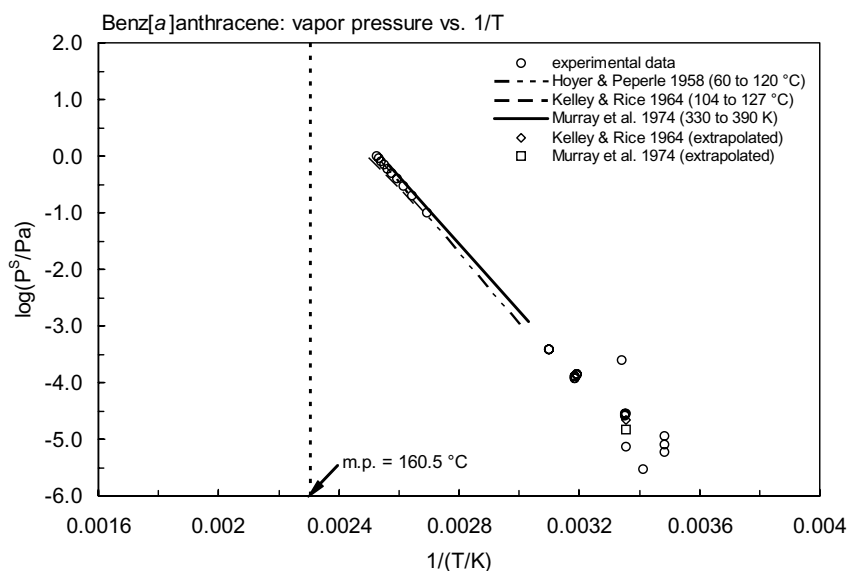


FIGURE 4.1.1.39.2 Logarithm of vapor pressure versus reciprocal temperature for benz[a]anthracene.

TABLE 4.1.1.39.3

Reported Henry's law constants of benz[a]anthracene at various temperatures and temperature dependence equations

$\ln K_{\text{AW}} = A - B/(T/K)$	(1)	$\log K_{\text{AW}} = A - B/(T/K)$	(1a)
$\ln (1/K_{\text{AW}}) = A - B/(T/K)$	(2)	$\log (1/K_{\text{AW}}) = A - B/(T/K)$	(2a)
$\ln (k_{\text{H}}/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{\text{AW}} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

Bamford et al. 1999

gas stripping-GC/MS

t/°C	H/(Pa m ³ /mol)	H/(Pa m ³ /mol)
		average
4.1	0.10, 0.22	0.15
11.0	0.24, 0.41	0.31
18.0	0.50, 0.79	0.63
25.0	0.91, 1.64	1.22
31.0	1.43, 3.13	2.11

 $\ln K_{\text{AW}} = A - B/(T/K)$

TABLE 4.1.1.39.3 (Continued)

Bamford et al. 1999		
gas stripping-GC/MS		
t/°C	H/(Pa m ³ /mol)	H/(Pa m ³ /mol)
A	19.124	
B	7986.5	
enthalpy, entropy change:		
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 66.4 \pm 6.9$		
$\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 159$		
at 25°C		

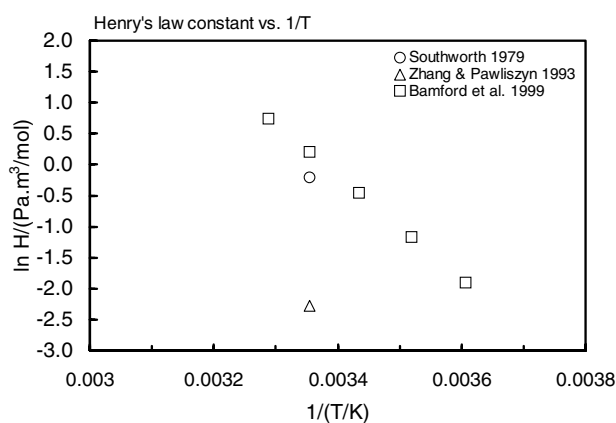
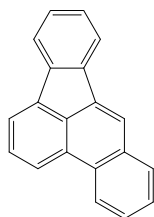


FIGURE 4.1.1.39.3 Logarithm of Henry's law constant versus reciprocal temperature for benz[a]anthracene.

4.1.1.40 Benzo[*b*]fluoranthene

Common Name: Benzo[*b*]fluoranthene

Synonym: 2,3-benzofluoranthene, 3,4-benzofluoranthene, benz[*e*]acephenanthrylene, B[*b*]F

Chemical Name: 2,3-benzofluoranthene

CAS Registry No: 205-99-2

Molecular Formula: C₂₀H₁₂

Molecular Weight: 252.309

Melting Point (°C):

168 (Bjørseth 1983; Pearlman et al. 1984; Lide 2003)

Boiling Point (°C):

481 (Bjørseth 1983)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

268.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0395 (mp at 168°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):

0.0015 (generator column-HPLC/fluorescence, Wise et al. 1981)

0.0015 (average lit. value, Pearlman et al. 1984)

0.00109 (generator column-HPLC/fluoro., De Maagd et al. 1998)

log [S_L/(mol/L)] = -0.351 - 1303/(T/K) (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

6.67 × 10⁻⁵ (20°C, estimated, Callahan et al. 1979)

2.12 × 10⁻⁵ (Yamasaki et al. 1984)

5.0 × 10⁻⁸; 1.30 × 10⁻⁶ (quoted solid P_s from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)

log (P_s/Pa) = 12.43 - 5880/(T/K) (solid, Passivirta et al. 1999)

log (P_L/Pa) = 9.48 - 4578/(T/K) (supercooled liquid, Passivirta et al. 1999)

7.55 × 10⁻⁶ (supercooled liquid P_L, calibrated GC-RT correlation, Lei et al. 2002)

log (P_L/Pa) = -4682/(T/K) + 10.58, ΔH_{vap} = -89.7 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations.):

0.051 (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)

log [H/(Pa m³/mol)] = 9.83 - 3274/(T/K) (Passivirta et al. 1999)

0.0485 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 2.955 - 2245/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{ow}:

5.78 (HPLC-RT correlation, Wang et al. 1986)

5.78 (recommended, Sangster 1989, 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

5.15	(microorganisms-water, Mabey et al. 1982)
4.00	(<i>Daphnia magna</i> , Newsted & Giesy 1987)
0.959, 0.230	(<i>Polychaete sp.</i> , <i>Capitella capitata</i> , Bayona et al. 1991)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

6.182; 6.00, 6.18	(sediment: concn ratio C_{sed}/C_w ; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
5.45	($\log K_{DOC}$ - Aldrich humic acid, RP-HPLC, Ozretich et al. 1995)
6.57	(10°C), 6.55, 6.61 (20°C), 6.26 (35°C), 6.44, 6.45 (45°C) ($\log K_{DOC}$, dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
6.20	(20°C, $\log K_{DOC}$, particulate organic material from lake, Lüers & ten Hulscher 1996)
6.15–8.02; 5.70–7.50	(range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001, for benzo[b + j + k]fluoranthenes)
5.91; 6.50, 6.26, 6.68	(20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001, for benzo[b + j + k]fluoranthenes)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric and aqueous $t_{1/2} = 8.7$ –720 h, based on measured rate of photolysis in heptane irradiated with light > 290 nm (Howard et al. 1991);

first order daytime decay rate constants: $k = 0.0065 \text{ min}^{-1}$ for 1000–2000 ng/mg soot particles loading and $k = 0.0090 \text{ min}^{-1}$ with 30–350 ng/mg loading (Kamens et al. 1988);

$t_{1/2}(\text{obs.}) = 4.31 \text{ h}$, $t_{1/2}(\text{calc}) = 1.49 \text{ h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Photodegradation $k = 3 \times 10^{-5} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002).

Oxidation: rate constant $k = 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 5 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 1.43$ –14.3 h, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991).

Hydrolysis: not hydrolyzable (Mabey et al. 1982; no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

aerobic $t_{1/2} = 8640$ –14640 h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$k = 0.0024 \text{ d}^{-1}$ with $t_{1/2} = 294 \text{ d}$ for Kidman sandy loam and $k = 0.0033 \text{ d}^{-1}$ with $t_{1/2} = 211 \text{ d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990);

$t_{1/2}(\text{aq. anaerobic}) = 34560$ –58560 h, based on estimated unacclimated aqueous aerobic degradation half-life (Howard et al. 1991).

Biotransformation: estimated to be $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.11$ –0.38 $\text{mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0029 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Sorption-Desorption Rate constants: desorption rate constant $k = 0.016 \text{ d}^{-1}$ with $t_{1/2} = 42.4 \text{ d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Half-Lives in the Environment:

Air: $t_{1/2} = 1.43$ –14.3 h, based on estimated photooxidation half-life in air (Howard et al. 1991)

half-lives under simulated atmospheric conditions: simulated sunlight $-t_{1/2} = 8.70 \text{ h}$, simulated sunlight + ozone (0.2 ppm) $t_{1/2} = 4.20 \text{ h}$, dark reaction ozone (0.2 ppm) $t_{1/2} = 52.70 \text{ h}$ (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

$t_{1/2} = 1.3 \text{ h}$ for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant $k = 0.0091 \text{ min}^{-1}$ at $1 \text{ cal cm}^{-2} \text{ min}^{-1}$, $10 \text{ g/m}^3 \text{ H}_2\text{O}$ and 20°C (Kamens et al. 1988).

Surface water: $t_{1/2} = 8.7$ –720 h, based on estimated aqueous photolysis half-life (Lane & Katz 1977; Muel & Saguem 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 17280\text{--}29280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

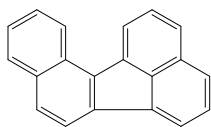
Sediment: desorption $t_{1/2} = 42.4$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: biodegradation rate constant $k = 0.0024\text{ d}^{-1}$ with $t_{1/2} = 294$ d for Kidman sandy loam soil, and $k = 0.0033\text{ d}^{-1}$ with $t_{1/2} = 211$ d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} = 8640\text{--}14640$ h, based on aerobic die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$t_{1/2} = 42$ wk, 9.0 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: elimination $t_{1/2} = 5.7\text{--}16.9$ d from mussel *Mytilus edulis*; $t_{1/2} = 7.7$ d from Oyster (isomer unspecified), $t_{1/2} = 3.9$ d from clam *Mercenaria mercenaria* (isomer unspecified) (quoted, Meador et al. 1995).

4.1.1.41 Benzo[*j*]fluoranthene

Common Name: Benzo[*j*]fluoranthene

Synonym: 7,8-benzofluoranthene, 10,11-fluoranthene

Chemical Name: benzo[*j*]fluoranthene

CAS Registry No: 205-82-3

Molecular Formula: C₂₀H₁₂

Molecular Weight: 252.309

Melting Point (°C):

166 (Bjørseth 1983; Pearlman et al. 1984; Lide 2003)

Boiling Point (°C):

480 (Bjørseth 1983)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

222.8 (Ruelle & Kesselring 1997)

268.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0414 (mp at 166°C)

Water Solubility (g/m³ or mg/L at 25°C):

0.0025 (generator column-HPLC/fluorescence, Wise et al. 1981)

0.0025 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log K_{OW}:

6.44 (calculated-MCI χ as per Rekker & De Kort 1979, Ruepert et al. 1985)

6.40 (Bayona et al. 1991)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

0.914; -0.222 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient, log K_{OC}:

6.15–8.02; 5.70–7.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001, for benzo[*b + j + k*]fluoranthenes)

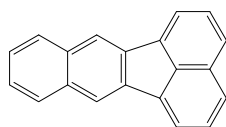
5.91; 6.50, 6.26, 6.68 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001, for benzo[*b + j + k*]fluoranthenes)

Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:

Half-Lives in the Environment:

Biota: elimination t_{1/2} = 7.7 d from Oyster (isomer unspecified), t_{1/2} = 3.9 d from clam *Mercenaria mercenaria* (isomer unspecified) (quoted, Meador et al. 1995).

4.1.1.42 Benzo[k]fluoranthene



Common Name: Benzo[k]fluoranthene

Synonym: 8,9-benzofluoranthene, 11,12-benzofluoranthene, B[k]F

Chemical Name: 8,9-benzofluoranthene

CAS Registry No: 207-08-9

Molecular Formula: $C_{20}H_{12}$

Molecular Weight: 252.309

Melting Point ($^{\circ}\text{C}$):

217 (Weast 1977; Bjørseth 1983; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

480 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

268.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

56.6 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 0.0131 (mp at 217°C)

0.0126 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C and reported temperature dependence equations):

0.0008 (generator column-HPLC/UV, Wise et al. 1981)

0.00081 (average lit. value, Pearlman et al. 1984)

0.00109 (generator column-HPLC/fluorescence, De Maagd et al. 1998)

$\log [S_L/(\text{mol}/\text{L})] = -0.351 - 1448/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

1.28×10^{-8} (20°C , Radding et al. 1976)

6.70×10^{-5} (20°C , Mabey et al. 1982)

2.07×10^{-5} (Yamasaki et al. 1984)

5.20×10^{-8} , 4.93×10^{-6} (20°C , lit. mean solid P_s , supercooled liquid value P_L , Bidleman & Foreman 1987)

1.29×10^{-7} (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 12.8907 - 6792/(T/\text{K})$; temp range 363–430 K (Antoine eq., Stephenson & Malanowski 1987)

2.09×10^{-5} (supercooled liquid P_L , calculated from Yamasaki et al. 1984, Finizio et al. 1997)

5.20×10^{-8} ; 4.14×10^{-6} (quoted solid P_s from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.43 - 5874/(T/\text{K})$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 9.48 - 4427/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)

8.96×10^{-6} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/\text{Pa}) = -4623/(T/\text{K}) + 10.46$; $\Delta H_{\text{vap}} = -88.5 \text{ kJ}\cdot\text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.111 (15°C , calculated, Baker & Eisenreich 1990)

0.043* (20°C , gas stripping-HPLC/fluorescence, measured range 10 – 55°C , ten Hulscher et al. 1992)

$\log (H/(\text{Pa m}^3/\text{mol})) = 9.83 - 2979/(T/\text{K})$ (Passivirta et al. 1999)

0.0422 (20°C , selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 3.498 - 2421/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.84	(calculated-fragment const., Callahan et al. 1979)
6.06	(calculated-f const., Mabey et al. 1982)
6.44	(calculated-MCI χ as per Rekker & De Kort 1979)
6.40	(Bayona et al. 1991)
6.50	(calculated-S and mp, Capel et al. 1991)
7.20	(calculated- K_{OC} , Broman et al. 1991)
6.00	(selected, Mackay et al. 1992; quoted, Finizio et al. 1997)
6.30	(computed-expert system SPARC, Kolliig 1995)
6.50–6.85; 6.73	(quoted lit. range; lit. mean, Meador et al. 1995)
6.11	(range 5.86–6.28) (shake flask/slow stirring-HPLC/fluor., De Maagd et al. 1998)
5.94; 6.16	(quoted lit.; calculated, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

11.19	(calculated, Finizio et al. 1997)
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Bioconcentration Factor, $\log BCF$:

5.15	(microorganisms-water, calculated from K_{ow} , Mabey et al. 1982)
4.12	(<i>Daphnia magna</i> , Newsted & Giesy 1987)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

5.99	(sediments average, Kayal & Connell 1990)
7.00	(Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
6.80 (10°C), 6.74, 6.89 (20°C), 6.46 (35°C), 6.44, 6.45 (45°C)	($\log K_{DOC}$ - dissolved organic material from lake, gas-purge technique- HPLC/fluorescence, Lüers & ten Hulscher 1996)
6.30	(20°C, $\log K_{POC}$ - particulate organic material from lake, Lüers & ten Hulscher 1996)
6.04 (5.93–6.12), 5.47 (5.39–5.54)	(sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
6.15–8.02; 5.70–7.50	(range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001, for benzo[<i>b</i> + <i>j</i> + <i>k</i>]fluoranthenes)
5.91; 6.50, 6.26, 6.68 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1, 2, 3-solvophobic approach, Krauss & Wilcke 2001, for benzo[<i>b</i> + <i>j</i> + <i>k</i>]fluoranthenes)	

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric and aqueous photolysis $t_{1/2} = 3.8$ –499 h, based on measured rate of photolysis in heptane under November sunlight and adjusted by ratio of sunlight photolysis half-lives in water versus heptane (Howard et al. 1991);

first-order daytime decay constants: $k = 0.0047 \text{ min}^{-1}$ for soot particles loading of 1000–2000 ng/mg and $k = 0.0013 \text{ min}^{-1}$ with 30–350 ng/mg loading (Kamens et al. 1988);

direct photolysis $t_{1/2}(\text{obs}) = 0.88 \text{ h}$, $t_{1/2}(\text{calc}) = 0.80 \text{ h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Photodegradation $k = 3 \times 10^{-5} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant $k = 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 5 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 1.1$ –11 h, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991).

Hydrolysis: not hydrolyzable (Mabey et al. 1982);

no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

aerobic $t_{1/2} = 21840$ –51360 h, based on aerobic soil die-away test data (Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 87360$ –205440 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated to be 3×10^{-12} mL cell⁻¹ h⁻¹ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 1.1\text{--}11$ h, based on estimated photooxidation half-life in air (Howard et al. 1991);

$t_{1/2} = 14.10$ h in simulated sunlight: $t_{1/2} = 3.90$ h in simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 34.90$ h in dark reaction ozone (0.2 ppm) u) under simulated atmospheric conditions (Katz et al. 1979);

$t_{1/2} = 0.8$ h for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant $k = 0.0138$ min⁻¹ at 1 cal cm⁻² min⁻¹ and 10 g/m³ H₂O at 20°C (Kamens et al. 1988).

Surface water: $t_{1/2} = 3.8\text{--}499$ h, based on photolysis half-life in water (Howard et al. 1991).

Groundwater: $t_{1/2} = 42680\text{--}102720$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption $t_{1/2} = 23.2$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} = 21840\text{--}51360$ h, based on aerobic soil die-away test data Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988);

mean $t_{1/2} = 8.7$ yr for Luddington soil (Wild et al. 1991).

Biota: elimination $t_{1/2} = 11.9$ d from mussel *Mytilus edulis*; $t_{1/2} = 7.7$ d from Oyster (isomer unspecified), $t_{1/2} = 3.9$ d from clam *Mercenaria mercenaria* (isomer unspecified) (quoted, Meador et al. 1995).

TABLE 4.1.1.42.1

Reported Henry's law constants of benzo[k]fluoranthene at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1) \quad \log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \quad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_p/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4) \quad \ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

ten Hulscher et al. 1992

gas stripping-HPLC/fluorescence

t/°C	H/(Pa m ³ /mol)
10.0	0.022
20.0	0.043
35.0	0.107
40.1	0.138
45.0	0.198
55.0	0.403
$\ln K_{AW} = -\Delta H_{vol}/RT + \Delta S_{vol}/R$ $R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$ $\Delta S_{vol} = 16.41$ $\Delta H_{vol} = 5893.7$ enthalpy of volatilization: $\Delta H_{vol}/(\text{kJ} \cdot \text{mol}^{-1}) = 49 \pm 1.9$ entropy of volatilization, ΔS $T\Delta S_{vol}/(\text{kJ} \cdot \text{mol}^{-1}) = 40 \pm 4$ at 20°C	

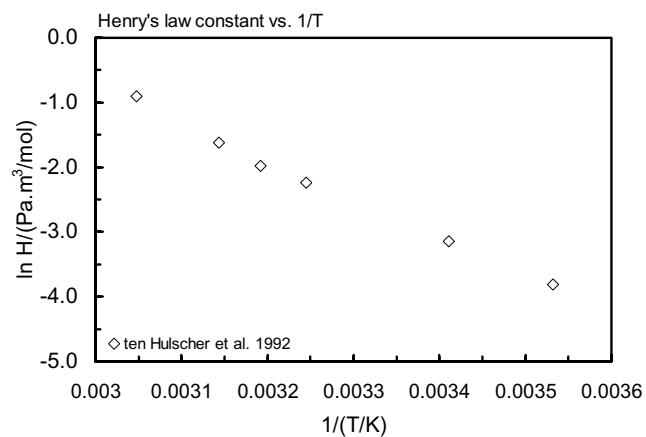
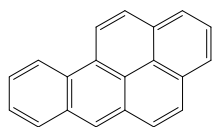


FIGURE 4.1.1.42.1 Logarithm of Henry's law constant versus reciprocal temperature for benzo[k]fluoranthrene.

4.1.1.43 Benzo[a]pyrene



Common Name: Benzo[a]pyrene

Synonym: BaP, B(a)P, 3,4-benzopyrene

Chemical Name: benzo[a]pyrene

CAS Registry No: 50-32-8

Molecular Formula: $C_{20}H_{12}$

Molecular Weight: 252.309

Melting Point ($^{\circ}C$):

181.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

495 (Stephenson & Malanowski 1987; Dean 1992)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

262.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.324 (Ruelle & Kesselring 1997)

8.49, 17.32; 25.61 (117.05, 181.05 $^{\circ}C$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

38.5 (differential scanning calorimetry, Hinckley et al. 1990)

21.77, 38.13 (117.05, 181.05 $^{\circ}C$, Chickos et al. 1999)

42.35, 43.7 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

38.2 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0294 (mp at 181.1 $^{\circ}C$)

0.0903 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.004 (27 $^{\circ}C$, nephelometry, Davis et al. 1942)

0.0043 (shake flask-UV/fluorescence, Barone et al. 1967)

0.0061 (average, Barone et al. 1967)

0.0005 (20 $^{\circ}C$, shake flask-UV, Eisenbrand & Baumann 1970)

0.000038, 0.0000606, 0.000038, 0.0000505 (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)

0.00121 (Haque & Schmedding 1975)

0.0038 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0002 (Rossi 1977; Neff 1979)

0.0012 (generator column-HPLC, Wise et al. 1981)

0.00162* (generator column-HPLC, measured range 10–30 $^{\circ}C$, May et al. 1983)

0.00158* (generator column-spectrofluorimetry, measured range 10–30 $^{\circ}C$, Velapoldi et al. 1983)

0.0038 (selected value, Pearlman et al. 1984)

0.00154* (generator column-HPLC/UV, measured 8.0–25.0 $^{\circ}C$, Whitehouse 1984)

0.0016 (generator column-HPLC/UV, Billington et al. 1988)

0.000504 (shake flask-LSC, Eadie et al. 1990)

0.00472 (shake flask-fluorescence, Haines & Sandler 1995)

0.00182 (generator column-HPLC/fluorescence, De Maagd et al. 1998)

0.00622 \pm 0.00023; 0.0038, 0.0018 \pm 0.0003 (shake flask-SPME (solid-phase micro-extraction)-GC; quoted lit. values; Paschke et al. 1999)

$\log S_L$ (mol/L) = $-1.310 - 906.6/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -2.59638 - 6046.87/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

7.32×10^{-7} (effusion method, extrapolated, Murray et al. 1974)

$\log (P/\text{mmHg}) = 9.601 - 6181/(T/K)$; temp range 358–431 K (Knudsen effusion method, Murray et al. 1974)

1.12×10^{-4} , 1.50×10^{-5} (P_{GC} , GC-RT correlation with different GC columns, Bidleman 1984)

2.35×10^{-5} (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)

1.22×10^{-5} (Yamasaki et al. 1984)

3.2×10^{-7} , 1.23×10^{-5} (lit. mean, supercooled liq. value, Bidleman & Foreman 1987)

7.51×10^{-7} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_S/\text{kPa}) = 11.6067 - 6181/(T/K)$; temp range 358–431 K (Antoine eq., Stephenson & Malanowski 1987)

1.12×10^{-4} , 7.24×10^{-5} (P_{GC} , GC-RT correlation with different reference standards, Hinckley et al. 1990)

2.35×10^{-5} , 7.28×10^{-6} (supercooled liquid P_L , converted from literature P_S with different ΔS_{fus} Hinckley et al. 1990)

$\log (P_L/\text{Pa}) = 11.59 - 4989/(T/K)$ (liquid phase, GC-RT correlation, Clausius-Clapeyron eq., Hinckley et al. 1990)

1.17×10^{-5} (supercooled liquid P_L , calculated from Yamasaki et al 1984, Finizio et al. 1997)

7.51×10^{-7} , 7.45×10^{-7} (quoted exptl., effusion, Delle Site 1997)

7.01×10^{-7} ; 3.51×10^{-6} , 4.73×10^{-7} , 2.25×10^{-7} (quoted lit., calculated-UNIFAC; GC-RT correlation, Delle Site 1997)

1.54×10^{-5} ; 1.39×10^{-6} (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/\text{Pa}) = 12.17 - 5371/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 10.71 - 4465/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

5.90×10^{-6} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/\text{Pa}) = -4755/(T/K) + 10.72$; $\Delta H_{vap.} = -91.0 \text{ kJ}\cdot\text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.009 (15°C, calculated, Baker & Eisenreich 1990)

0.0079 (10°C, estimated, McLachlan et al. 1990)

0.034* (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)

0.074 (wetted wall column-GC, Altschuh et al. 1999)

$\log [H/(\text{Pa m}^3/\text{mol})] = 12.02 - 3558/(T/K)$ (Passivirta et al. 1999)

0.035 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 1.732 - 1927/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.04 (Radding et al. 1976)

6.31 (Smith et al. 1978)

5.99, 5.78 (calculated-fragment const., Hansch & Leo 1979)

6.34 (Steen & Karickhoff 1981)

6.50 (RP-TLC- k' correlation, Bruggeman et al. 1982)

6.20 (shake flask-GC, Hanai et al. 1982)

5.85–5.12; 5.88–6.04; 5.99, 6.00 ± 0.1 (23°C, shake flask- concentration ratio/UV spec.; shake flask-HPLC/UV; exptl. mean value, recommended value; Mallon & Harris 1984)

6.74, 7.77, 7.99 (HPLC-RT correlation, Sarna et al. 1984)

6.42 (HPLC-RT correlation, Rapaport et al. 1984)

5.97 (Hansch & Leo 1985)

6.78 (HPLC-RT correlation, Webster et al. 1985)

6.04 (HPLC-RT correlation, Wang et al. 1986)

6.44 (TLC retention time correlation, De Voogt et al. 1990)

6.35 (recommended, Sangster 1993)

5.97 (recommended, Hansch et al. 1995)

- 6.02 ± 0.19, 6.14 ± 0.71 (HPLC- k' correlation: ODS column; Diol column, Helweg et al. 1997)
 6.13 (5.91–6.28) (slow stirring-HPLC/fluorescence, De Maagd et al. 1998)
 6.27 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} :

- 10.80 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
 10.77 (calculated, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.09; 2.22; 3.45 (steady-state, bluegills; midge larva; periphyton, Leversee et al. 1981)
 4.74 (*P. hoyi*, Eadie et al. 1982)
 3.90 (*Daphnia magna*, McCarthy 1983)
 3.69, 4.45 (*Lepomis macrochirus*, bluegill sunfish, Spacie et al., 1983)
 4.00 (activated sludge, Freitag et al. 1984)
 3.42 (bluegills, McCarthy & Jimenez 1985)
 2.35, 2.45 (bluegills-with dissolved humic material, McCarthy & Jimenez 1985)
 2.68, 3.52, 4.0 (fish, algae, activated sludge, Freitag et al. 1985)
 3.51 (worms, Frank et al. 1986)
 6.95, 6.51 (*P. hoyi* of Lake Michigan interstitial waters, Landrum et al. 1985)
 3.34 (*P. hoyi* of Government Pond of Grand Haven in Michigan, Landrum et al. 1985)
 2.69 (Gobas et al. 1987)
 4.11 (*Daphnia magna*, Newsted & Giesy 1987)
 3.77 (10–20°C, *H. limbata*, Landrum & Poore 1988)
 4.61, 3.86, 3.87 (4°C, *P. hoyi*, *S. heringianus*, *Mysis relicta*, Landrum & Poore 1988)
 4.69, 3.93 (calculated for amphipods and mysids, Evans & Landrum 1989)
 3.22–3.59; 2.96–3.32 (*Daphnia magna* in natural waters with humic substances, measured range; predicted range, Kokkonen et al. 1989)
 1.140, –0.155 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)
 6.22, 6.04; 3.68, 5.01, 4.90, 5.15 (oligochaetes; chironomid larvae, Bott & Standley 2000)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 5.95 (Aldrich humic acid, RP-HPLC separation, Landrum et al. 1984)
 4.59, 4.72, 4.26 (humic materials in natural water: Huron River 6.1% OC winter, Grand River 10.7% DOC spring, Lake Michigan 5.5% DOC spring, RP-HPLC separation method, Landrum et al. 1984)
 6.66 (LSC, Eadie et al. 1990)
 6.26 (sediments average, Kayal & Connell 1990)
 8.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 7.0 (Rotterdam Harbor sediment 4.6% OC, batch sorption equilibrium, Hegeman et al. 1995)
 6.00, 6.28, 6.17; 5.81 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island; quoted lit., McGroddy & Farrington 1995)
 5.93 (Aldrich humic acid, Ozretich et al. 1995)
 6.54 (10°C), 6.46, 6.60 (20°C), 6.14 (35°C), 6.07, 6.09 (45°C) (log K_{DOC} - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
 6.30 (20°C, log K_{POC} - particulate organic material from lake, Lüers & ten Hulscher 1996)
 6.27; 6.30 (humic acid, HPLC- k' correlation; quoted lit., Nielsen et al. 1997)
 5.72, 5.89, 5.51 (pH 5, 6.5, 8, humic acid from sediments of River Arno, De Paolis & Kukkonen 1997)
 4.81, 4.87, 4.49 (pH 5, 6.5, 8, fulvic acid from sediments of River Arno, De Paolis & Kukkonen 1997)
 5.54, 5.59, 5.37 (pH 5, 6.5, 8, HA + FA extracted from sediments of River Arno, De Paolis & Kukkonen 1997)
 5.51, 5.74, 5.68 (pH 5, 6.5, 8, HA extracted from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)
 4.93, 4.84, 4.85 (pH 5, 6.5, 8, FA extracted from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)
 5.66, 5.46, 5.60 (pH 5, 6.5, 8, HA + FA from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)
 5.22, 5.46, 5.60 (pH 5, 6.5, 8, HA extracted from water of River Arno, De Paolis & Kukkonen 1997)
 4.67, 4.80, 4.45 (pH 5, 6.5, 8, FA extracted from water of River Arno, De Paolis & Kukkonen 1997)
 5.21, 5.29, 5.18 (pH 5, 6.5, 8, HA + FA extracted from water of River Arno, De Paolis & Kukkonen 1997)
 4.62, 4.52, 4.61 (pH 5, 6.5, 8, FA extracted from water of Tyrrhenian Sea, De Paolis & Kukkonen 1997)

- 5.99 (5.92–6.04), 5.53 (5.43–5.61) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
- 5.25–6.18 (Lake Michigan sediment, Kukkonen & Landrum 1998)
- 5.48–5.69, 5.56, 5.55, 5.49, 5.30 (log K_{DOC} : humic acid from Lake Hohlohsee in Black Forest, soil leachate, fulvic acid from brown coal-derived production effluent, fulvic acid from groundwater, fulvic acid from effluent of a waste water plant near Karlsruhe, Haitzer et al. 1999)
- 5.53 (Clay Creek sediment with organic matter content 0.45%, Bott & Standley. 2000)
- 6.23 (sediment: organic carbon OC -0.5%, average, Delle Site 2001)
- 6.39–8.17; 6.30–8.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 3.12; 6.67, 6.58, 6.79 (20°C, batch equilibrium method, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
- 6.15; 6.34 (Plym river sediment; plym sea sediment, batch equilibrium-LSC, Turner & Rawling 2002)
- 6.49; 6.31 (Carnon river sediment; Carnon sea sediment, batch equilibrium-LSC, Turner & Rawling 2002)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

- Volatilization: aquatic fate rate of 300 h^{-1} with $t_{1/2} = 22$ h (Callahan et al. 1979);
 half-lives predicted by one compartment model: $t_{1/2} = 140$ h in river water, $t_{1/2} = 350$ h in eutrophic pond, $t_{1/2} = 700$ h in eutrophic lake and oligotrophic lake (Smith et al. 1978);
 calculated $t_{1/2} = 1500$ h for a river of 1-m deep with water velocity of 0.5 m s^{-1} and wind velocity of 1 m/s (Southworth 1979; Herbes et al. 1980);
 sublimation rate constant from glass surface of $< 1 \times 10^{-5} \text{ s}^{-1}$ was measured at 24°C at an airflow rate of 3 L/min (Cope & Kalkwarf 1987).
- Photolysis: photolysis $t_{1/2} = 2$ h in methanol solution when irradiated at 254 nm (Lu et al. 1977);
 $k = 0.58 \text{ h}^{-1}$ for winter at midday at 40°N latitude (Smith et al. 1978);
 direct photochemical transformation $t_{1/2}(\text{calc}) = 0.54$ h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis $t_{1/2} = 3.2$ d and 13 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)
- $k(\text{aq.}) = 2.8 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 1\text{--}2$ h (Callahan et al. 1979)
 photolytic $t_{1/2}(\text{aq}) = 0.53$ h (quoted of EPA Report 600/7-78-074, Haque et al. 1980)
 $k = 1.30 \text{ h}^{-1}$ (Zepp 1980)
- half-lives predicted by one compartment model: $t_{1/2} = 3.0$ h in river water based on the photolysis rates estimated for summer sunlight, $t_{1/2} = 7.5$ h in eutrophic pond or eutrophic lake, and $t_{1/2} = 1.5$ h in oligotrophic lake (Smith et al. 1978; quoted, Harris 1982)
- $k = 2.8 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 1\text{--}2$ h (Callahan et al., 1979)
 calculated direct photolysis $k = 3.86 \times 10^{-4} \text{ s}^{-1}$ in late January with $t_{1/2} = 0.69$ h in pure water at 366 nm and in sunlight at 23–28°C and $k = 1.05 \times 10^{-5} \text{ s}^{-1}$ in mid-December with $t_{1/2} = 1.1$ h at 313 nm with 1–20% acetonitrile as cosolvent in filter-sterilized natural water (Mill et al. 1981)
 $t_{1/2} = 0.37\text{--}1.1$ h, based on estimated photolysis half-life in air (Howard et al. 1991)
 sunlight photolysis $t_{1/2} = 0.045$ d for mid-December (Mill & Mabey 1985)
 half-lives on different atmospheric particulate substrates (approx. 25 $\mu\text{g/g}$ on substrate): $t_{1/2} = 4.7$ h on silica gel, $t_{1/2} = 1.4$ h on alumina and $t_{1/2} = 31$ h on fly ash (Behymer & Hites 1985)
 ozonation rate constant $k < 6.1 \times 10^{-4} \text{ m/s}$ was measured at 24°C with $[\text{O}_3] = 0.16$ ppm and light intensity of 1.3 kW/m^2 (Cope & Kalkwarf 1987)
 first order daytime decay $k = 0.0090 \text{ min}^{-1}$ for soot particles loading of 1000–2000 ng/mg and $k = 0.0211 \text{ min}^{-1}$ with 30–350 ng/mg loading (Kamens et al. 1988)
 photodegradation half-life was found ranging from 1 h in summer to days in winter (Valerio et al. 1991)
 photodegradation $k = 0.0322 \text{ min}^{-1}$ and $t_{1/2} = 0.35$ h in ethanol-water (3:7, v/v) solution for initial concentration of 2.5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
 pseudo-first-order direct photolysis $k(\text{exptl}) = 0.0322 \text{ min}^{-1}$ with the calculated $t_{1/2} = 0.35$ h and the predicted $t_{1/2} = 0.0416 \text{ min}^{-1}$ calculated by QSPR method, in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
 direct photolysis $t_{1/2}(\text{obs}) = 0.50$ h, $t_{1/2}(\text{calc}) = 0.57$ h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001)

photochemical degradation under atmospheric conditions: $k = (1.18 \pm 0.50) \times 10^{-4} \text{ s}^{-1}$ and $t_{1/2} = (1.63 \pm 0.48) \text{ h}$ in diesel particulate matter, rate constant $k = (3.09 \pm 0.23) \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = (6.22 \pm 0.51) \text{ h}$ in diesel particulate matter/soil mixture, and $t_{1/2} = 0.35$ to 1.62 h in various soil components using a 900-W photo-irradiator as light source; rate constant $k = (2.92 \pm 0.20) \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = (6.59 \pm 0.49) \text{ h}$ in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation $k = 2.1 \times 10^{-3} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$t_{1/2} > 340 \text{ h}$ in river water, eutrophic pond or lake and oligotrophic lake, half-lives predicted by one compartment model (Smith et al. 1978)

$k(\text{aquatic fate rate}) = 1680 \text{ M}^{-1} \text{ s}^{-1}$, with half-life of 96 h (Callahan et al. 1979)

$t_{1/2} = 1500 \text{ h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N , midday, midsummer (Zepp & Schlotzhauer 1979)

$k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $2 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k = 0.62 \times 10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with O_3 in water at pH 7 and 25°C with $t_{1/2} = 1.0 \text{ s}$ in presence of 10^{-4} M of ozone at pH 7 (Butković et al. 1983)

$k(\text{aq.}) = 3.6 \times 10^{-4} \text{ h}^{-1}$ with $t_{1/2} = 0.5 \text{ h}$ under natural sunlight conditions; $k(\text{aq.}) = 1.9 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ with $t_{1/2} = 4.3 \text{ d}$ free-radicals oxidation in air-saturated water (NRCC 1983)

photooxidation $t_{1/2} = 0.428\text{--}4.28 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{\text{HO}\cdot}(\text{calc}) = 1 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ with hydroxyl radical in aqueous solutions (Haag & Yao 1992)

Hydrolysis: not hydrolyzable (Mabey et al. 1982; Howard et al. 1991).

Biodegradation:

$t_{1/2} > 10000 \text{ h}$ (quoted, Smith et al. 1978)

$k = 0.2\text{--}0.9 \mu\text{mol}^{-1} \text{ mg}^{-1}$ for bacterial protein (Callahan et al. 1979)

$k = 3.4 \times 10^{-4} \text{ h}^{-1}$ with $t_{1/2} = 83 \text{ h}$ for mixed bacterial populations in stream sediment (NRCC 1983)

$k < 3 \times 10^{-5} \text{ h}^{-1}$ with $t_{1/2} > 2.5 \text{ yr}$; $k < 3.0 \times 10^{-5} \text{ h}^{-1}$ with $t_{1/2} > 2.5 \text{ yr}$ for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)

$k = 3.5 \times 10^{-5} \text{ h}^{-1}$ estimated in water and soil (Ryan & Cohen 1986)

$t_{1/2}(\text{aq. aerobic}) = 57 \text{ d}$ to 1.45 yr at $10\text{--}30^\circ\text{C}$, soil die-away test (Coover & Sims 1987; quoted, Howard et al. 1991); $k = 0.0022 \text{ d}^{-1}$ with $t_{1/2} = 309 \text{ d}$ for Kidman sandy loam and $k = 0.0030 \text{ d}^{-1}$ with $t_{1/2} = 229 \text{ d}$ for McLaren sandy loam all at -0.33 bar soil moisture (Park et al. 1990)

$t_{1/2}(\text{aq. anaerobic}) = 228 \text{ d}$ to 5.8 yr , based on estimated unacclimated aqueous aerobic biodegradation half-life (Coover & Sims 1987; quoted, Howard et al. 1991).

Biotransformation: estimated to be $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 49 \text{ h}^{-1}$; $k_2 = 0.010 \text{ h}^{-1}$ (bluegill sunfish, Spacie et al. 1983)

$k_1 = 131.1 \text{ mL g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0033 \text{ h}^{-1}$ (4°C , *P. hoyi*, Landrum 1988)

$k_1 = 81.3 \text{ h}^{-1}$; $k_2 = 0.014 \text{ h}^{-1}$ ($10\text{--}20^\circ\text{C}$, *H. limbata*, Landrum & Poore 1988)

$k_1 = 16.8 \text{ h}^{-1}$; $k_2 = 0.0016 \text{ h}^{-1}$ (4°C , *P. hoyi*, Landrum & Poore 1988)

$k_1 = 87.8 \text{ h}^{-1}$; $k_2 = 0.012 \text{ h}^{-1}$ (4°C , *S. heringianus*, quoted, Landrum & Poore 1988)

$k_1 = 112.0 \text{ h}^{-1}$; $k_2 = 0.013 \text{ h}^{-1}$ (4°C , *Mysis relicta*, quoted, Landrum & Poore 1988)

$k_1 = 75.9 \text{ mL g}^{-1} \text{ h}^{-1}$ (*Pontoporeia hoyi*, Evans & Landrum 1989)

$k_1 = 39.9 \text{ mL g}^{-1} \text{ h}^{-1}$ (*Mysis relicta*, Evans & Landrum 1989)

$k_2 = 0.0017 \text{ h}^{-1}$ (*Amphipods*, Evans & Landrum 1989)

$k_2 = 0.0047 \text{ h}^{-1}$ (*Mysids*, Evans & Landrum 1989)

$k_1 = 0.11\text{--}0.36 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0032 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.37\text{--}1.1 \text{ h}$, based on estimated photolysis half-life (Lyman et al. 1982; quoted, Howard et al. 1991);

half-lives under simulated atmospheric conditions: $t_{1/2} = 5.30 \text{ h}$ in simulated sunlight, $t_{1/2} = 0.58 \text{ h}$ in simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 0.62 \text{ h}$ in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

$t_{1/2} = 14 \text{ h}$ with a steady-state concn of tropospheric ozone of $2 \times 10^{-9} \text{ M}$ in clean air (Butković et al. 1983);

- photooxidation $t_{1/2} = 0.428\text{--}4.28$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- $t_{1/2} = 0.5$ h for adsorption on soot particles in an outdoor Teflon chamber with an estimated $k = 0.0234 \text{ min}^{-1}$ at $1 \text{ cal cm}^{-2} \text{ min}^{-1}$, $10 \text{ g m}^{-3} \text{ H}_2\text{O}$ and 20°C (Kamens et al. 1988).
- Surface Water: $t_{1/2} = 2$ h in methanol solution irradiated at 254 nm (Lu et al. 1977);
- half-lives predicted by one compartment model: $t_{1/2} > 340$ h in river water, eutrophic pond or lake and oligotrophic lake (Smith et al. 1978);
- very slow, not an important process (Callahan et al. 1979);
- computed near-surface half-life for direct photochemical transformation of a natural water body $t_{1/2} = 0.54$ h at latitude 40°N , midday, midsummer, and direct photolysis, $t_{1/2} = 3.2$ d (no sediment-water partitioning) and $t_{1/2} = 13$ d (with sediment-water partitioning) in a 5-m deep inland water body (Zepp & Schlottzauer 1979);
- $t_{1/2} = 0.37\text{--}1.1$ h, based on photolysis half-life in water (Lyman et al. 1982; quoted, Howard et al. 1991);
- $t_{1/2} = 1.0$ s in presence of 10^{-4} M of ozone at pH 7 (Butković et al. 1983);
- $t_{1/2} = 4.3$ d free-radical oxidation in air-saturated water (NRCC 1983);
- $t_{1/2} = 0.045$ d under mid-December sunlight (Mill & Mabey 1985);
- photolysis $t_{1/2} = 0.35$ h in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
- Groundwater: $t_{1/2} = 2736\text{--}25440$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Sediment: uptake clearance from sediment $k = (0.0023 \pm 0.001) \text{ g of dry sediment} \cdot \text{g}^{-1} \text{ of organism} \cdot \text{h}^{-1}$ for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C (Landrum 1989);
- desorption $t_{1/2} = 19.5$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
- Soil: $t_{1/2} > 2$ d (Sims & Overcash 1983; quoted, Bulman et al. 1987);
- $t_{1/2} = 347$ d for 5 mg/kg treatment and $t_{1/2} = 218$ d for 50 mg/kg treatment (Bulman et al. 1987);
- biodegradation $k = 0.002 \text{ d}^{-1}$ with $t_{1/2} = 309$ d for Kidman sandy loam soils and $k = 0.0030 \text{ d}^{-1}$ with $t_{1/2} = 229$ d for McLaurin sandy loam soils (Park et al. 1990);
- $t_{1/2} = 1368\text{--}12720$ h, based on aerobic soil dieaway test data at $10\text{--}30^\circ\text{C}$ (Groenewegen & Stolp 1976; Coover & Sims 1987; quoted, Howard et al. 1991);
- $t_{1/2} > 50$ d (Ryan et al. 1988);
- $t_{1/2} = 0.3$ to > 300 wk, 8.2 yr (literature, Luddington soil, Wild et al. 1991).
- Biota: depuration $t_{1/2} = 18$ d by oysters (Lee et al. 1978; quoted, Verschueren 1983);
- $t_{1/2} = 67$ h in bluegill sunfish (Spacie et al. 1983);
- depuration $t_{1/2} = 52$ h in *s. heringianus* (Frank et al. 1986);
- calculated half-lives in different tissues of sea bass: $t_{1/2} = 12.4$ d for fat, $t_{1/2} = 6.5$ d for kidney, $t_{1/2} = 5.1$ d for kidney, $t_{1/2} = 5.1$ d for intestine, $t_{1/2} = 4.8$ d for gallbladder, $t_{1/2} = 4.5$ d for spleen, $t_{1/2} = 2.9$ d for muscle, $t_{1/2} = 2.4$ d for whole body, $t_{1/2} = 2.3$ d for gonads, $t_{1/2} = 2.3$ d for gills, and $t_{1/2} = 2.2$ d for liver (Lemaire et al. 1990);
- elimination $t_{1/2} = 4.8\text{--}16$ d from mussel *Mytilus edulis*; $t_{1/2} = 7$ d from polychaete *Abarenicola pacifica*, $t_{1/2} = 21.7$ d from Oyster, $t_{1/2} = 8.0$ d from clam *Mercenaria mercenaria*, $t_{1/2} = 8$ d from clam *Rangia cuneata* (quoted, Meador et al. 1995);
- $t_{1/2} = 15\text{--}17$ d for blue mussel *Mytilus edulis* in 32-d exposure laboratory studies (Magnusson et al. 2000).

TABLE 4.1.1.43.1

Reported aqueous solubilities and Henry's law constants of benzo[a]pyrene at various temperatures

$$\ln x = A + B/(T/K) + C \cdot \ln (T/K)$$

(1)

Aqueous solubility						Henry's law constant	
May et al. 1983		Velapoldi et al. 1983		Whitehouse 1984		ten Hulscher et al. 1992	
generator column-HPLC		generator column-fluorescence		generator column-HPLC		gas stripping-HPLC/fluorescence	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	Pa m ³ /mol
10	0.00056	10	0.00061	8.0	0.00066	10.0	0.022
15	0.00080	15	0.00082	12.4	0.00077	20.0	0.034
20	0.00114	20	0.00113	16.7	0.00094	35.0	0.074
25	0.00162	25	0.00158	20.9	0.00116	40.1	0.092
30	0.00229	30	0.00224	25.0	0.00154	45.0	0.110
						55.0	0.239
		eq. 1	x				
		A	-677.4109				ln K _{AW} = -ΔH/RT + ΔS/R
		B	23963.0				R = 8.314 Pa m ³ mol ⁻¹ K ⁻¹
		C	100.767				ΔS/R 11.90
							ΔH/R 4690.88
		ΔH _{sol} /(kJ mol ⁻¹) = 50.6					
		at 25°C					enthalpy of volatilization:
							ΔH/(kJ·mol ⁻¹) = 39 ± 3
							entropy of volatilization, ΔS :
							TΔS/(kJ·mol ⁻¹) = 29 ± 3
							at 20°C

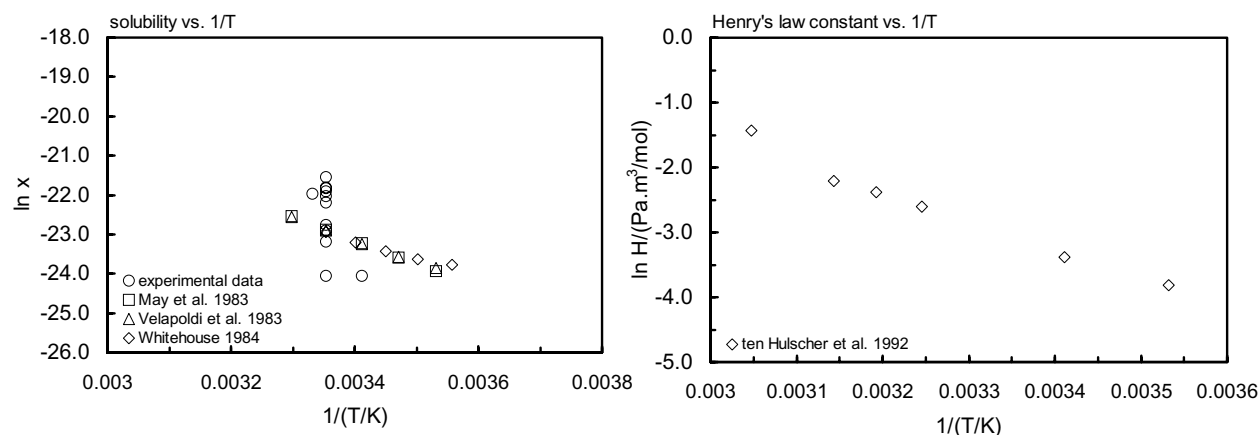
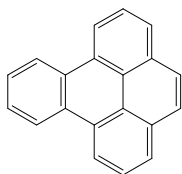


FIGURE 4.1.1.43.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for benzo[a]pyrene.

4.1.1.44 Benzo[e]pyrene



Common Name: Benzo[e]pyrene

Synonym: B[e]P, 4,5-benzopyrene

Chemical Name: 4,5-benzopyrene

CAS Registry No: 192-97-2

Molecular Formula: $C_{20}H_{12}$

Molecular Weight: 252.309

Melting Point ($^{\circ}\text{C}$):

181.4 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

311 (Lide 2003)

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

262.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

16.57 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

42.30 (differential scanning calorimetry, Hinckley et al. 1990)

36.5 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 0.0292 (mp at 181.4°C)

0.010 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0035 (27°C , shake flask-nephelometry, Davis et al. 1942)

0.00732 (shake flask-UV/fluorescence, Barone et al. 1967)

0.00014, 0.000172, 0.0000252 (HPLC-relative retention correlation, different stationary and phases, Locke 1974)

0.0050* (23°C , shake flask-fluorescence, measured range $8.6\text{--}31.7^{\circ}\text{C}$, Schwarz 1977)

0.00732, 0.004; 0.0063 (quoted values; lit. mean, Pearlman et al. 1984)

$\log S_L$ (mol/L) = $-1.398 - 866.8/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -11.8754 - 2916.84/(T/K)$; temp range $5\text{--}50^{\circ}\text{C}$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

7.40×10^{-7} (Knudsen effusion method, extrapolated, Murray et al. 1974)

$\log (P/\text{mmHg}) = 9.736 - 6220/(T/K)$; temp range $359\text{--}423 \text{ K}$ (Knudsen effusion method, Murray et al. 1974)

7.58×10^{-7} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 11.7417 - 6220/(T/K)$; temp range $358\text{--}423 \text{ K}$ (Antoine eq., Stephenson & Malanowski 1987)

3.20×10^{-7} , 1.28×10^{-5} (20°C , literature solid P_s , converted to supercooled liquid P_L with ΔS_{fus} Bidleman & Foreman 1987)

8.59×10^{-5} (P_{GC} , GC-RT correlation with p,p' -DDT as reference standard, Hinckley et al. 1990)

2.53×10^{-5} , 1.02×10^{-5} (supercooled liquid values P_L , converted from literature P_s with different ΔS_{fus} values, Hinckley et al. 1990)

$\log (P_L/\text{Pa}) = 11.11 - 4803/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)

1.29×10^{-5} (supercooled liquid values P_L , calculated from Yamasaki et al. 1984, Finizio et al. 1997)

1.78×10^{-5} ; 1.78×10^{-6} (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.15 - 5333/(T/K)$ (solid, Passivirta et al. 1999)

$$\log (P_L/Pa) = 10.14 - 4467/(T/K) \text{ (supercooled liquid, Passivirta et al. 1999)}$$

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

$$0.02 \quad (\text{calculated-P/C, Mackay et al. 1992})$$

$$\log [H/(\text{Pa m}^3/\text{mol})] = 11.64 - 3660/(T/K) \text{ (Passivirta et al. 1999)}$$

Octanol/Water Partition Coefficient, $\log K_{ow}$:

$$6.44 \quad (\text{calculated-MCI } \chi \text{ as per Rekker \& De Kort 1979, Ruepert et al. 1985})$$

$$7.40 \quad (\text{calculated-}K_{OC}, \text{Broman et al. 1991})$$

$$6.44 \quad (\text{TLC retention time correlation, De Voogt et al. 1990})$$

$$6.44 \quad (\text{recommended, Sangster 1993})$$

$$6.10 \quad (\text{quoted, Meador et al. 1995})$$

$$5.68 \quad (\text{calculated, Passivirta et al. 1999})$$

Octanol/Air Partition Coefficient, $\log K_{OA}$:

$$11.13 \quad (\text{calculated, Finizio et al. 1997})$$

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

$$7.20 \quad (\text{Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991})$$

$$4.00 \quad (\text{predicted dissolved } \log K_{OC}, \text{Broman et al. 1991})$$

$$6.11\text{--}7.90; 7.20\text{--}8.30 \quad (\text{range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001})$$

$$5.84; 6.12, 6.11, 6.62 \quad 20^\circ\text{C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss \& Wilcke 2001})$$

Environmental Fate Rate Constants or Half-Lives:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$$k_1 = 0.13\text{--}0.36 \text{ mg g}^{-1} \text{ h}^{-1}; k_2 = 0.0031 \text{ h}^{-1} \text{ (freshwater oligochaete from sediment, Van Hoof et al. 2001)}$$

Half-Lives in the Environment:

Air: half-lives under simulated atmospheric conditions: $t_{1/2} = 21.10 \text{ h}$ in simulated sunlight, $t_{1/2} = 5.38 \text{ h}$ in simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 7.6 \text{ h}$ in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 6.9\text{--}14.4 \text{ d}$ from mussel *Mytilus edulis*; $t_{1/2} = 30.1 \text{ d}$ from Oyster, $t_{1/2} = 4.7 \text{ d}$ from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.44.1
Reported aqueous solubilities of benzo[e]pyrene at various temperatures

Schwarz 1977

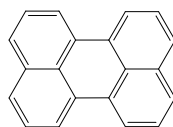
shake flask-fluorescence

$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
8.6	3.25×10^{-3}
14.0	3.58×10^{-3}
17.0	4.44×10^{-3}
17.5	3.94×10^{-3}

TABLE 4.1.1.44.1 (*Continued*)

Schwarz 1977	
shake flask-fluorescence	
<i>t</i> /°C	<i>S</i> /g·m ⁻³
20.2	4.79 × 10 ⁻³
23.2	5.35 × 10 ⁻³
23.0	5.07 × 10 ⁻³
29.2	6.38 × 10 ⁻³
29.2	6.48 × 10 ⁻³
31.7	6.81 × 10 ⁻³
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 25.56$	
at 25°C	

4.1.1.45 Perylene



Common Name: Perylene

Synonym: peri-dinaphthalene

Chemical Name: perylene

CAS Registry No: 198-55-0

Molecular Formula: $C_{20}H_{12}$

Molecular Weight: 252.309

Melting Point ($^{\circ}C$):

277.76 (Lide 2003)

Boiling Point ($^{\circ}C$):

503 (Pearlman et al. 1984)

Density (g/cm^3 at $25^{\circ}C$):

1.35 (Lide 2003)

Molar Volume (cm^3/mol):

186.9 ($25^{\circ}C$, calculated-density)

222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

262.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.51 (quoted, Tsonopoulos & Prausnitz 1971)

31.753 (Ruelle & Kesselring 1997)

31.88 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

42.68 (quoted, Tsonopoulos & Prausnitz 1971)

57.4 (Passivirta et al. 1999)

67.87, 43.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.00331 (mp at $277.76^{\circ}C$)

0.00268 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0005 ($27^{\circ}C$, shake flask-nephelometry Davis et al. 1942)

< 0.0005 (Weimer & Prausnitz 1965)

0.00011 ($20^{\circ}C$, shake flask-UV, Eisenbrand & Baumann 1970)

0.0004 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0003 (average lit. value, Pearlman et al. 1984)

0.0007 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)

$\log [S_L/(mol/L)] = -0.306 - 1662/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

$\log (P/mmHg) = 13.95 - 7260/(T/K)$; temp range $110-180^{\circ}C$ (Knudsen effusion method, Hoyer & Peperle 1958)

5.31×10^{-9} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 13.075 - 7260/(T/K)$; temp range $383-453\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.9379 - 7210/(T/K)$; temp range $383-516\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

7.00×10^{-7} (quoted, Riederer 1990)

$1.84 \times 10^{-8*}$ (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range $118-210^{\circ}C$, Oja & Suuberg 1998)

$\ln (P/Pa) = 35.702 - 15955/(T/K)$; temp range $391-424\ K$ (Clausius-Clapeyron eq., Knudsen effusion, Oja & Suuberg 1998)

1.40×10^{-8} ; 5.22×10^{-6} (quoted solid P_s from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F , Passivirta et al. 1999)

$\log (P_s/Pa) = 12.53 - 6074/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.53 - 4414/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

4.88×10^{-6} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -4694/(T/K) + 10.43$; $\Delta H_{vap} = -89.9 \text{ kJ}\cdot\text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C and the report temperature dependence equations):

0.440 (calculated-P/C, Riederer 1990)

$\log [H/(\text{Pa m}^3/\text{mol})] = 9.84 - 2752/(T/K)$, (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.30, 5.10 (HPLC-RV predicted, Brooke et al. 1986)

5.30 (HPLC-RV measured, Brooke et al. 1986)

5.82 (HPLC-RT correlation, Wang et al. 1986)

6.25 (recommended, Sangster 1989, 1994)

6.40 (Bayona et al. 1991)

5.82 (recommended, Hansch et al. 1995)

6.50 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

6.25; 6.53 (quoted lit.; calculated, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.86, 3.73 (*Daphnia pulex*, kinetic estimation, Southworth et al. 1978)

4.36 (activated sludge, Freitag et al. 1984)

3.30, 4.36, < 1.0 (algae, activated sludge, fish, Klein et al. 1984)

3.85 (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

3.30, 4.36, < 1.0 (algae, activated sludge, fish, Freitag et al. 1985)

3.86 (*Daphnia magna*, Newsted & Giesy 1987)

1.196, -0.398 (*Polychaete sp.*, *Capitella capitata*, Bayona et al. 1991)

Sorption Partition Coefficient, $\log K_{oc}$ at 25°C or as indicated:

6.39–7.93 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.88; 6.73, 6.63, 6.76 (20°C , batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

6.30; 5.89; 4.15–6.38 (calculated- K_{ow} ; calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)

6.05 at pH 4, 5.98 at pH 7, 5.71 at pH 10 in 0.001 M NaCl; 6.01 at pH 4, 5.95 at pH 7, 5.29 at pH 10 in 0.01 M NaCl; 5.98 at pH 4, 5.67 at pH 7, 4.86 at pH 10 in 0.1 M NaCl; 5.97 at pH 4, 5.61 at pH 7, 4.78 at pH 10 in 1 mM Ca^{2+} in 0.1 M total ionic strength solutions (shake flask/fluorescence, dissolved humic substances-humic acid; Schlautman & Morgan 1993)

5.17 at pH 4 in 0.001 M NaCl; 5.14 at pH 4 in 0.01 M NaCl; 5.08 at pH 4 in 0.1 M NaCl; 5.11 at pH 4 in 1 mM Ca^{2+} in 0.1 M total ionic strength solutions (shake flask/fluorescence, dissolved humic substances-fulvic acid; Schlautman & Morgan 1993a, b)

5.82 at pH 4, < 4.49 at pH 7, < 4.18 at pH 10 in 0.001 M NaCl; 5.65 at pH 4, < 4.46 at pH 7, < 3.85 at pH 10 in 0.01 M NaCl; 5.67 at pH 4, < 4.17 at pH 7, < 3.78 at pH 10 in 0.1 M NaCl; 5.74 at pH 4, 5.02 at pH 7, 4.43 at pH 10 in 1 mM Ca^{2+} in 0.1 M total ionic strength solutions (shake flask/fluorescence, adsorbed humic substances-humic acid; Schlautman & Morgan 1993b)

< 3.48 at pH 4 in 0.001 M NaCl; < 3.30 at pH 4 in 0.01 M NaCl; < 3.48 at pH 4 in 0.1 M NaCl; < 3.48 at pH 4 in 1 mM Ca^{2+} in 0.1 M total ionic strength solutions (shake flask/fluorescence, adsorbed humic substances-fulvic acid; Schlautman & Morgan 1993b)

6.00 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: sublimation $k < 1 \times 10^{-5} \text{ s}^{-1}$ from glass surface was measured at 24°C at an airflow rate of 3 L/min (Cope & Kalkwarf 1987).

Photolysis:

half-lives on different atmospheric particulate substrates (appr. 25 $\mu\text{g/g}$ on substrate): $t_{1/2} = 3.9 \text{ h}$ on silica gel, $t_{1/2} = 1.2 \text{ h}$ on alumina and $t_{1/2} = 35 \text{ h}$ on fly ash (Behymer & Hites 1985)

ozonation $k < 4.7 \times 10^{-5} \text{ m/s}$ was measured from glass surface at 24°C with $[\text{O}_3] = 0.16 \text{ ppm}$ and light intensity of 1.3 kW/m^2 (Cope & Kalkwarf 1987)

photodegradation $k = 0.0152 \text{ min}^{-1}$ and $t_{1/2} = 0.78 \text{ h}$ in ethanol-water (2:3, v/v) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)

$k(\text{expt}) = 0.0152 \text{ min}^{-1}$ the pseudo-first-order rate constant with the calculated $t_{1/2} = 0.78 \text{ h}$ and the predicted $k = 0.0406 \text{ min}^{-1}$, calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);

$t_{1/2} = 0.53 \text{ h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001)

Photodegradation $k = 4.4 \times 10^{-4} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 752 \text{ h}^{-1}$; $k_2 = 0.139 \text{ h}^{-1}$ (*Daphnia pulex*, Southworth et al. 1978)

$\log k_1 = 2.88 \text{ h}^{-1}$; $\log k_2 = -0.86 \text{ h}^{-1}$ (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 0.12\text{--}0.38 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0034 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: direct photolysis $t_{1/2} = 0.53 \text{ h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis $t_{1/2} = 0.78 \text{ h}$ (reported in units of minutes) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: elimination half-lives: $t_{1/2} = 2.0 \text{ d}$ from rainbow trout, $t_{1/2} = 26.2 \text{ d}$ from clam *Mya arenaria*, $t_{1/2} = 6.3\text{--}13.3 \text{ d}$ from mussel *Mytilus edulis*; $t_{1/2} = 9.2 \text{ d}$ from Oyster, $t_{1/2} = 1.2 \text{ d}$ from shrimp, $t_{1/2} = 5.7 \text{ d}$ from polychaete *Nereis virens*, $t_{1/2} = 8.0 \text{ d}$ from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

TABLE 4.1.1.45.1

Reported vapor pressures of perylene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Hoyer & Peperle 1958		Oja & Suuberg 1998	
effusion		Knudsen effusion	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
data presented by equation		124.10	0.0114
eq. 1	P/mmHg	127.37	0.0164
A	13.95	131.82	0.0249
B	7260	135.96	0.0373

TABLE 4.1.1.45.1 (Continued)

Hoyer & Peperle 1958		Oja & Suuberg 1998	
effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
for temp range 110–180°C		141.87	0.0638
mp/°C	270.5–273.5	mp/K	551
$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 140.1$		eq. 1a	P/Pa
		A	35.702
		B	15955
		for temp range 391–424 K	
		$\Delta H_{\text{sub}}/(\text{kJ/mol}) = 132.6$	

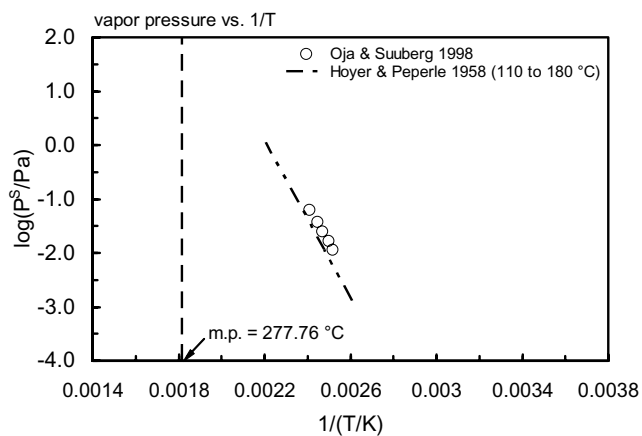
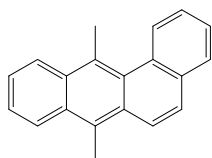


FIGURE 4.1.1.45.1 Logarithm of vapor pressure versus reciprocal temperature for perylene.

4.1.1.46 7,12-Dimethylbenz[a]anthracene



Common Name: 7,12-Dimethylbenz[a]anthracene

Synonym: 7,12-dimethylbenz[a]anthracene, 9,10-dimethyl-1,2-benzanthracene, 7,12-dimethylbenzanthracene

Chemical Name: 7,12-dimethylbenz[a]anthracene

CAS Registry No: 57-97-6

Molecular Formula: $C_{20}H_{16}$

Molecular Weight: 256.341

Melting Point ($^{\circ}C$):

122.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

245.8 (Ruelle & Kesselring 1997)

292.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

104.56 (Kelley & Rice 1964)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.09 (Kelley & Rice 1964)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.111 (mp at $122.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.043 ($27^{\circ}C$, shake flask-nephelometry, Davis et al. 1942)

0.061 (shake flask-fluorescence, Mackay & Shiu 1977)

0.053 ($24^{\circ}C$, shake flask-nephelometry, Hollifield 1979)

0.025 ($24^{\circ}C$, shake flask-LSC, Means et al. 1979)

0.0244 (shake flask-LSC, Means et al. 1980b)

0.043, 0.061, 0.053; 0.054 (quoted lit. values; lit. mean, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.73×10^{-7} (solid vapor pressure, extrapolated, effusion method, Kelley & Rice 1974)

3.70×10^{-6} (extrapolated, supercooled liquid value P_L , Kelley & Rice 1974)

$\log(P_s/mmHg) = 15.108 - 7051/(T/K)$; temp range: $106-122^{\circ}C$ (effusion method, Kelley & Rice 1964)

$\log(P_L/mmHg) = 12.232 - 5987/(T/K)$; temp range: $122-135^{\circ}C$ (effusion method, Kelley & Rice 1964)

3.84×10^{-7} (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 14.233 - 7051/(T/K)$; temp range 379–396 K (Antoine eq.-I, Stephenson & Malanowski 1987)

6.78×10^{-6} (extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.70417 - 5629.911/(T/K)$; temp range 379–390 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 11.357 - 5897/(T/K)$, temp range 396–408 K (Antoine eq.-III, Stephenson & Malanowski 1987)

6.38×10^{-6} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -4643/(T/K) + 10.38$; $\Delta H_{vap} = -88.9 kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($Pa m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.98 (shake flask-LSC, concn. ratio, Means et al. 1979)

5.80 (shake flask-LSC, Means et al. 1980b)

6.16	(UNIFAC activity coeff., Banerjee & Howard 1988)
5.80	(recommended, Sangster 1989)
5.89	(recommended, Sangster 1993)
5.80	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.68	(average of 3 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1979)
5.37	(average of 12 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1980b)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 0.32\text{--}3.2$ h estimated, based on estimated rate constant for the reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991); photooxidation $t_{1/2}(\text{aq.}) = 1.57\text{--}157$ yr estimated, based on measured rate constant for the reaction with singlet oxygen in benzene (Stevens et al. 1974; quoted, Howard et al. 1991).

Biodegradation: biodegradation $k = 0.0339\text{ d}^{-1}$ with $t_{1/2} = 20$ d for Kidman sandy loam soil and $k = 0.0252\text{ d}^{-1}$ with $t_{1/2} = 28$ d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2}(\text{aq. aerobic}) \sim 480\text{--}672$ h, based on aerobic soil die-away test data (Sims 1990; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) \sim 1920\text{--}2688$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.32\text{--}3.2$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

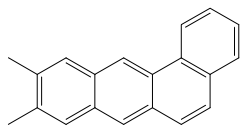
Surface water: $t_{1/2} = 480\text{--}672$ h, based on aerobic soil die-away test data (Howard et al. 1991).

Groundwater: $t_{1/2} = 960\text{--}1344$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: biodegradation rate constant $k = 0.0339\text{ d}^{-1}$ with $t_{1/2} = 20$ d for Kidman sandy loam soil and $k = 0.0252\text{ d}^{-1}$ with $t_{1/2} = 28$ d for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} \sim 480\text{--}672$ h, based on aerobic soil die-away test data (Howard et al. 1991).

4.1.1.47 9,10-Dimethylbenz[a]anthracene

Common Name: 9,10-Dimethylbenz[a]anthracene

Synonym:

Chemical Name: 9,10-dimethylbenz[a]anthracene

CAS Registry No: 56-56-4

Molecular Formula: C₂₀H₁₆

Molecular Weight: 256.341

Melting Point (°C):

122 (Yalkowsky et al. 1983; Ruelle & Kesselring 1997)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

245.8 (Ruelle & Kesselring 1997)

292.7 (calculated-Le Bas method at normal boiling point)

Entropy of Fusion, ΔS_{fus} (J/mol K):

54.81 (Kelley & Rice 1974)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.112 (mp at 122°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.0435 (27°C, shake flask-nephelometry, Davis et al. 1942)

0.0435 (recommended, Shaw 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):

log (P/mmHg) = 15.108 – 7051/(T/K); temp range: 106–135°C (effusion method, Kelley & Rice 1964)

log (P/mmHg) = 12.232 – 5897/(T/K) (liquid, effusion method, Kelley & Rice 1964)

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:

6.93 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient, log K_{OA}:

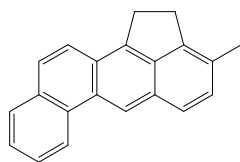
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:

Half-Lives in the Environment:

4.1.1.48 3-Methylcholanthrene



Common Name: 3-Methylcholanthrene

Synonym: 20-methylcholanthrene, 1,2-dihydro-3-methyl-benz[j]aceanthrylene

Chemical Name: 3-methylcholanthrene

CAS Registry No: 56-49-5

Molecular Formula: $C_{21}H_{16}$

Molecular Weight: 268.352

Melting Point ($^{\circ}C$):

180 (Bjørseth 1983)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.28 (Lide 2003)

Molar Volume (cm^3/mol):

247.8 (Ruelle & Kesselring 1997)

209.6 ($20^{\circ}C$, calculated-density)

296.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0301 (mp at $180^{\circ}C$)

0.003 (Mackay et al. 1980)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0015 (Weimer & Prausnitz 1965)

0.0029 (shake flask-fluorescence, Mackay & Shiu 1977)

0.00323 (shake flask-liquid scintillation counting, Means et al. 1980)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 13.168 - 6643/(T/K)$; temp range $128-152^{\circ}C$ (effusion method, Kelley & Rice 1964)

1.03×10^{-7} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 12.293 - 6643/(T/K)$; temp range $401-425 K$ (Antoine eq., Stephenson & Malanowski 1987)

1.48×10^{-6} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -4901/(T/K) + 10.61$; $\Delta H_{vap} = -93.8 kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($Pa m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.42 (shake flask-LSC, Means et al. 1980)

7.11 (calculated-f const., Valvani & Yalkowsky 1980)

6.69 (calculated-S and mp, Mackay et al. 1980)

7.11 (Hansch & Leo 1985)

6.45, 7.07 (calculated-UNIFAC, calculated-fragment const., Banerjee & Howard 1988)

6.75 ± 0.50 (recommended, Sangster 1989)

6.45 (recommended, Sangster 1993)

6.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

4.12 (*Daphnia magna*, McCarthy et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

6.09 (soil/sediment, sorption isotherm by batch equilibrium-LSC, Means et al. 1980b)
 6.25 (average of 14 soil/sediment samples, sorption isotherm by shake flask-LSC, Means et al. 1980)
 6.09, 6.10 (calculated-regression of K_p versus substrate properties, calculated- K_{OW} , Means et al. 1980)
 4.02 (soil, calculated- K_{OW} , Briggs 1981)
 6.18 (soil, calculated- K_{OW} , Means et al. 1982)
 5.07 (soil, calculated- K_{OW} , Chiou et al. 1983)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 0.317\text{--}3.17$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aerobic $t_{1/2} = 14616\text{--}33600$ h, based on mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991);
 anaerobic $t_{1/2} = 58464\text{--}134400$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.317\text{--}3.17$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 14616\text{--}33600$ h, based on mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991).

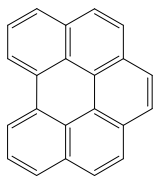
Groundwater: $t_{1/2} = 29232\text{--}672000$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 14616\text{--}33600$ h, based on estimated mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991).

Biota:

4.1.1.49 Benzo[ghi]perylene



Common Name: Benzo[ghi]perylene

Synonym: 1,12-benzoperylene, benzoperylene

Chemical Name: 1,12-benzoperylene

CAS Registry No: 191-24-2

Molecular Formula: $C_{22}H_{12}$

Molecular Weight: 276.330

Melting Point ($^{\circ}C$):

272.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

525 (Pearlman et al. 1984)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

233.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

277.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.365 (Ruelle & Kesselring 1997)

17.37 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

31.34, 43.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

31.4 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, $F = 0.00373$ (mp at $272.5^{\circ}C$))

0.039 (calculated, $\Delta S_{fus} = 31.4 J/mol K$, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00026 (shake flask-fluorescence, Mackay & Shiu 1977)

0.0007 (generator column-HPLC/fluor., Wise et al. 1981)

0.00083 (quoted, Pearlman et al. 1984)

0.000137 (generator column-HPLC/fluor., De Maagd et al. 1998)

$\log [S_L/(mol/L)] = -2.073 - 908.7/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.39×10^{-8} (Knudsen effusion method, Murray et al. 1974)

$\log (P/atm) = 9.519 - 6674/(T/K)$; temp range: 389–468 K (Knudsen effusion method, Murray et al. 1974)

1.33×10^{-8} ($20^{\circ}C$, estimated, Callahan et al. 1979)

6.69×10^{-7} (Yamasaki et al. 1984)

1.38×10^{-8} ; 7.51×10^{-9} (extrapolated-Antoine eq. I, II, Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 11.5247 - 6674/(T/K)$; temp range 389–468 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_S/kPa) = 10.945 - 6580/(T/K)$; temp range 391–513 K (Antoine eq.-II, Stephenson & Malanowski 1987)

7.20×10^{-6} ; 1.84×10^{-6} (quoted solid P_S from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/Pa) = 12.40 - 5824/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 10.76 - 4915/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

4.28×10^{-7} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -5018/(T/K) + 10.46$; $\Delta H_{vap} = -96.1 kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.027* (20°C , gas stripping-HPLC/fluorescence, measured range $10\text{--}55^\circ\text{C}$, ten Hulscher et al. 1992)

$\log (H/(\text{Pa m}^3/\text{mol})) = 12.83 - 4006/(T/K)$ (Passivirta et al. 1999)

0.0278 (20°C , selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = -0.651 - 1258/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

7.10 (RP-TLC- k' correlation, Bruggeman et al. 1982)

7.05 (HPLC-RT correlation, Rapaport et al. 1984)

6.63 (HPLC-RT correlation, Wang et al. 1986)

6.90 (recommended, Sangster 1989, 1993)

7.04 (TLC retention time correlation, De Voogt et al. 1990)

6.63 (recommended, Hansch et al. 1995)

6.22 (range $5.95\text{--}6.38$) (shake flask/slow stirring-HPLC/fluor., De Maagd et al. 1998)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

5.54 (microorganisms-water, calculated from K_{OW} , Mabey et al. 1982)

4.45 (*Daphnia magna*, Newsted & Giesy 1987)

Sorption Partition Coefficient, $\log K_{\text{OC}}$ at 25°C or as indicated:

6.70 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)

7.215 (10°C), 7.08, 6.93 (20°C), 6.68 (35°C), 6.46, 6.51 (45°C) ($\log K_{\text{DOC}}$ - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)

6.80 (20°C , $\log K_{\text{POC}}$ - particulate organic material from lake, Lüers & ten Hulscher 1996)

6.82–8.25; 6.20–9.20 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

5.87; 6.84, 6.82, 7.26 (20°C , batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: half-lives on different atmospheric particulate substrates (approx. $25\text{ }\mu\text{g/g}$ on substrate): $t_{1/2} = 7.0\text{ h}$ on silica gel, $t_{1/2} = 22\text{ h}$ on alumina and $t_{1/2} = 29\text{ h}$ on fly ash (Behymer & Hites 1985);

first order daytime photodegradation rate constants for adsorption on wood soot particles in an outdoor Teflon chamber: $k = 0.0077\text{ min}^{-1}$ with $1000\text{--}2000\text{ ng/mg}$ loading and $k = 0.0116\text{ min}^{-1}$ with $30\text{--}350\text{ ng/mg}$ loading (Kamens et al. 1988);

direct photolysis $t_{1/2}(\text{obs}) = 0.89\text{ h}$, $t_{1/2}(\text{calc}) = 0.86\text{ h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Oxidation: rate constants $k < 60\text{ M}^{-1}\text{ h}^{-1}$ for singlet oxygen and $k < 6\text{ M}^{-1}\text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982); photooxidation $t_{1/2} = 0.321\text{--}3.21\text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aerobic $t_{1/2} = 14160\text{--}15600\text{ h}$, based on aerobic soil die-away test data at $10\text{--}30^\circ\text{C}$ (Coover & Sims 1987; quoted, Howard et al. 1991); anaerobic $t_{1/2} = 56640\text{--}62400\text{ h}$, based on aerobic soil die-away test data at $10\text{--}30^\circ\text{C}$ (Coover & Sims 1987; quoted, Howard et al. 1991).

Biotransformation: estimated to be $3 \times 10^{-12}\text{ mL cell}^{-1}\text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.076\text{--}0.21\text{ mg g}^{-1}\text{ h}^{-1}$; $k_2 = 0.0012\text{--}0.0014\text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.321\text{--}3.21$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991); $t_{1/2} = 0.6$ h for adsorption on wood soot particles in an outdoor Teflon chamber with an estimated first order rate constant $k = 0.0179 \text{ min}^{-1}$ at $1 \text{ cal cm}^{-2} \text{ min}^{-1}$, $10 \text{ g/m}^3 \text{ H}_2\text{O}$ and 20°C (Kamens et al. 1988).

Surface water: $t_{1/2} = 14160\text{--}15600$ h, based on aerobic soil die-away test data at $10\text{--}30^\circ\text{C}$ (Coover & Sims 1987; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 28320\text{--}31200$ h, based on aerobic soil die-away test data at $10\text{--}30^\circ\text{C}$ (Coover & Sims 1987; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 14160\text{--}15600$ h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988);

mean $t_{1/2} = 9.1$ yr for Luddington soil (Wild et al. 1991).

Biota: elimination $t_{1/2} = 12.4$ d from Oyster, $t_{1/2} = 4.8$ d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

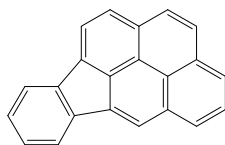
TABLE 4.1.1.49.1

Reported Henry's law constants of benzo[ghi]perylene at various temperatures

ten Hulscher et al. 1992

gas stripping-HPLC/fluor.

$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
10.0	0.019
20.0	0.027
35.0	0.052
40.1	0.054
45.0	0.066
55.0	0.087
enthalpy of volatilization:	
$\Delta H_{\text{vol}}/(\text{kJ}\cdot\text{mol}^{-1}) = 26.1 \pm 1.0$	
entropy of volatilization, ΔS	
$T\Delta S_{\text{vol}}/(\text{kJ}\cdot\text{mol}^{-1}) = 15.9 \pm 1.3$	
at 20°C	
$\ln K_{\text{AW}} = -\Delta H_{\text{vol}}/RT + \Delta S_{\text{vol}}/R$	
$R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$	

4.1.1.50 Indeno[1,2,3-*cd*]pyrene

Common Name: Indeno[1,2,3-*cd*]pyrene

Synonym: 2,3-*o*-phenylenepyrene,

Chemical Name: indeno[1,2,3-*cd*]pyrene

CAS Registry No: 193-39-5

Molecular Formula: C₂₂H₁₂

Molecular Weight: 276.330

Melting Point (°C):

162 (Lide 2003)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):

233.8 (Ruelle & Kesselring 1997, Passivirta et al. 1999)

283.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.51 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

49.41, 36.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

56.5 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0453 (mp at 162°C)

0.043 (Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):

0.00019 (generator column-HPLC/UV, Wise et al. 1981)

0.000438; 0.0023, 0.000191 (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

log [S_L/(mol/L)] = -0.758 - 1631/(T/K) (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):

1.33 × 10⁻⁷ (estimated, Callahan et al. 1979)

1.00 × 10⁻⁸; 2.32 × 10⁻⁷ (quoted solid P_s from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)

log (P_s/Pa) = 12.56 - 6126/(T/K) (solid, Passivirta et al. 1999)

log (P_L/Pa) = 9.60 - 4839/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa·m³/mol at 25°C and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.029* (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)

log [H/(Pa m³/mol)] = 10.36 - 3208/(T/K) (Passivirta et al. 1999)

0.0285 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 0.033 - 1455/(T/K) (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{ow}:

7.66 (calculated-π substituent const., Callahan et al. 1979)

8.20 (calculated, Broman et al. 1991)

6.72 (calculated, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 8.00 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 6.93 (10°C), 6.88, 6.84 (20°C), 6.42 (35°C), 6.32, 6.31 (45°C) ($\log K_{DOC}$ - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
 6.80 (20°C, $\log K_{POC}$ - particulate organic material from lake, Lüers & ten Hulscher 1996)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 0.067\text{--}0.20 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0010\text{--}0.0013 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

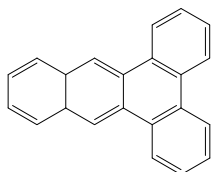
TABLE 4.1.1.50.1
Reported Henry's law constants of indeno[123-cd]pyrene at various temperatures

ten Hulscher et al. 1992

gas stripping-HPLC/fluor.

$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
10.0	0.018
20.0	0.029
35.0	0.057
40.1	0.061
45.0	0.077
55.0	0.105
enthalpy of volatilization: $\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 30.0 \pm 1.1$	
entropy of volatilization, ΔS : $T\Delta S/(\text{J}\cdot\text{K}^{-1} \text{ mol}^{-1}) = 19.9 \pm 1.3$	
at 20°C	
$\ln K_{AW} = -\Delta H/RT + \Delta S/R$	
$R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$	

4.1.1.51 Dibenz[a,c]anthracene



Common Name: Dibenz[a,c]anthracene

Synonym: 1,2:3,4-Dibenzanthracene, naphtho-2',3':9,10-phenanthrene

Chemical Name: dibenz[a,c]anthracene

CAS Registry No: 215-58-7

Molecular Formula: C₂₂H₁₄

Molecular Weight: 278.346

Melting Point (°C):

205 (Bjørseth 1983; Lide 2003)

Boiling Point (°C):

518 (Weast 1982–83)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

299.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.82 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

46.65, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0171 (mp at 205°C)

Water Solubility (g/m³ or mg/L at 25°C):

0.0016 (generator column-HPLC/UV, Billington et al. 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.30 × 10⁻⁹* (effusion method, extrapolated, De Kruif 1980)

log (P/Pa) = 16.25 – 7322.2/(T/K); temp range: 152–179°C (torsion-effusion, de Kruif 1980)

log (P/Pa) = 16.011 – 7207.2/(T/K); temp range: 152–179°C (weighing-effusion, de Kruif 1980)

log (P/Pa) = 16.131 – 7265/(T/K); temp range: 152–179°C (mean, de Kruif 1980)

3.44 × 10⁻⁷ (supercooled liquid P_L, calibrated GC-RT correlation, Lei et al. 2002)

log (P_L/Pa) = -5094/(T/K) + 10.62; ΔH_{vap} = -97.5 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:

7.19 (calculated, Miller et al. 1985)

7.11 (calculated-MCI χ as per Rekker & De Kort 1979, Ruepert et al. 1985)

7.19 (recommended, Sangster 1989, 1993)

7.11 (TLC retention time correlation, De Voogt et al. 1990)

8.0068 (calculated-UNIFAC group contribution, Chen et al. 1993)

6.17 (recommended, Hansch et al. 1995)

6.40 ± 0.19, 6.48 ± 0.78 (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, $\log K_{OC}$:

6.54 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: half-lives under simulated atmospheric conditions: $t_{1/2} = 9.20$ h in simulated sunlight, $t_{1/2} = 4.60$ h in simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 3.82$ h in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983).

TABLE 4.1.1.51.1

Reported vapor pressures of dibenz[a,c]anthracene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

de Kruif 1980

torsion-, weighing effusion

$t/^{\circ}\text{C}$	P/Pa
151.65	0.1
158.52	0.2
163.08	0.3
166.38	0.4
168.97	0.5
171.11	0.6
172.94	0.7
174.53	0.8
175.95	0.9
177.22	1.0
298.15	1.3×10^{-9}
	extrapolated
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 138.0$	

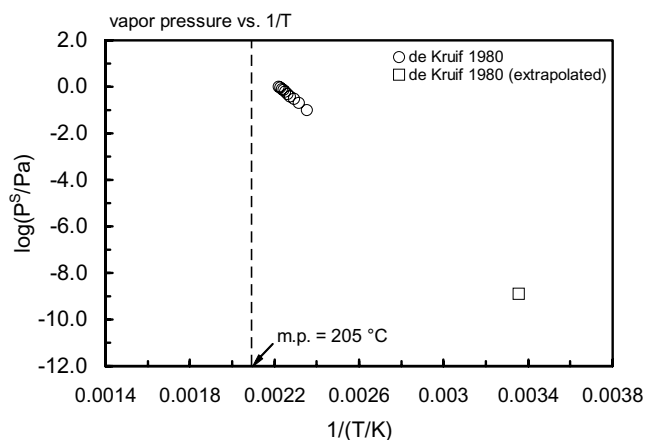
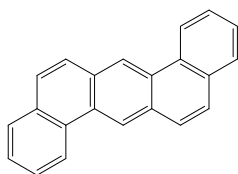


FIGURE 4.1.1.51.1 Logarithm of vapor pressure versus reciprocal temperature for dibenz[a,c]anthracene.

4.1.1.52 Dibenz[a,h]anthracene



Common Name: Dibenz[a,h]anthracene

Synonym: DB[a,h]A, 1,2,5,6-dibenzanthracene, 1,2:5,6-dibenzanthracene

Chemical Name: 1,2:5,6-dibenzanthracene

CAS Registry No: 53-70-3

Molecular Formula: $C_{22}H_{14}$

Molecular Weight: 278.346

Melting Point ($^{\circ}C$):

269.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

524 (Weast 1977)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

252.6 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

299.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

31.165 (Ruelle & Kesselring 1997)

31.16 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

58.26, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

57.3 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.00399 (mp at $269.5^{\circ}C$)

0.00389 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and the reported temperature dependence equations):

0.0005 ($27^{\circ}C$, shake flask-nephelometry, Davis et al. 1942)

0.0006 (shake flask-UV, Klevens 1950)

0.0025 (shake flask-LSC, Means et al. 1980b)

0.00056 (lit. mean, Pearlman et al. 1984)

$\log [S_L/(mol/L)] = -1.409 - 1631/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.33×10^{-8} ($20^{\circ}C$, estimated, Callahan et al. 1979)

3.70×10^{-10} * (effusion method, De Kruif 1980)

$\log (P/Pa) = 16.049 - 7395.4/(T/K)$; temp range: $163-189^{\circ}C$ (torsion-effusion, de Kruif 1980)

$\log (P/Pa) = 15.876 - 7312/(T/K)$; temp range: $163-189^{\circ}C$ (weighing-effusion, de Kruif 1980)

$\log (P/Pa) = 15.962 - 7730/(T/K)$; temp range: $163-189^{\circ}C$ (mean, de Kruif 1980)

4.25×10^{-10} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.515 - 7420/(T/K)$; temp range $403-513\ K$ (Antoine eq., Stephenson & Malanowski 1987)

3.70×10^{-10} ; 9.31×10^{-8} (quoted solid P_s from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.82 - 5824/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.82 - 5002/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

2.51×10^{-7} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log (P_L/Pa) = -5193/(T/K) + 10.82$; $\Delta H_{vap} = -99.4\ kJ\cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

- 0.0074 (calculated-P/C, Mabey et al. 1982)
- 0.0076 (calculated-P/C, Eastcott et al. 1988)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 11.23 - 3371/(T/K)$, (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.50 (shake flask-LSC, Means et al. 1980b)
- 6.88 (HPLC-RT/MS, Burkhard et al. 1985)
- 5.80 (Hansch & Leo 1985)
- 6.75 ± 0.40 (recommended, Sangster 1989, 1993)
- 7.11 (TLC retention time correlation, De Voogt et al. 1990)
- 6.60 (shake flask-UV, pH 7.4, Alcorn et al. 1993)
- 6.50 (recommended, Hansch et al. 1995)
- 6.54 ± 0.19 , 6.60 ± 0.78 (HPLC- k' correlation: ODS column; Diol column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 5.84 (microorganisms-water, calculated from K_{OW} , Mabey et al. 1982)
- 4.63 (activated sludge, Freitag et al. 1984)
- 3.38, 4.63, 1.0 (algae, activated sludge, fish, Freitag et al. 1985)
- 4.00 (*Daphnia magna*, Newsted & Giesy 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.31 (average of 14 soil/sediment samples, equilibrium sorption isotherms by shake flask-LSC, Means et al. 1980b)
- 6.22, 6.18 (calculated-regression of k_p versus substrate properties, calculated- K_{OW} , Means et al. 1980b)
- 6.22; 6.11, 5.30, 5.62 (quoted; calculated- K_{OW} , calculated-S and mp, calculated-S, Karickhoff 1981)
- 6.52 (calculated- K_{OW} , Mabey et al. 1982)
- 5.20 (calculated, Pavlou 1987)
- 6.31; 6.44; 3.75–5.77 (soil, quoted exptl.; calculated-MCI $^1\chi$, calculated- K_{OW} range, Sabljic 1987a,b)
- 5.77 (soil, calculated- K_{OW} based on model of Karickhoff et al. 1979, Sabljic 1987b)
- 5.66 (soil, calculated- K_{OW} based on model of Means et al. 1982, Sabljic 1987b)
- 4.60 (soil, calculated- K_{OW} based on model of Chiou et al. 1983, Sabljic 1987b)
- 4.61 (soil, calculated- K_{OW} based on model of Kenaga 1980, Sabljic 1987b)
- 3.75 (soil, calculated- K_{OW} based on model of Briggs 1981, Sabljic 1987b)
- 6.22 (calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 6.44 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)
- 6.00; 6.30 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
- 6.76–8.42; 5.80–8.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 6.03; 7.0, 6.76, 7.32 (20°C , batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric and aqueous photolysis $t_{1/2} = 782$ h, based on measured rate of photolysis in heptane under November sunlight (Muel & Saguim 1985; quoted, Howard et al. 1991) and $t_{1/2} = 6$ h after adjusting the ratio of sunlight photolysis in water versus heptane (Smith et al. 1978; Muel & Saguim 1985; quoted, Howard et al. 1991);

pseudo-first-order direct photolysis rate constant $k(\text{exptl}) = 0.014 \text{ min}^{-1}$ with the calculated $t_{1/2} = 0.83$ h and the predicted $k = 0.0216 \text{ min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);

direct photolysis $t_{1/2}(\text{obs.}) = 0.31$ h, $t_{1/2} = 0.38$ h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Oxidation: rate constant $k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1.5 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 0.428\text{--}4.28 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aerobic $t_{1/2} = 8664\text{--}22560 \text{ h}$, based on aerobic soil die-away test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);

$k = 0.0019 \text{ d}^{-1}$ with $t_{1/2} = 361 \text{ d}$ for Kidman sandy loam and $k = 0.0017 \text{ d}^{-1}$ with $t_{1/2} = 420 \text{ d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990).

Biotransformation: estimated to be $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: half-lives under simulated atmospheric conditions: $t_{1/2} = 9.6 \text{ h}$ in simulated sunlight, $t_{1/2} = 4.8 \text{ h}$ in simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 2.71 \text{ h}$ in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

$t_{1/2} = 0.428\text{--}4.28 \text{ h}$, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 6\text{--}782 \text{ h}$, based on sunlight photolysis half-life in water (Smith et al. 1978; Muel & Saguem 1985; quoted, Howard et al. 1991);

photolysis $t_{1/2} = 0.83 \text{ h}$ in aqueous solution when irradiated with a 500 W medium-pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2} = 17328\text{--}45120 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: biodegradation rate constant $k = 0.0019 \text{ d}^{-1}$ with $t_{1/2} = 361 \text{ d}$ for Kidman sandy loam soil and $k = 0.117 \text{ d}^{-1}$ with $t_{1/2} = 420 \text{ d}$ for McLaurin sandy loam soil (Park et al. 1990);

$t_{1/2} \sim 8664\text{--}22560 \text{ h}$, based on aerobic soil dieaway test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);

mean $t_{1/2} = 20.607 \text{ wk}$ (quoted, Wild et al. 1991).

Biota:

TABLE 4.1.1.52.1

Reported vapor pressures of dibenz[a,h]anthracene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

de Kruif 1980

torsion-, weighing effusion

$t/^{\circ}\text{C}$	P/Pa
160.38	0.1
168.21	0.2
172.93	0.3
176.33	0.4
179.01	0.5
181.22	0.6
183.11	0.7
184.76	0.8

TABLE 4.1.1.52.1 (Continued)

de Kruif 1980	
torsion-, weighing effusion	
t/°C	P/Pa
186.22	0.9
187.54	1.0
25.0	3.7×10^{-10}
	extrapolated
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 140.0$	

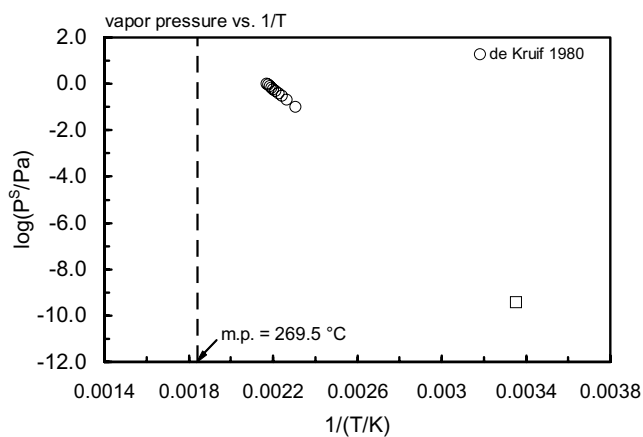
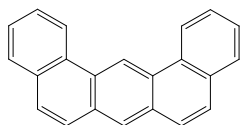


FIGURE 4.1.1.52.1 Logarithm of vapor pressure versus reciprocal temperature for dibenz[a,h]anthracene.

4.1.1.53 Dibenz[*a,j*]anthracene

Common Name: Dibenz[*a,j*]anthracene

Synonym: 1,2:7,8-dibenzanthracene, 1,2:7,8-dibenzanthracene, *a,a'*-dibenzanthracene, dinaphthanthracene

Chemical Name: dibenz[*a,j*]anthracene

CAS Registry No: 58-70-3

Molecular Formula: C₂₂H₁₄

Molecular Weight: 278.346

Melting Point (°C):

197.5 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

222.8 (Ruelle & Kesselring 1997)

299.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S = 56$ J/mol K), F: 0.0203 (mp at 197.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.012 (27°C, shake flask-nephelometry, Davis et al. 1942; quoted, Shaw 1989)

0.012 (quoted, Yalkowsky et al. 1983; Pearlman et al. 1984)

0.000041, 0.00022 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:

7.19 (calculated-fragment const., Yalkowsky et al. 1983)

7.11 (calculated-MCI χ as per Rekker & De Kort 1979, Ruepert et al. 1985)

7.11 (TLC retention time correlation, De Voogt et al. 1990)

7.11 (quoted and recommended, Sangster 1993)

6.54 ± 0.19, 6.44 ± 0.75 (HPLC-*k'* correlation: ODS column; Diol column, Helweg et al. 1997; quoted, Nielsen et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

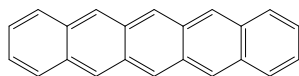
Sorption Partition Coefficient, log K_{oc}:

6.58 (humic acid, HPLC-*k'* correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, *k* or Half-Lives, *t*_{1/2}:

Half-Lives in the Environment:

4.1.1.54 Pentacene



Common Name: Pentacene

Synonym: 2,3,6,7-dibenzanthracene, 2,3:6,7-dibenzanthracene

Chemical Name: pentacene

CAS Registry No: 135-48-8

Molecular Formula: $C_{22}H_{14}$

Molecular Weight: 278.346

Melting Point ($^{\circ}C$):

270–271 (Weast 1982–83)

Boiling Point ($^{\circ}C$):

290–300 (sublimation, Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

299.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

35.19 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

55.22, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.00395 (mp at $270^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.0×10^{-13} * (effusion method, De Kruif 1980)

$\log(P_s/kPa) = 12.725 - 8260/(T/K)$; temp range 444–566 K (Antoine eq., Stephenson & Malanowski 1987)

1.19×10^{-12} * (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 170 – $210^{\circ}C$, Oja & Suuberg 1998)

$\log(P/Pa) = 35.823 - 18867/(T/K)$; temp range 443–483 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

Henry's Law Constant ($Pa\ m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.19 (calculated-f const., Miller et al. 1985)

7.19 (recommended, Sangster 1989, 1993)

7.11 (TLC retention time correlation, De Voogt et al. 1990)

8.0068 (calculated-UNIFAC group contribution, Chen et al. 1993)

7.19 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 4.1.1.54.1

Reported vapor pressures of pentacene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
de Kruif 1980		Oja & Suuberg 1998	
torsion-, weighing effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
220.51	0.1	171.33	0.00161
229.8	0.2	184.8	0.00413
235.4	0.3	185.99	0.00421
239.45	0.4	190.98	0.00760
242.63	0.5	200.29	0.0171
245.27	0.6	203.1	0.0157
247.51	0.7	212.6	0.0515
249.47	0.8		
251.22	0.9	mp/K	> 573
252.79	1.0		
25.0	1.0×10^{-13}	eq. 1a	P/Pa
	extrapolated	A	35.823
		B	18823
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 155.0$		for temp range 443–483 K	
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 155.9$	

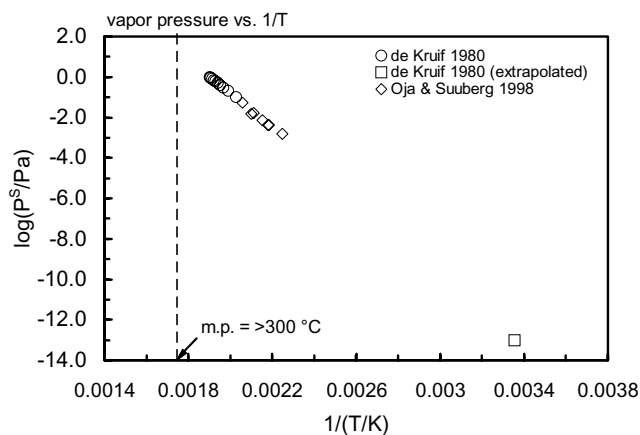
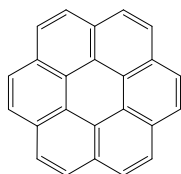


FIGURE 4.1.1.54.1 Logarithm of vapor pressure versus reciprocal temperature for pentacene.

4.1.1.55 Coronene



Common Name: Coronene

Synonym: hexabenzobenzene

Chemical Name: coronene

CAS Registry No: 191-07-1

Molecular Formula: $C_{24}H_{12}$

Molecular Weight: 300.352

Melting Point ($^{\circ}C$):

437.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

525 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

1.371 (Lide 2003)

Molar Volume (cm^3/mol):

244.8 (Ruelle & Kesselring 1997)

219.1 ($25^{\circ}C$, calculated-density)

292.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.202 (Ruelle & Kesselring 1997)

19.2 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

27.02, 42.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 8.99×10^{-5} (mp at $437.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00014 (shake flask-fluorescence, Mackay & Shiu 1977)

0.00014 (average lit. value, Pearlman et al. 1984)

0.00010 (generator column-HPLC/UV, Billington et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

$\log(P/mmHg) = 12.62 - 7675/(T/K)$; temp range $160-240^{\circ}C$ (Knudsen effusion method, Hoyer & Peperle 1958)

1.95×10^{-10} (Knudsen effusion method, extrapolated, Murray et al. 1974)

$\log(P/atm) = 9.110 - 7100/(T/K)$; temp range $427-510 K$ (Knudsen effusion method, Murray et al. 1974)

2.00×10^{-10} (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.1157 - 7100/(T/K)$; temp range $427-510 K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.886 - 5764/(T/K)$; temp range not specified (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.318 - 5362/(T/K)$; temp range not specified (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

2.89×10^{-10} * (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range $148-231^{\circ}C$, Oja & Suuberg 1998)

$\log(P/Pa) = 31.72 - 16006/(T/K)$; temp range $421-504 K$ (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

2.55×10^{-8} (supercooled liquid P_L , calibrated GC-RT correlation, Lei et al. 2002)

$\log(P_L/Pa) = -5446/(T/K) + 10.67$; $\Delta H_{vap} = -104.2 kJ \cdot mol^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

7.64	(average lit. value, Yalkowsky et al. 1983)
7.64	(calculated-MCI χ as per Rekker & De Kort 1979, Ruepert et al. 1985)
8.20, 6.70	(HPLC-RV correlation, different mobile phases, Brooke et al. 1986)
5.40	(shake flask/slow stirring-GC, Brooke et al. 1986)
6.50	(recommended, Sangster 1989, 1993)
7.64	(TLC retention time correlation, De Voogt et al. 1990)
8.0	(calculated-K _{OC} , Broman et al. 1991)
5.40, 6.70	(Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

7.80	(Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
5.0	(predicted dissolved log K _{OC} , Broman et al. 1991)

Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:

Half-Lives in the Environment:

Soil: mean t_{1/2} = 16.5 yr for Luddington soil (Wild et al. 1991).

TABLE 4.1.1.55.1

Reported vapor pressures of coronene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		
Hoyer & Peperle 1958	Murray et al. 1974	Oja & Suuberg 1998	
effusion	Knudsen effusion	Knudsen effusion	
t/°C P/Pa	t/°C P/Pa	t/°C	P/Pa
data presented by equation	data presented by graph and	147.9	0.00191
eq. 1 P/mmHg	eq. 1 P/atm	163.6	0.00686
A 12.62	A 9.110	178.1	0.0236
B 7676	B 7100	196.9	0.0895
for temp range 160–240°C	for temp range 427–510 K	109.9	0.222
		210.0	0.309
ΔH _{sub} /(kJ/mol) = 147.0	25.0 2.0 × 10 ⁻¹⁰	231.11	0.927
	extrapolated		
		mp/K	711
	mp/°C ~440		
		eq. 1a	P/Pa
	ΔH _{sub} /(kJ/mol) = 135.9	A	31.72
	at av. temp measurements	B	16006
		temp range 421–504 K	
		ΔH _{sub} /(kJ/mol) = 133.1	

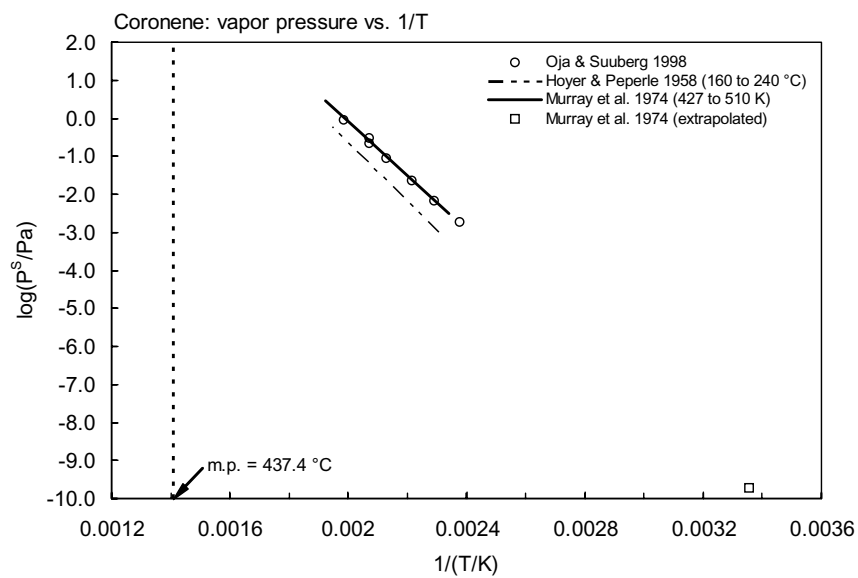
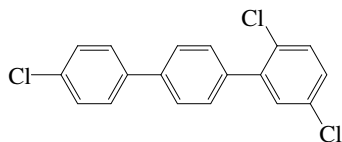


FIGURE 4.1.1.55.1 Logarithm of vapor pressure versus reciprocal temperature for coronene.

4.1.2 CHLORINATED POLYNUCLEAR AROMATIC HYDROCARBONS

4.1.2.1 2,4'',5-Trichloro-*p*-terphenyl



Common Name: 2,4'',5-Trichloro-*p*-terphenyl

Synonym:

Chemical Name:

CAS Registry No: 61576-93-0

Molecular Formula: $C_{18}H_{11}Cl_3$

Molecular Weight: 333.639

Melting Point ($^{\circ}C$):

92 (Dickhut et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.9 (calculated-Le Bas method at normal boiling point)

Heat of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.22 (mp at $92^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

3.8×10^{-4} ; 3.37×10^{-4} (exptl. mean by generator column-GC method; calculated-TSA, Dickhut et al. 1994)
 1.01×10^{-4} , 6.56×10^{-4} , 8.56×10^{-4} (5, 25, $30^{\circ}C$, generator column-GC, Dickhut et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

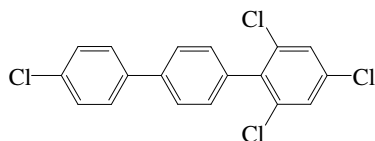
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.2.2 2,4,4'',6-Tetrachloro-*p*-terphenyl

Common Name: 2,4,4'',6-Tetrachloro-*p*-terphenyl

Synonym:

Chemical Name:

CAS Registry No:

Molecular Formula: $C_{18}H_{11}Cl_4$

Molecular Weight: 368.084

Melting Point ($^{\circ}C$):

114 (Dickhut et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

356.8 (calculated-Le Bas method at normal boiling point)

Heat of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.134 (m.p at $114^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.79×10^{-4} ; 7.91×10^{-5} (exptl. mean by generator column-GC method; calculated-TSA, Dickhut et al. 1994)

5.91×10^{-5} , 1.74×10^{-4} , 4.07×10^{-4} (5, 25, $40^{\circ}C$, generator column-GC, Dickhut et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

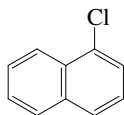
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3 POLYCHLORINATED NAPHTHALENES

4.1.3.1 1-Chloronaphthalene



Common Name: 1-Chloronaphthalene

Synonym: PCN-1, α -chloronaphthalene

Chemical Name: 1-chloronaphthalene

CAS Registry No: 90-13-1

Molecular Formula: $C_{10}H_7Cl$

Molecular Weight: 162.616

Melting Point ($^{\circ}C$):

−2.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

259 (Lide 200)

Density (g/cm^3):

1.1938 ($20^{\circ}C$, Weast 1982–83; Windholz 1983; Budavari 1989)

1.1976, 1.1938 ($15^{\circ}C$, $20^{\circ}C$, Riddick et al. 1986)

1.188 ($25^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

136.2 ($20^{\circ}C$, calculated-density)

168.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

22.4 (shake flask-fluorescence, Mackay & Shiu 1981)

19.0; 8.93 (quoted; calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)

2.87 (quoted, Crookes & Howe 1993, Alcock et al. 1999)

6.75; 36.3 (quoted exptl value; calculated-molar volume, Wang et al. 1992)

19.1; 25.8 (quoted; calculated-group contribution method, Kühne et al. 1995)

19.1; 25.2 (quoted; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($80.6^{\circ}C$, static-Hg manometer, measured range 80.6 – $269.3^{\circ}C$, Kahlbaum 1898)

133.3* ($80.6^{\circ}C$, summary of literature data, temp range 80.6 – $269.3^{\circ}C$, Stull 1947)

3.055 (extrapolated from Antoine eq., temp range 353–533 K, Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.15143 - [1861.65/(T/K - 83.337)]$; temp range: 353–533 K (Antoine eq., Stephenson & Malanowski 1987)

2.133 (estimated, Crookes & Howe 1993)

1.2×10^{-4} (estimated, Alcock et al. 1999)

3.597, 3.84 (calibrated GC-RT correlation, GC-RT correlation, P_L supercooled liquid values, Lei et al. 1999)

$\log(P_L/Pa) = -3058/(T/K) + 10.81$ (HPLC-RT correlation, Lei et al. 1999)

5.588 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3054/(T/K) + 9.97$; (regression with GC-RT from literature, supercooled liquid, Lei et al. 1999)

6.89* ($23.15^{\circ}C$, transpiration method, measured range 289.1–332.3 K, Verevkin 2003)

$\ln (P/P^\circ) = 299.001/R - 83941.481/R \cdot (T/K) - (73.5/R) \cdot \ln[(T/K)/298.15]$, where $P^\circ = 101.325$ kPa, gas constant $R = 8.31451$ J·K⁻¹·mol⁻¹ (vapor pressure eq. from transpiration measurement, temp range 289.1–332.3 K, Verevkin 2003)

Henry's Law Constant (Pa·m³/mol at 25°C):

- 35.5 (gas stripping-GC, Mackay & Shiu 1981)
36.3 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, log K_{ow} at 25°C and the reported temperature dependence equations:

- 3.80 (HPLC-k'correlation, Hanai et al. 1981)
4.08 (calculated-fragment constant, Yalkowsky et al. 1983)
3.90 (shake flask, Opperhuizen 1987)
4.08 (estimated, Abernethy & Mackay 1987)
3.80 (calculated-molar volume, Wang et al. 1992)
4.24 (recommended, Hansch et al. 1995)
4.0; 3.97 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
 $\log K_{ow} = 0.841 + 940.09/(T/K)$, temp range 5–55°C (temperature dependence HPLC-k'correlation, Lei et al. 2000)
4.06 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

- 6.39, 6.10, 5.52, 5.30, 5.13 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
 $\log K_{OA} = 58300/(2.303 \cdot RT) - 4.40$; temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

- 2.28 (*Cyprinus carpio*, for monochloronaphthalenes, Matsuo 1984; quoted, Crookes & Howe 1993)

Sorption Partition Coefficient, log K_{OC} :

- 2.97 (estimated for mono-chloronaphthalenes, Crookes & Howe 1993)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 4.1.3.1.1

Reported vapor pressures of 1-chloronaphthalene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^\circ\text{C}) & (2) & \ln P = A - B/(C + t/^\circ\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & \ln P/P^\circ = A - B/(T/K) - C \cdot \ln [(T/K)/298.15] & (4a) \end{array}$$

Kahlbaum 1898		Stull 1947		Verevkin 2003	
static-Hg manometer		summary of lit. data		transpiration-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
80.6	133.3	80.6	133.3	15.95	3.57
104.8	666.6	104.8	666.6	5.55	1.47
118.6	1333	118.6	1333	7.15	1.75
134.7	2666	134.4	2666	13.85	3.12
140.3	2333	153.2	5333	20.05	5.29
145.1	3999	165.6	7999	23.15	6.89
149.4	4666	180.4	13332	26.05	8.43
153.0	5333	204.2	26664	30.25	11.51

(Continued)

TABLE 4.1.3.1.1 (Continued)

Kahlbaum 1898		Stull 1947		Verevkin 2003	
static-Hg manometer		summary of lit. data		transpiration-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
159.3	6666	230.8	53329	32.15	14.07
171.4	9999	269.3	101325	35.35	18.30
180.4	13332	mp/°C	-20	38.35	24.71
204.2	26664			40.35	28.10
218.3	39997			41.15	29.56
230.8	53329			44.05	35.53
240.5	66661			47.05	46.62
248.6	79993			50.15	55.93
255.5	93326			53.15	69.72
269.3	101325			56.15	84.66
				59.15	105.54
				eq. 4a	P/kPa
				P ^o	101.325 kPa
				A	299.011/R
				B	83941.481/R
				C	73.5/R
				R = 8.314 J K ⁻¹ mol ⁻¹	
				$\Delta H_v/(kJ\ mol^{-1}) = 62.03$	
				at 298.15 K	

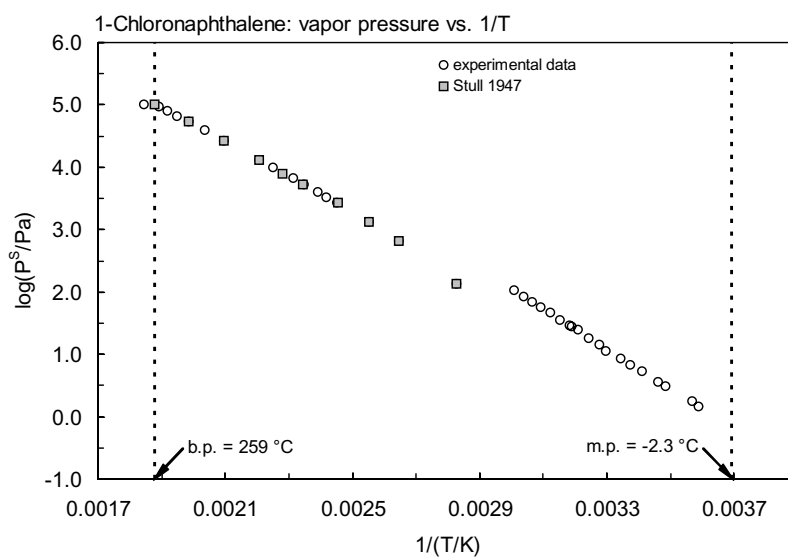
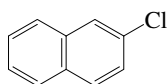


FIGURE 4.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chloronaphthalene.

4.1.3.2 2-Chloronaphthalene



Common Name: 2-Chloronaphthalene

Synonym: PCN-2, β -chloronaphthalene

Chemical Name: 2-chloronaphthalene

CAS Registry No: 91-58-7

Molecular Formula: $C_{10}H_7Cl$

Molecular Weight: 162.616

Melting Point ($^{\circ}C$):

58 (Lide 2003)

Boiling Point ($^{\circ}C$):

256 (Weast 1982–83; Windholz 1983; Budavari 1989; Järnberg et al. 1994; Lide 2003)

Density (g/cm^3):

1.1377 (71 $^{\circ}C$, Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

142.9 (71 $^{\circ}C$, calculated from density, Stephenson & Malanowski 1987)

168.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

3.346 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K, F: 0.474 (mp at 58 $^{\circ}C$))

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

11.7 (shake flask-fluorescence, Mackay & Shiu 1981)

0.924 (shake flask, Opperhuizen et al. 1985, 1986)

8.93 (calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)

16.3 (calculated-group contribution method, Kühne et al. 1995)

7.80 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5.34 (supercooled liquid value, extrapolated from Antoine eq., temperature range 400–435 K, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.8608 - [3021.2/(T/K)]$; temp range 400–435 K (Antoine eq., Stephenson & Malanowski 1987)

3.679, 3.84 (supercooled liquid values P_L : calibrated GC-RT correlation, GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3054/(T/K) + 10.81$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

2.526 (supercooled liquid P_L , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3054/(T/K) + 9.97$ (regression with GC-RT data from literature, Lei et al. 1999)

2.301* (24.15 $^{\circ}C$, transpiration method, measured range 280.2–330.7 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 301.255/R - 87496.950/R \cdot (T/K) - (39.5/R) \cdot \ln[(T/K)/298.15]$, where $P^{\circ} = 101.325$ kPa, gas constant $R = 8.31451$ J·K $^{-1}$ ·mol $^{-1}$ (vapor pressure eq. from transpiration measurement, solid, temp range 280.2–330.7 K, Verevkin 2003)

53.71* (59.05 $^{\circ}C$, transpiration method, measured range 332.2–362.2 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 294.501/R - 84197.803/R \cdot (T/K) - (73.5/R) \cdot \ln[(T/K)/298.15]$, where $P^{\circ} = 101.325$ kPa, gas constant $R = 8.31451$ J·K $^{-1}$ ·mol $^{-1}$ (vapor pressure eq. from transpiration measurements, liquid, temp range 332.2–362.2 K, Verevkin 2003)

Henry's Law Constant (Pa·m 3 /mol at 25 $^{\circ}C$):

31.9 (gas stripping-GC, Mackay & Shiu 1981)

33.5 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C and the reported temperature dependence equations:

- 4.80 (calculated-fragment constant, Yalkowsky et al. 1983)
- 4.19 (HPLC-RT correlation, Opperhuizen et al. 1985, 1986)
- 4.08 (estimated, Abernethy & Mackay 1987)
- 3.98 (shake flask, Opperhuizen 1987)
- 4.07 (selected, Isnard & Lambert 1988; 1989)
- 4.6024 (calculated-UNIFAC group contribution, Chen et al. 1993)
- 4.14 (selected, Hansch et al. 1995)
- 3.90; 3.91 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
- $\log K_{OW} = 0.821 + 924.42/(T/K)$, temp range 5–55°C (temperature dependence HPLC- k' correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 6.36, 6.08, 5.50, 5.28, 5.11 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
- $\log K_{OA} = 58000/(2.303 \cdot RT) - 4.40$; temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 2.28 (*Cyprinus carpio*, for monochloronaphthalenes, Matsuo 1981)
- 3.63 (guppies, Opperhuizen et al. 1985)
- 3.63, 4.81 (whole fish, fish lipid, Gobas et al. 1987)
- 4.52 (guppy, lipid-weight based, Gobas et al. 1989)
- 3.63; 3.06 (quoted means; calculated- K_{OW} and S_0 , Banerjee & Baughman 1991)
- 3.63 (*Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)
- 2.496, 2.721 (calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.97 (estimated for monochloronaphthalenes, Crookes & Howe 1993)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis: laboratory determined hydrolysis rate constant $k = (9.5 \pm 2.8) \times 10^{-6} \text{ h}^{-1}$ at neutral conditions, calculated $t_{1/2} = 8.3 \text{ yr}$ at pH 7 (Ellington et al. 1988).

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_1 = 7.3 \times 10^2 \text{ d}^{-1}$; $k_2 = 3.1 \times 10^{-1} \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1985; quoted, Connell & Hawker 1988)
- $\log k_1 = 2.83 \text{ d}^{-1}$; $\log k_2 = -0.51 \text{ d}^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil: experimentally measured abiotic disappearance $t_{1/2} = 11.3 \text{ d}$ in two different soil types, a Captina silt loam (Typic Fragiudult) and McLaurin sandy loam (Typic Paleudults) (Anderson et al. 1991).

Biota: $t_{1/2} = 2.3 \text{ d}$ (female guppies, Opperhuizen et al. 1985, quoted, Crookes & Howe 1993)

TABLE 4.1.3.2.1

Reported vapor pressures of 2-chloronaphthalene at various temperatures and the coefficients for the vapor pressure equations

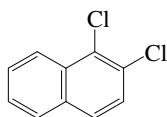
$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & \quad \ln P/P^{\circ} = A - B/(T/K) - C \cdot \ln[(T/K)/298.15] & (4a)\end{aligned}$$

Verevkin 2003

transpiration-GC

t/°C	P/Pa	t/°C	P/Pa
	solid		liquid
7.05	0.342	59.05	53.71
10.15	0.494	62.05	64.43
15.05	0.881	65.05	77.53
17.05	1.103	68.05	95.98
19.05	1.394	71.05	111.91
21.05	1.716	74.05	134.91
24.15	2.301	77.05	161.0
27.15	3.162	80.05	190.2
29.05	3.854	83.05	223.41
30.15	4.361	85.05	252.43
32.05	5.167	89.05	310.78
34.05	6.297		
36.05	7.569	$\Delta H_v/(\text{kJ mol}^{-1}) = 62.3 \pm 1.1$ at 298.15 K	
38.05	9.386		
40.05	10.941		
42.05	13.466	eq. 4a	P/kPa
44.04	15.786	P ^o	101.325 kPa
46.05	18.715	A	294.501/R
48.05	22.307	B	84197.803/R
50.05	26.990	C	73.5/R
52.05	31.158	R = 8.314 J K ⁻¹ mol ⁻¹	
54.05	36.801		
56.05	43.420		
57.55	49.194		
eq. 4a	P/kPa		
P ^o	101.325 kPa		
A	301.255/R		
B	87496.95/R		
C	39.5/R		
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 75.72$ at 298.15 K			

4.1.3.3 1,2-Dichloronaphthalene



Common Name: 1,2-Dichloronaphthalene

Synonym: PCN-3

Chemical Name: 1,2-dichloronaphthalene

CAS Registry No: 2050-69-3

Molecular Formula: $C_{10}H_6Cl_2$

Molecular Weight: 197.061

Melting Point ($^{\circ}C$):

36 (Lide 2003)

Boiling Point ($^{\circ}C$):

295.6 (Lide 2003)

Density (g/cm^3): 1.3147 (49 $^{\circ}C$, Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

156 (Ruelle & Kesselring 1997)

189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.78 (mp at 36 $^{\circ}C$)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

0.137 (generator column-GC/ECD, Opperhuizen 1987)

4.31 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations):

0.344; 0.333 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3172/(T/K) + 10.18$; (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.301 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3172/(T/K) + 10.11$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25 $^{\circ}C$ and the reported temperature dependence equations:

4.40 (HPLC-RT correlation, Opperhuizen et al. 1985)

4.42 (shake flask, Opperhuizen 1987; quoted, Sangster 1993, Crookes & Howe 1993, Hansch et al. 1995)

4.66 (selected, Alcock et al. 1999)

4.60; 4.45 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 1.064 + 1060.21/(T/K)$, temp range 5–55 $^{\circ}C$ (temperature dependence HPLC- k' correlation, Lei et al. 2000)

4.69 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations:

6.93 (generator column-GC, Harner & Bidleman 1998)

7.35, 7.01, 6.44, 6.13, 5.91 (10, 20, 30, 40, 50 $^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 66000/(2.303 \cdot RT) - 4.800$; temp range 10–50 $^{\circ}C$ (GC-RT correlation, Su et al. 2002)

6.89; 7.01 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

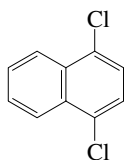
3.40 (fish, Opperhuizen et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.4 1,4-Dichloronaphthalene



Common Name: 1,4-Dichloronaphthalene

Synonym: PCN-5

Chemical Name: 1,4-dichloronaphthalene

CAS Registry No: 1825-31-6

Molecular Formula: $C_{10}H_6Cl_2$

Molecular Weight: 197.061

Melting Point ($^{\circ}C$):

67.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

288 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

156.0 (Ruelle & Kesselring 1997)

189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.383 (mp at $288^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.314 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.314 (generator column-GC/ECD, Opperhuizen et al. 1987)

4.02 (calculated-TSA, Dickhut et al. 1994)

1.98 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.173 (estimated, Crookes & Howe 1993)

9.98×10^{-6} (estimated, Alcock et al. 1999)

0.428; 0.416 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3067/(T/K) + 9.92$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.353 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3067/(T/K) + 10.17$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ and the reported temperature dependence equations:

4.88 (HPLC-RT correlation, Opperhuizen et al. 1985)

4.66 (shake flask, Opperhuizen 1987; quoted, Gobas et al. 1987; 1989; Clark et al. 1990; Sangster 1993; Crookes & Howe 1993; Hansch et al. 1995; Devillers et al. 1996; Alcock et al. 1999)

4.79 (calculated, Oliver & Niimi 1984; Oliver 1987)

4.80; 4.57 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{ow} = 1.269 + 1049.8/(T/K)$, temp range $5-55^{\circ}C$ (temperature dependence HPLC- k' correlation, Lei et al. 2000)

4.56 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations:

6.93 (generator column-GC/MS, Harner & Bidleman 1998)

7.52, 7.13, 6.72, 6.38, 6.13 (10, 20, 30, 40, $50^{\circ}C$, generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -3.97 + 3248/(T/K)$, temp range: 10–50°C (generator column-GC/MS, Harner & Bidleman 1998)
6.78; 6.91 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

3.75 (*Oncorhynchus mykiss*, Oliver & Niimi 1984)
3.36 (female guppies, Opperhuizen et al. 1985)
3.80 (Opperhuizen et al. 1985)
4.04 (Opperhuizen et al. 1985)
3.36, 4.54 (guppies: whole fish, fish lipid, Gobas et al. 1987)
3.75 (rainbow trout, Oliver & Niimi 1984; Oliver 1987)
5.18 (guppy, lipid-weight based, Gobas et al. 1989)
3.36; 4.63 (quoted means; calculated- K_{OW} and S_0 , Banerjee & Baughman 1991)
3.75 (*Oncorhynchus mykiss*, under flow-through condition, quoted Devillers et al. 1996)
3.36 (*Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation: rate constant $k = 5.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at $298 \pm 2 \text{ K}$ (Atkinson 1989).

Hydrolysis:

Biodegradation:

Biotransformation:

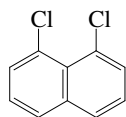
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 1.2 \times 10^3 \text{ d}^{-1}$; $k_2 = 1.1 \times 10^{-1} \text{ d}^{-1}$ (guppies, Opperhuizen et al. 1985)
 $\log k_1 = 3.04 \text{ d}^{-1}$; $\log k_2 = -0.96 \text{ d}^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: $t_{1/2} = 6.2 \text{ d}$ (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)

4.1.3.5 1,8-Dichloronaphthalene



Common Name: 1,8-Dichloronaphthalene

Synonym: PCN-9

Chemical Name: 1,8-dichloronaphthalene

CAS Registry No: 2050-74-0

Molecular Formula: $C_{10}H_6Cl_2$

Molecular Weight: 197.061

Melting Point ($^{\circ}C$):

89 (Weast 1982-83; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

156.0 (Ruelle & Kesselring 1997)

189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.236 (mp at $89^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.315 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.059 (generator column-GC/ECD, Opperhuizen et al. 1987)

0.309 (Isnard & Lambert 1988, 1989; quoted, Crookes & Howe 1993)

1.27 (calculated-molar volume mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equation):

0.198 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3169/(T/K) + 9.93$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.41 (HPLC-RT, Opperhuizen et al. 1985)

4.19 (shake flask-GC, Opperhuizen 1987; quoted, Sangster 1993; Hansch et al. 1995)

5.4348 (calculated-UNIFAC, Chen et al. 1993)

4.85 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.79 (guppies, Opperhuizen et al. 1985)

3.79. 4.96 (guppies: whole fish, fish lipid, Gobas et al. 1987)

4.95 (guppy, lipid-weight based, Gobas et al. 1989)

3.79 (*Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

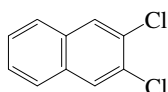
$k_1 = 9.8 \times 10^2 d^{-1}$; $k_2 = 1.6 \times 10^{-1} d^{-1}$ (guppies, Opperhuizen et al. 1985)

$\log k_1 = 2.97 d^{-1}$; $\log k_2 = -0.80 d^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 4.3 d$ (guppies, Opperhuizen et al. 1985; Crookes & Howe 1993)

4.1.3.6 2,3-Dichloronaphthalene



Common Name: 2,3-Dichloronaphthalene

Synonym: PCN-10

Chemical Name: 2,3-dichloronaphthalene

CAS Registry No: 2050-75-1

Molecular Formula: $C_{10}H_6Cl_2$

Molecular Weight: 197.061

Melting Point ($^{\circ}C$):

120 (Weast 1982-83; Ruelle & Kesselring 1997; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

156.0 (Ruelle & Kesselring 1997)

189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K, F: 0.117 (mp at $120^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0862 (generator column-GC/ECD, Opperhuizen et al. 1985; 1987)

0.623 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equation):

0.333 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3169/(T/K) + 10.15$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.71 (HPLC-RT correlation, Opperhuizen et al. 1985)

4.51 (shake flask, Opperhuizen 1987)

4.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.04 (guppies, Opperhuizen et al. 1985)

4.04, 5.22 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.08 (guppy, lipid-weight based, Gobas et al. 1989)

4.04 (*Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

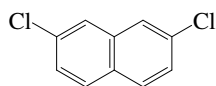
$k_1 = 1.6 \times 10^3 d^{-1}$; $k_2 = 1.4 \times 10^{-1} d^{-1}$ (guppies, Opperhuizen et al. 1985)

$\log k_1 = 3.05 d^{-1}$; $\log k_2 = -0.85 d^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 5.1 d$ (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)

4.1.3.7 2,7-Dichloronaphthalene



Common Name: 2,7-Dichloronaphthalene

Synonym: PCN-12

Chemical Name: 2,7-dichloronaphthalene

CAS Registry No: 2198-77-8

Molecular Formula: $C_{10}H_6Cl_2$

Molecular Weight: 197.061

Melting Point ($^{\circ}C$):

115 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

156.0 (Ruelle & Kesselring 1997)

189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.131 (mp at $115^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.236 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.235 (reported as 2,8-dichloronaphthalene, generator column-GC/ECD, Opperhuizen 1987)

0.699 (calculated-molar volume mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.344 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3169/(T/K) + 10.16$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.81 (HPLC-RT correlation, Opperhuizen et al. 1985)

4.56 (shake flask-GC, Opperhuizen 1987)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ and reported temperature dependence equation:

7.28, 6.95, 6.38, 6.08, 5.85 (10, 20, 30, 40, $50^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 65400/(2.303 \cdot RT) - 4.80$; temp range 10 – $50^{\circ}C$ (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.04 (guppies, Opperhuizen et al. 1985; Crookes & Howe 1993, Lu et al. 1999)

4.04 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.11 (guppy, lipid-weight based, Gobas et al. 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

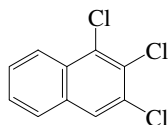
$k_1 = 1.6 \times 10^3$ d^{-1} ; $k_2 = 1.4 \times 10^{-1}$ d^{-1} (guppies, Opperhuizen et al. 1985)

$\log k_1 = 3.08$ d^{-1} ; $\log k_2 = -0.85$ d^{-1} (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: depuration $t_{1/2} = 5.1$ d (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)

4.1.3.8 1,2,3-Trichloronaphthalene



Common Name: 1,2,3-Trichloronaphthalene

Synonym: PCN-13

Chemical Name: 1,2,3-trichloronaphthalene

CAS Registry No: 50402-52-3

Molecular Formula: $C_{10}H_5Cl_3$

Molecular Weight: 231.506

Melting Point ($^{\circ}C$):

81–84 (Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

210.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.071; 0.0652 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log (P_L/Pa) = -3551/(T/K) + 10.76$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.0791 (supercooled liquid P_L , regression with GC-RT data from literature, Lei et al. 1999)

$\log (P_L/Pa) = -3485/(T/K) + 10.59$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ and reported temperature dependence equation:

8.24, 7.85, 7.30, 6.91, 6.63 (10, 20, 30, 40, $50^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 73200/(2.303 \cdot RT) - 5.20$; temp range 10 – $50^{\circ}C$ (GC-RT correlation, Su et al. 2002)

7.66; 7.72 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

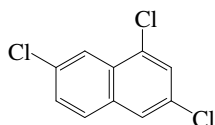
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.9 1,3,7-Trichloronaphthalene



Common Name: 1,3,7-Trichloronaphthalene

Synonym: PCN-21

Chemical Name: 1,3,7-trichloronaphthalene

CAS Registry No: 55720-37-1

Molecular Formula: $C_{10}H_5Cl_3$

Molecular Weight: 231.506

Melting Point ($^{\circ}C$):

113 (Crookes & Howe 1993)

Boiling Point ($^{\circ}C$): 274

Density (g/cm^3):

Molar Volume (cm^3/mol):

168.9 (Ruelle & Kesselring 1997)

210.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.137 (mp at $113^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0644 (generator column-GC/ECD, Opperhuizen et al. 1985, 1987)

0.049 (Opperhuizen et al. 1986)

2.85 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.127 (estimated, Crookes & Howe 1993)

7.10×10^{-6} (estimated, Alcock et al. 1999)

0.114 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3485/(T/K) + 10.74$ (regression with GC-RT from literature, Lei et al. 1999)

$0.0778 - P_S, 0.359 - P_L$ (estimated for trichloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.59 (HPLC-RT correlation, Opperhuizen et al. 1985)

5.60 (selected, Opperhuizen et al. 1986)

5.35 (shake flask, Opperhuizen 1987)

5.08 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.94 (*Cyprinus carpio*, for trichloronaphthalenes, Matsuo 1981)

4.43 (guppies, Opperhuizen et al. 1985)

4.43, 5.61 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.96 (guppy, lipid-weight based, Gobas et al. 1989)

4.08 (calculated- K_{OW} and solubility, Banerjee & Baughman 1991)

4.43 (*Poecilia reticulata*, under static and semi-static conditions, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$$k_1 = 2.3 \times 10^3 \text{ d}^{-1}; k_2 = 8.4 \times 10^{-2} \text{ d}^{-1} \text{ (guppy, Opperhuizen et al. 1985)}$$

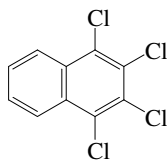
$$k_1 = 1.7 \times 10^3 \text{ d}^{-1} \text{ (estimated, Opperhuizen et al. 1985)}$$

$$\log k_1 = 3.14 \text{ d}^{-1}; \log k_2 = -1.64 \text{ d}^{-1} \text{ (guppy, Gobas et al. 1989)}$$

Half-Lives in the Environment:

$$\text{Biota: } t_{1/2} = 8.3 \text{ d (guppies, Opperhuizen et al. 1985; quoted, Crookes \& Howe 1993)}$$

4.1.3.10 1,2,3,4-Tetrachloronaphthalene



Common Name: 1,2,3,4-Tetrachloronaphthalene

Synonym: PCN-27

Chemical Name: 1,2,3,4-tetrachloronaphthalene

CAS Registry No: 20020-02-4

Molecular Formula: $C_{10}H_4Cl_4$

Molecular Weight: 265.951

Melting Point ($^{\circ}C$):

199 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

181.8 (Ruelle & Kesselring 1997)

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0196 (mp at $199^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00426 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.0042 (generator column-GC/ECD, Opperhuizen 1987)

0.0172 (calculated-AQUAFAC, Myrdal et al. 1995)

0.016 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0197; 0.0173 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3825/(T/K) + 11.12$; (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.0162(supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3825/(T/K) + 10.96$ (regression with GC-RT from literature, Lei et al. 1999)

0.00536 – P_S ; 0.0975 – P_L (estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ and the reported temperature dependence equations:

5.94 (HPLC-RT correlation, Opperhuizen et al. 1985)

5.90 (HPLC-RT correlation, Opperhuizen et al. 1985)

5.75 (shake flask-GC, Opperhuizen 1987)

6.30; 5.76 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{ow} = 1.832 + 1347.46/(T/K)$, temp range $5-55^{\circ}C$ (temperature dependence HPLC- k' correlation, Lei et al. 2000)

5.91 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equation:

9.03, 8.59, 8.05, 7.59, 7.26 (10, 20, 30, 40, $50^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 79500/(2.303 \cdot RT) - 5.60$; temp range $10-50^{\circ}C$ (GC-RT correlation, Su et al. 2002)

8.30; 8.29 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

3.94	(<i>Cyprinus carpio</i> , Matsuo 1981)
3.71	(<i>Oncorhynchus mykiss</i> , Oliver & Niimi 1984)
4.52	(guppies, Opperhuizen et al. 1985)
4.50	(fish, Opperhuizen et al. 1985)
4.66, 5.71	(whole fish, fish lipid, Gobas et al. 1987)
3.71	(rainbow trout, mean value, Oliver & Niimi 1985)
5.96	(guppy, lipid-weight based, Gobas et al. 1989)

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 3.3 \times 10^3 \text{ d}^{-1}$; $k_2 = 9.9 \times 10^{-2} \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1985)

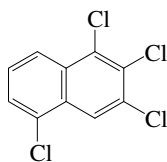
$k_1 = 1.3 \times 10^3 \text{ d}^{-1}$ (estimated, Opperhuizen et al. 1985)

$\log k_1 = 3.70 \text{ d}^{-1}$; $\log k_2 = -1.08 \text{ d}^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: $t_{1/2} = 7 \text{ d}$ (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)

4.1.3.11 1,2,3,5-Tetrachloronaphthalene



Common Name: 1,2,3,5-Tetrachloronaphthalene

Synonym: PCN-28

Chemical Name: 1,2,3,5-tetrachloronaphthalene

CAS Registry No: 53555-63-8

Molecular Formula: $C_{10}H_4Cl_4$

Molecular Weight: 265.951

Melting Point ($^{\circ}C$):

141 (Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0728 (mp at $141^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0203; 0.0179 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3836/(T/K) + 11.17$; (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.0205 (supercooled liquid P_L , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3800/(T/K) + 11.06$ (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equation:

8.98, 8.55, 8.00, 7.55, 7.22 (10, 20, 30, 40, $50^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 79100/(2.303 \cdot RT) - 5.60$; temp range 10 – $50^{\circ}C$ (GC-RT correlation, Su et al. 2002)

8.29; 8.28 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

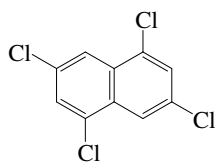
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.12 1,3,5,7-Tetrachloronaphthalene



Common Name: 1,3,5,7-Tetrachloronaphthalene

Synonym: PCN-42

Chemical Name: 1,3,5,7-tetrachloronaphthalene

CAS Registry No: 53555-64-9

Molecular Formula: $C_{10}H_4Cl_4$

Molecular Weight: 265.951

Melting Point ($^{\circ}C$):

179 (Crookes & Howe 1993)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

181.8 (Ruelle & Kesselring 1997)

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0308 (mp at $179^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00426 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.0040 (generator column-GC/ECD, Opperhuizen 1987)

0.0237 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0480 (estimated, Crookes & Howe 1993)

2.70×10^{-6} (estimated, Alcock et al. 1999)

0.0415 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3800/(T/K) + 11.36$ (regression with GC-RT from literature, Lei et al. 1999)

$0.00536 - P_S$; $0.0975 - P_L$ (estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.38 (HPLC-RT correlation, Opperhuizen et al. 1985)

6.40 (Opperhuizen 1986)

6.19 (shake flask, Opperhuizen 1987; selected, Hansch et al. 1995)

5.54 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equation:

8.39 (estimated value for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

8.58, 8.18, 7.62, 7.21, 6.90 (10, 20, 30, 40, $50^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 75000/(2.303 \cdot RT) - 5.40$; temp range $10-50^{\circ}C$ (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.53 (guppies, Opperhuizen et al. 1985)

4.50 (guppies, Opperhuizen et al. 1985)

5.06, 5.71 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.81 (guppy, lipid-weight based, Gobas et al. 1989)
4.53; 4.37 (quoted means; calculated- K_{OW} and S, Banerjee & Baughman 1991)
4.701, 4.961 (calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

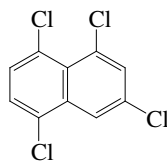
$k_1 = 7.5 \times 10^2 \text{ d}^{-1}$; $k_2 = 2.2 \times 10^{-2} \text{ d}^{-1}$ (guppies, Opperhuizen et al. 1985)

$\log k_1 = 2.97 \text{ d}^{-1}$; $\log k_2 = -1.66 \text{ d}^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: $t_{1/2} = 30 \text{ d}$ (guppies, Opperhuizen et al. 1985)

4.1.3.13 1,3,5,8-Tetrachloronaphthalene



Common Name: 1,3,5,8-Tetrachloronaphthalene

Synonym: PCN-43

Chemical Name: 1,3,5,8-tetrachloronaphthalene

CAS Registry No: 31604-28-1

Molecular Formula: $C_{10}H_4Cl_4$

Molecular Weight: 265.951

Melting Point ($^{\circ}C$):

131 (Crookes & Howe 1993; Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

181.8 (Ruelle & Kesselring 1997)

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0912 (mp at $131^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00825 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.0030 (Opperhuizen 1986)

0.0082 (generator column-GC/ECD, Opperhuizen 1987)

0.0716 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0208 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -3800/(T/K) + 11.07$ (regression with GC-RT from literature, Lei et al. 1999)

$0.00536 - P_S$; $0.0975 - P_L$ (estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.96 (HPLC-RT correlation, Opperhuizen et al. 1985; selected, Sangster 1993)

6.00 (Opperhuizen et al. 1985; Opperhuizen 1986)

5.76 (shake flask, Opperhuizen 1987; selected, Hansch et al. 1995)

5.81 (selected, Gobas et al. 1987, 1989)

5.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations:

8.39 (value for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

8.98, 8.55, 8.00, 7.55, 7.22 (10, 20, 30, 40, $50^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 79100/(2.303 \cdot RT) - 5.60$; temp range $10-50^{\circ}C$ (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.40 (guppies, Opperhuizen et al. 1985)

4.69, 5.57 (guppies: whole fish, fish lipid, Gobas et al. 1987)

5.62 (guppy, lipid-weight based, Gobas et al. 1989)

4.701, 4.582 (calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$$k_1 = 1.2 \times 10^3 \text{ d}^{-1}; k_2 = 4.5 \times 10^{-2} \text{ d}^{-1} \quad (\text{guppies, Opperhuizen et al. 1985})$$

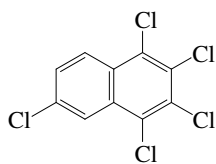
$$k_1 = 1.4 \times 10^3 \text{ d}^{-1} \quad (\text{fish, Opperhuizen 1986})$$

$$\log k_1 = 3.10 \text{ d}^{-1}; \log k_2 = -1.35 \text{ d}^{-1} \quad (\text{guppy, Gobas et al. 1989})$$

Half-Lives in the Environment:

$$\text{Biota: } t_{1/2} = 15.5 \text{ d (guppies, Opperhuizen et al. 1985)}$$

4.1.3.14 1,2,3,4,6-Pentachloronaphthalene



Common Name: 1,2,3,4,6-Pentachloronaphthalene

Synonym: PCN-50

Chemical Name: 1,2,3,4,6-pentachloronaphthalene

CAS Registry No: 67922-25-2

Molecular Formula: $C_{10}H_3Cl_5$

Molecular Weight: 300.396

Melting Point ($^{\circ}C$):

147 (Crookes & Howe 1993; Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0635 (mp at $147^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$):

0.00562; 0.00475 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4123/(T/K) + 11.58$; (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.0055 (supercooled liquid P_L , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4116/(T/K) + 11.55$ (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$ at $25^{\circ}C$ and the reported temperature dependence equations:

7.0; 6.27 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 2.166 + 1446.69/(T/K)$, temp range $5-55^{\circ}C$ (temperature dependence HPLC-k' correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and the reported temperature dependence equations:

8.91 (generator column-GC/MS, Harner & Bidleman 1998)

9.73, 9.20, 8.63, 8.11, 7.75 (10, 20, 30, 40, $50^{\circ}C$, generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.63 + 4629/(T/K)$, temp range: $10-50^{\circ}C$ (generator column-GC/MS, Harner & Bidleman 1998)

8.92; 8.85 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

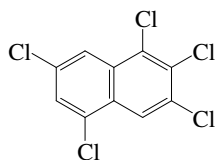
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.15 1,2,3,5,7-Pentachloronaphthalene



Common Name: 1,2,3,5,7-Pentachloronaphthalene

Synonym: PCN-52

Chemical Name: 1,2,3,5,7-pentachloronaphthalene

CAS Registry No: 53555-65-0

Molecular Formula: $C_{10}H_3Cl_5$

Molecular Weight: 300.396

Melting Point ($^{\circ}C$):

171 (Crookes & Howe 1993; Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

313 (estimated, Crookes & Howe 1993)

Density (g/cm^3):

Molar Volume (cm^3/mol):

252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0369 (mp at $171^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0073 (estimated, Crookes & Howe 1993)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

4.266×10^{-3} (estimated, Crookes & Howe 1993)

2.40×10^{-6} (estimated, Alcock et al. 1999)

0.00696; 0.00593 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4082/(T/K) + 11.53$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00798 (supercooled liquid P_L , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4082/(T/K) + 11.71$ (regression with GC-RT data from literature, Lei et al. 1999)

0.0–133 – P_S ; 0.0277 – P_L (estimated for pentachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.46 (selected, Hawker 1990)

6.87 (estimated, Crookes & Howe 1993, quoted, Alcock et al. 1999)

6.87 (quoted, Falandysz et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations:

8.73 (generator-column-GC, Harner & Bidleman 1998)

9.50, 9.04, 8.47, 7.97, 7.63 (10, 20, 30, 40, $50^{\circ}C$, generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.02 + 4394/(T/K)$; temp range: 10– $50^{\circ}C$ (generator column-GC/MS, Harner & Bidleman 1998)

9.00 (estimated, Kaupp & McLachlan 1999)

8.82; 8.76 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.23 (selected, Hawker 1990)

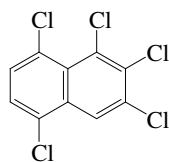
Sorption Partition Coefficient, $\log K_{oc}$:

4.36 (estimated, Crookes & Howe 1993)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.16 1,2,3,5,8-Pentachloronaphthalene



Common Name: 1,2,3,5,8-Pentachloronaphthalene

Synonym: PCN-53

Chemical Name: 1,2,3,5,8-pentachloronaphthalene

CAS Registry No: 150224-24-1

Molecular Formula: $C_{10}H_3Cl_5$

Molecular Weight: 300.396

Melting Point ($^{\circ}C$):

174–176 (Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00394; 0.00329 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4204/(T/K) + 11.70$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00428 (supercooled liquid P_L , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4116/(T/K) + 11.44$ (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$ at $25^{\circ}C$ and the temperature dependence equations:

6.80; 6.13 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 2.305 + 1431.02/(T/K)$, temp range 5 – $55^{\circ}C$ (temperature dependence HPLC- k' correlation, Lei et al. 2000)

6.46 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations:

9.13 (generator column-GC/MS, Harner & Bidleman 1998)

9.97, 9.44, 8.86, 8.34, 7.96 (10, 20, 30, 40, $50^{\circ}C$, generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.59 + 4684/(T/K)$; temp range: 10 – $50^{\circ}C$ (generator column-GC/MS, Harner & Bidleman 1998)

9.10; 9.01 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

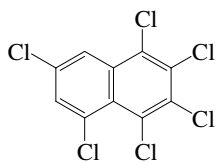
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.17 1,2,3,4,5,7-Hexachloronaphthalene



Common Name: 1,2,3,4,5,7-Hexachloronaphthalene

Synonym: PCN-64

Chemical Name: 1,2,3,4,5,7-hexachloronaphthalene

CAS Registry No: 67927-67-4

Molecular Formula: $C_{10}H_2Cl_6$

Molecular Weight: 334.842

Melting Point ($^{\circ}C$):

194 (Crookes & Howe 1993)

164–166 (Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

331 (estimated, Crookes & Howe 1993)

Density (g/cm^3):

Molar Volume (cm^3/mol):

273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.022 (mp at $194^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00011 (estimated, Crookes & Howe 1993)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

9.47×10^{-4} (estimated, Crookes & Howe 1993)

5.30×10^{-8} (estimated, Alcock et al. 1999)

0.00134 (supercooled liquid P_L , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4432/(T/K) + 11.99$ (regression with GC-RT data from literature, Lei et al. 1999)

$0.000257 - P_S$; $0.00809 - P_L$ (estimated for hexachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.58 (estimated, Crookes & Howe 1993, quoted, Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and the reported temperature dependence equations:

9.80 (generator-column-GC, Harner & Bidleman 1998)

10.07, 9.57, 8.95, 8.54 (20, 30, 40, $50^{\circ}C$, generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.77 + 4393/(T/K)$; temp range: 20 – $50^{\circ}C$ (generator column-GC/MS, Harner & Bidleman 1998)

10.02 (value for hexachloronaphthalenes, Kaupp & McLachlan 1999)

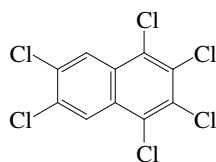
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.18 1,2,3,4,6,7-Hexachloronaphthalene



Common Name: 1,2,3,4,6,7-Hexachloronaphthalene

Synonym: PCN-66

Chemical Name: 1,2,3,4,6,7-hexachloronaphthalene

CAS Registry No: 103426-96-6

Molecular Formula: $C_{10}H_2Cl_6$

Molecular Weight: 334.842

Melting Point ($^{\circ}C$):

205-206 (Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

0.0015; 0.00121 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4411/(T/K) + 11.97$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00157 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4432/(T/K) + 12.06$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ and the temperature dependence equations:

7.70; 6.79 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{ow} = 2.489 + 1556.37/(T/K)$; temp range $5-55^{\circ}C$ (temperature dependence HPLC-k' correlation, Lei et al. 2000)

6.77 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations:

9.70 (generator column-GC/MS, Harner & Bidleman 1998)

10.58, 10.01, 9.46, 8.84, 8.42 (10, 20, 30, 40, $50^{\circ}C$, generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -7.09 + 5003/(T/K)$; temp range: $10-50^{\circ}C$ (generator column-GC/MS, Harner & Bidleman 1998)

9.58; 9.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

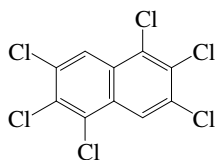
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.19 1,2,3,5,6,7-Hexachloronaphthalene



Common Name: 1,2,3,5,6,7-Hexachloronaphthalene

Synonym: PCN-67

Chemical Name: 1,2,3,5,6,7-hexachloronaphthalene

CAS Registry No: 103426-97-7

Molecular Formula: $C_{10}H_2Cl_6$

Molecular Weight: 334.842

Melting Point ($^{\circ}C$):

234–235 (Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$):

0.00150; 0.00121 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4411/(T/K) + 11.97$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00157 (supercooled liquid P_L , regression with GC-RT data from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4432/(T/K) + 12.06$ (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ and reported temperature dependence equation:

9.70 (generator column-GC/MS, Harner & Bidleman 1998)

10.58, 10.01, 9.46, 8.84, 8.42 (10, 20, 30, 40, $50^{\circ}C$, generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -7.09 + 5003/(T/K)$; temp range: 10– $50^{\circ}C$ (generator column-GC/MS, Harner & Bidleman 1998)

9.58; 9.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

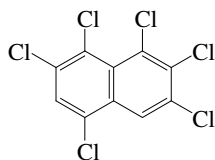
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.20 1,2,3,5,7,8-Hexachloronaphthalene



Common Name: 1,2,3,5,7,8-Hexachloronaphthalene

Synonym: PCN-69

Chemical Name: 1,2,3,5,7,8-hexachloronaphthalene

CAS Registry No: 103426-94-4

Molecular Formula: $C_{10}H_2Cl_6$

Molecular Weight: 334.842

Melting Point ($^{\circ}C$):

148–149 (Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

0.00124; 0.0010 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4441/(T/K) + 11.99$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.00134(supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4432/(T/K) + 11.99$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ and the reported temperature dependence equations:

7.50; 6.69 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{ow} = 2.413 + 1535.48/(T/K)$; temp range 5 – $55^{\circ}C$ (temperature dependence HPLC- k' correlation, Lei et al. 2000)

6.87 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equation:

9.83 (generator column-GC/MS, Harner & Bidleman 1998)

10.09, 9.62, 8.99, 8.57 (20, 30, 40, $50^{\circ}C$, generator column-GC/MS, Harner & Bidleman 1998)

$\log K_{OA} = -6.64 + 4909/(T/K)$; temp range: 20 – $50^{\circ}C$ (generator column-GC, Harner & Bidleman 1998)

9.67; 9.53 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

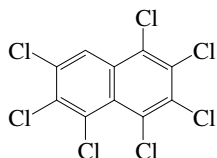
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.21 1,2,3,4,5,6,7-Heptachloronaphthalene



Common Name: 1,2,3,4,5,6,7-Heptachloronaphthalene

Synonym: PCN-73

Chemical Name: 1,2,3,4,5,6,7-heptachloronaphthalene

CAS Registry No: 58863-14-2

Molecular Formula: $C_{10}HCl_7$

Molecular Weight: 369.287

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

293.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00062 (generator column-GC/ECD, Opperhuizen 1985; quoted, Opperhuizen 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$5.44 \times 10^{-4} - P_S$; $0.00258 - P_L$ (estimated for heptachloronaphthalenes, Kaupp & McLachlan 1999)

2.93×10^{-4} , 2.78×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4745/(T/K) + 12.38$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)

0.000278 (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4745/(T/K) + 12.37$ (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$ at $25^{\circ}C$ and the reported temperature dependence equations:

8.20 (HPLC-RT, Opperhuizen et al. 1985; quoted, Opperhuizen 1986)

7.69 (calculated-fragment const., Burreau et al. 1997)

8.20; 7.18 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

$\log K_{OW} = 2.638 + 1660.82/(T/K)$; temp range $5-55^{\circ}C$ (HPLC- k' correlation, Lei et al. 2000)

7.33 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equation:

11.52, 10.96, 10.44, 9.75, 9.28 (10, 20, 30, 40, $50^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 99500/(2.303 \cdot RT) - 6.80$; temp range $10-50^{\circ}C$ (GC-RT correlation, Su et al. 2002)

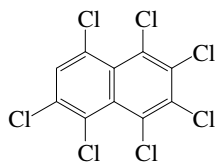
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.22 1,2,3,4,5,6,8-Heptachloronaphthalene



Common Name: 1,2,3,4,5,6,8-Heptachloronaphthalene

Synonym: PCN-74

Chemical Name: 1,2,3,4,5,6,8-heptachloronaphthalene

CAS Registry No: 58863-15-3

Molecular Formula: $C_{10}HCl_7$

Molecular Weight: 369.287

Melting Point ($^{\circ}C$):

194 (Crookes & Howe 1993; Järnberg et al. 1994)

Boiling Point ($^{\circ}C$):

348 (estimated, Crookes & Howe 1993)

Density (g/cm^3):

Molar Volume (cm^3/mol):

293.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.022 (mp at $194^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00004 estimated, Crookes & Howe 1993; quoted, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.73×10^{-4} (estimated, Crookes & Howe 1993)

2.10×10^{-8} (estimated, Alcock et al. 1999)

2.46×10^{-4} (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -4748/(T/K) + 12.31$ (regression with GC-RT from literature, Lei et al. 1999)

$5.44 \times 10^{-4} - P_S$; $0.00258 - P_L$ (estimated for heptachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.30 (estimated, Crookes & Howe 1993, quoted, Alcock et al. 1999)

8.50; 7.46 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equation:

11.56, 10.99, 10.47, 9.79, 9.31 (10, 20, 30, 40, $50^{\circ}C$, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 99800/(2.303 \cdot RT) - 6.80$; temp range 10 – $50^{\circ}C$ (GC-RT correlation, Su et al. 2002)

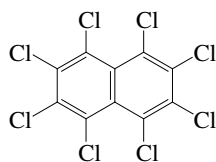
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.3.23 Octachloronaphthalene



Common Name: Octachloronaphthalene

Synonym: PCN-75

Chemical Name: octachloronaphthalene

CAS Registry No: 2234-13-1

Molecular Formula: $C_{10}Cl_8$

Molecular Weight: 403.731

Melting Point ($^{\circ}C$):

197.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

365 (estimated, Crookes & Howe 1993)

Density (g/cm^3):

Molar Volume (cm^3/mol):

314.8 (calculated-Le Bas method at normal boiling point)

233.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0203 (mp at $197.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.000078, 0.00008 (generator column-GC/ECD, Opperhuizen 1986)

0.00008 (generator column-GC/ECD, Opperhuizen 1987)

0.00008; 0.00027 (quoted; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.33×10^{-4} (estimated, Crookes & Howe 1993)

7.50×10^{-9} (estimated, Alcock et al. 1999)

7.61×10^{-5} , 5.60×10^{-5} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -5021/(T/K) + 12.72$ (Antoine eq., GC-RT correlation, supercooled liquid, Lei et al. 1999)

6.84×10^{-5} (supercooled liquid P_L , regression with GC-RT from literature, Lei et al. 1999)

$\log(P_L/Pa) = -5021/(T/K) + 12.82$ (regression with GC-RT from literature, Lei et al. 1999)

$1.60 \times 10^{-5} - P_S$; $8.71 \times 10^{-4} - P_L$ (estimated for heptachloronaphthalenes, Kaupp & McLachlan 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ and the reported temperature dependence equations.

6.50 (calculated, Kaiser 1983)

8.40 (HPLC-RT correlation, Opperhuizen et al. 1985)

8.50 (Opperhuizen 1986)

6.42 (shake flask, Opperhuizen)

7.90 (calculated, Banerjee & Baughman 1991)

8.50, 7.47 (calibrated HPLC- k' correlation, HPLC- k' correlation, Lei et al. 2000)

$\log K_{ow} = 2.998 + 1660.82/(T/K)$, temp range $5-55^{\circ}C$ (temperature dependence HPLC- k' correlation, Lei et al. 2000)

7.70 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and the reported temperature dependence equations:

12.39, 11.78, 11.27, 10.51, 9.98 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)

$\log K_{OA} = 10600/(2.303 \cdot RT) - 7.20$; temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.50 (*Oncorhynchus mykiss*, Oliver & Niimi 1985; quoted, Crookes & Howe 1993)

2.52 (rainbow trout, mean value, Oliver & Niimi 1985)

5.0 (calculated- K_{OW} and S_0 , Banerjee & Baughman 1991)

2.52 (*Oncorhynchus mykiss*, under flow-through condition, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

5.38 (estimated, Crookes & Howe 1993)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation: $t_{1/2} = 1608$ – 16082 h based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aerobic biodegradation $t_{1/2} = 4320$ – 8760 h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991);

anaerobic biodegradation $t_{1/2} = 17280$ – 35040 h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 1608$ – 16082 h in air based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

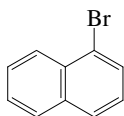
Surface water: $t_{1/2} = 4320$ – 8760 h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 8640$ – 17520 h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 4320$ – 8760 h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

Biota:

4.1.4 BROMINATED POLYNUCLEAR AROMATIC HYDROCARBONS**4.1.4.1 1-Bromonaphthalene**

Common Name: 1-Bromonaphthalene

Synonym: α -bromonaphthalene

Chemical Name: 1-bromonaphthalene

CAS Registry No: 90-11-9

Molecular Formula: $C_{10}H_7Br$

Molecular Weight: 207.067

Melting Point ($^{\circ}C$):

6.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

281 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4834 (Dean 1992)

1.4785 (Lide 2003)

Molar Volume (cm^3/mol):140.6 ($30^{\circ}C$, calculated from density, Stephenson & Malanowski 1987)140.0 ($20^{\circ}C$, calculated-density)

170.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.33 (at normal bp, Hon et al. 1976)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at $25^{\circ}C$, F: 1.0Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9.95 (Yalkowsky et al. 1983)

7.72 (calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)

9.08, 9.80, 13.35, and 18.98 (4, 10, 25, and $40^{\circ}C$, generator column-UV spec., Dickhut et al. 1994)

25.3 (calculated-TSA, Dickhut et al. 1994)

14.0 (calculated-group contribution method, Kühne et al. 1995)

23.3 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):266.6* ($97.9^{\circ}C$, static-Hg manometer, measured range 97.9 – $281.1^{\circ}C$, Kahlbaum 1898)133* ($84.2^{\circ}C$, summary of literature data, temp range 84.2 – $281.1^{\circ}C$, Stull 1947) $\log (P/mmHg) = [-0.2185 \times 13274.9/(T/K)] + 8.131285$; temp range 84.2 – $281.1^{\circ}C$, (Antoine eq., Weast 1972–73)18681* ($196.27^{\circ}C$, ebulliometry, measured range 97.9 – $285.92^{\circ}C$, Hon et al. 1976) $\log (P/mmHg) = 5.38175 - 929.64/(91.06 + t/^{\circ}C)$; temp range: 196.27 – $285.93^{\circ}C$ (Antoine eq., twin ebulliometry, Hon et al. 1976)0.713*, 1.07* (torsion effusion, measured range 295 – 359 K, Urbani et al. 1980) $\log (P/kPa) = (6.90 - 2950/(T/K))$, temp range 295 – 359 K (torsion and Knudsen effusion, Urbani et al. 1980) $\log (P/mmHg) = 7.00350 - 1927.05/(186.0 + t/^{\circ}C)$; temp range: liquid (Antoine eq., Dean 1985, 1992) $\log (P_L/kPa) = 6.56365 - 2303.73/[-48.841 + (T/K)]$; temp range 357 – 555 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 4.50679 - 929.871/[182.045 + (T/K)]$, temp range 469–559 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

2.754* (30.15°C, transpiration method, measured range 303.3–336.3 K, Verevkin 2003)

$\ln (P/P^\circ) = 299.001/R - 8.3941.481/R \cdot (T/K) - (73.5/R) \cdot \ln[(T/K)/298.15]$, where $P^\circ = 101.325$ kPa, gas constant $R = 8.31451 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ (vapor pressure eq. from transpiration measurement, temp range 303.3–336.3 K, Verevkin 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.35 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 4.1.4.1.1

Reported vapor pressures of 1-bromonaphthalene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Kahlbaum 1898		Stull 1947		Hon et al. 1976		Urbani et al. 1980	
static method-manometer		summary of literature data		ebulliometry		torsion effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						Run A.01	
97.9	266.6	84.2	133.3	196.27	18681	25	0.713
117.5	666.6	117.5	666.6	213.14	28206	28	0.950
134.0	1333	133.6	1333	228.08	39235	30	1.37
151.3	2666	150.2	2666	234.45	44740	33	1.31
157.2	3333	170.2	5333	244.51	54504	34	1.43
162.3	3999	183.5	7999	245.13	55150	40	2.85
166.7	4666	198.8	13332	250.71	61192	42	3.05
170.5	5333	224.2	26664	256.24	67574	45	3.62
177.1	6666	252.2	53329	262.78	75759	46	3.72
189.6	9999	281.1	101325	275.35	93151	47	4.16
198.8	13332			279.49	99510	48	4.51
223.8	26664	mp/°C	5.5	281.40	102474	49	4.75
239.7	39997			284.04	106737	50	4.99
252.0	53329			285.92	109863	52	5.82
261.6	66661					58	7.78
269.8	79993			bp/°C	280.56	61	8.94
277.2	93326					66	12.8

TABLE 4.1.4.1.1 (Continued)

Kahlbaum 1898		Stull 1947		Hon et al. 1976		Urbani et al. 1980	
static method-manometer		summary of literature data		ebulliometry		torsion effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
281.1	101325			eq. 2	P/mmHg	74	20.2
				A	5.38157	77	24.3
				B	929.64	86	42.0
				C	91.06		
				ΔH _v /(kJ mol ⁻¹) = 39.33 at bp			

2.

Urbani et al. 1980 (Continued)				Verevkin 2003			
torsion effusion		Knudsen effusion		transpiration-GC			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa		
Run A.02							
50	8.33	42	4.95	30.15	2.754		
53	8.54	49	9.26	33.15	3.466		
55	10.4	50	8.97	36.15	4.388		
58	12.5	54	11.6	39.14	5.529		
58	11.7	60	16.1	42.15	7.095		
67	17.3	65	18.4	45.15	8.644		
Run A.04		70	28.3	48.15	10.97		
26	1.07			51.25	13.66		
34	1.72	For Knudsen effusion:		54.15	16.64		
36	2.32	eq. 1	P/kPa	57.15	20.95		
38	2.61	A	6.33 ± 0.33	60.15	25.50		
43	3.86	B	2710 ± 110	63.15	30.34		
50	6.18						
51	6.21			ΔH _v /(kJ mol ⁻¹) = 63.91			
55	7.00			at 298.15 K			
60	8.58						
63	10.3			eq. 4a	P/kPa		
68	12.9			P ⁰	101.325 kPa		
70	17.5			A	303.761/R		
82	38.7	Overall temp dependence eq.		B	89574.863/R		
		eq. 1	P/kPa	C	78.8/R		
for torsion effusion:		A	6.90 ± 1.1	R = 8.314 J K ⁻¹ mol ⁻¹			
eq. 1	P/kPa	B	2950 ± 300				
A	6.96 ± 0.18						
B	2980 ± 57	ΔH _v /(kJ mol ⁻¹) = 56 ± 6					

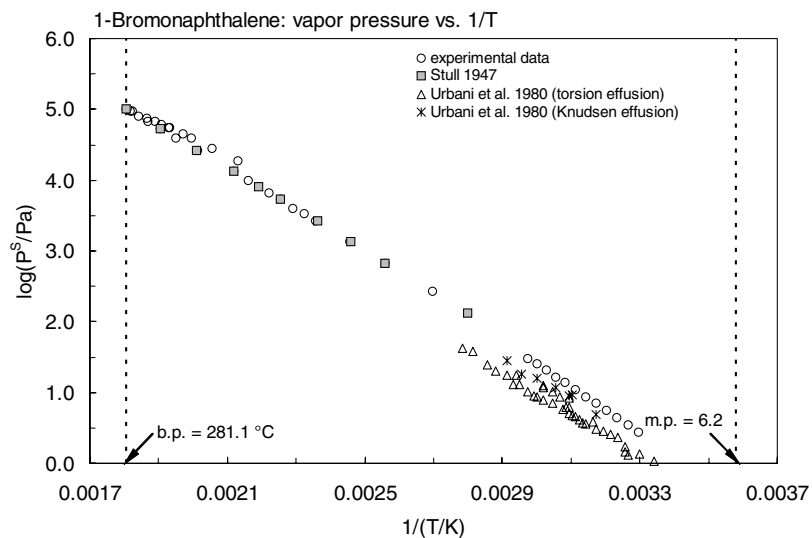
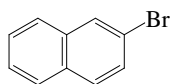


FIGURE 4.1.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1-bromonaphthalene.

4.1.4.2 2-Bromonaphthalene



Common Name: 2-Bromonaphthalene

Synonym: β -bromonaphthalene

Chemical Name: 2-bromonaphthalene

CAS Registry No: 580-13-2

Molecular Formula: $C_{10}H_7Br$

Molecular Weight: 207.067

Melting Point ($^{\circ}C$):

55.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

281.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

146.3 (Ruelle & Kesselring 1997)

170.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.97 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.498 (mp at $55.9^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

8.27 (Yalkowsky et al. 1983)

7.72 (calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)

3.80, 8.04, 15.76 (4, 25, $40^{\circ}C$, generator column-UV spec., Dickhut et al. 1994)

10.1 (calculated-TSA, Dickhut et al. 1994)

9.04 (calculated-group contribution method, Kühne et al. 1995)

8.06 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.501* ($25.15^{\circ}C$, solid I, transpiration method-GC, measured range 280.4–318.3 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 314.110/R - 94001.596/R \cdot (T/K) - (41.6/R) \cdot \ln[(T/K)/298.15]$, where $P^{\circ} = 101.325$ kPa, gas constant $R = 8.31451$ J·K $^{-1}$ ·mol $^{-1}$ (solid I, vapor pressure eq. from transpiration measurement, temp range 280.4–318.3 K, Verevkin 2003)

7.34* ($46.05^{\circ}C$, solid-II, transpiration method-GC, measured range 319.2–328.2 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 302.672/R - 90417.272/R \cdot (T/K) - (41.6/R) \cdot \ln[(T/K)/298.15]$, where $P^{\circ} = 101.325$ kPa, gas constant $R = 8.31451$ J·K $^{-1}$ ·mol $^{-1}$ (solid II, vapor pressure eq. from transpiration measurements, temp range 319.2–328.2 K, Verevkin 2003)

18.75* ($57.05^{\circ}C$, liquid, transpiration method-GC, measured range 330.2–360.2 K, Verevkin 2003)

$\ln(P/P^{\circ}) = 303.761/R - 89574.863/R \cdot (T/K) - (78.8/R) \cdot \ln[(T/K)/298.15]$, where $P^{\circ} = 101.325$ kPa, gas constant $R = 8.31451$ J·K $^{-1}$ ·mol $^{-1}$ (liquid, vapor pressure eq. from transpiration measurements, temp range 330.2–360.2 K, Verevkin 2003)

Henry's Law Constant (Pa·m 3 /mol):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.35 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 4.1.4.2.1

Reported vapor pressures of 2-bromonaphthalene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log(T/K) & (4) & \ln P/P^{\circ} = A - B/(T/K) - C \cdot \ln [(T/K)/298.15] & (4a) \end{array}$$

Verevkin 2003

transpiration-GC					
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
solid I		solid II		liquid	
7.25	0.105	46.05	77.34	57.05	18.75
10.35	0.152	47.15	8.04	60.15	23.55
15.15	0.287	48.05	8.68	63.15	28.58
20.05	0.501	49.15	9.73	66.15	34.83
25.05	0.886	51.05	11.47	69.15	41.76
28.15	1.239	51.15	11.59	72.15	52.31
31.15	1.709	53.15	13.60	75.15	61.76
34.15	2.285	54.65	15.68	78.05	75.34
37.15	3.107	55.05	16.20	81.05	88.25
40.05	4.219			85.05	103.89
41.15	4.588			87.05	125.40
43.15	5.703				
45.15	6.686				
eq. 4a		eq. 4a		eq. 4a	
P/kPa		P/kPa		P/kPa	
P°		P°		P°	
101.325 kPa		101.325 kPa		101.325 kPa	
A		A		A	
314.110/R		302.672/R		303.761/R	
B		B		B	
94001.596/R		90417.272/R		89574.863/R	
C		C		C	
41.6/R		41.6/R		78.8/R	
$R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$		$R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$		$R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 81.60$		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 78.01$		$\Delta H_v/(\text{kJ mol}^{-1}) = 66.08$	
at 298.15 K		at 298.15 K		at 298.15 K	

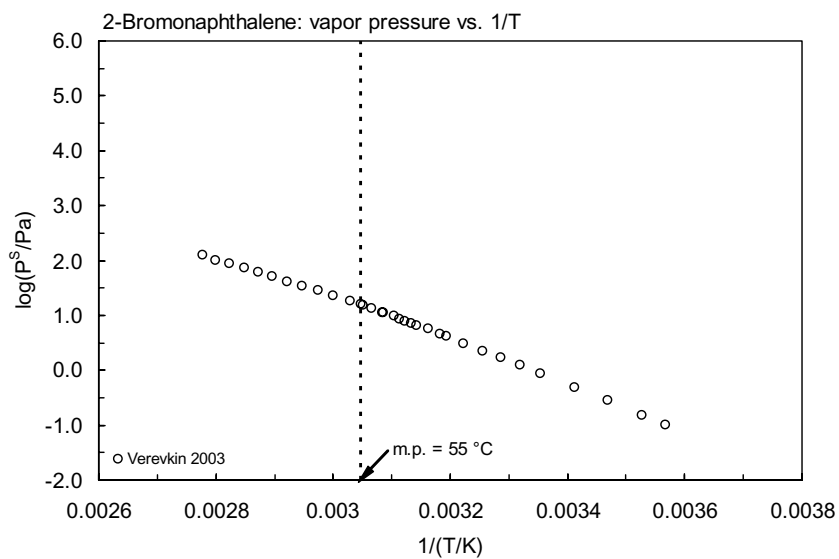
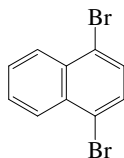


FIGURE 4.1.4.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2-bromonaphthalene.

4.1.4.3 1,4-Dibromonaphthalene



Common Name: 1,4-Dibromonaphthalene

Synonym:

Chemical Name: 1,4-dibromonaphthalene

CAS Registry No: 83-53-4

Molecular Formula: $C_{10}H_6Br_2$

Molecular Weight: 285.963

Melting Point ($^{\circ}C$):

83 (Lide 2003)

Boiling Point ($^{\circ}C$):

310 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

194.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.27 (mp at $83^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.125, 0.35, and 0.866 (4, 25, and $40^{\circ}C$, generator column-GC/ECD, Dickhut et al. 1994)

1.92 (calculated-TSA, Dickhut et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

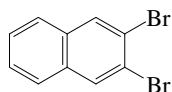
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.4.4 2,3-Dibromonaphthalene

Common Name: 2,3-Dibromonaphthalene

Synonym:

Chemical Name: 2,3-dibromonaphthalene

CAS Registry No:

Molecular Formula: $C_{10}H_6Br_2$

Molecular Weight: 285.963

Melting Point ($^{\circ}C$):

140 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

194.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0744 (mp at $140^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0554, 0.138, and 0.352 (4, 25, and $40^{\circ}C$, generator column-GC/ECD, Dickhut et al. 1994)

0.432 (calculated-TSA, Dickhut et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

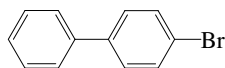
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.4.5 4-Bromobiphenyl



Common Name: 4-Bromobiphenyl

Synonym:

Chemical Name: 4-bromobiphenyl

CAS Registry No: 92-66-0

Molecular Formula: $C_{12}H_9Br$

Molecular Weight: 233.103

Melting Point ($^{\circ}C$):

91.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

310 (Weast 1983–84; Stephenson & Malanowski 1987, Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

0.9327 (Weast 1983–84, Lide 2003)

Molar Volume (cm^3/mol):

176.1 (Ruelle & Kesselring 1997)

250.0 ($25^{\circ}C$, calculated-density)

207.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

26.86 (Doucette & Andren 1988)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.223 (mp at $91.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations.):

0.235, 0.653, 0.874 ($4.9, 25, 40^{\circ}C$, generator column-GC, Doucette & Andren 1988a)

$S/(mol/L) = 9.36 \times 10^{-7} \exp(0.037 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range 4.9 – $40^{\circ}C$, Doucette & Andren 1988a); or

$\log x = -1436/(T/K) - 1.541$, temp range 4.9 – $40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

0.546 (calculated-TSA, Dickhut et al. 1994)

0.256 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P_L/kPa) = 2.24643 - 2174.97/[(T/K) - 70.067]$; (Antoine eq., liquid state, temp range 371 – $583 K$, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.96; 4.89, 5.00 (generator column-GC; calculated-group contribution method, estimated-TSA and K_{OW} , Doucette & Andren 1987)

4.96; 4.89, 4.83, 5.10, 5.14, 5.10 (generator column-GC; calculated- π const., HPLC-RT correlation, calculated-MW, calculated-MCI χ , calculated-TSA and K_{OW} , Doucette & Andren 1988b)

4.96 (recommended, Sangster 1993)

4.95 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

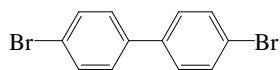
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.4.6 4,4'-Dibromobiphenyl



Common Name: 4,4'-Dibromobiphenyl

Synonym: PBB-15, 4,4'-dibromo-1,1'-biphenyl

Chemical Name: 4,4'-dibromobiphenyl

CAS Registry No: 92-86-4

Molecular Formula: $C_{12}H_8Br_2$

Molecular Weight: 312.000

Melting Point ($^{\circ}C$):

164 (Ruelle & Kesselring 1997, Lide 2003)

Boiling Point ($^{\circ}C$):

357.5 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

192.2 (Ruelle & Kesselring 1997)

231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0433 (mp at $164^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00574 (generator column-GC, Gobas et al. 1988)

0.104 (quoted, Chessells et al. 1992)

0.0164 (calculated-MCI χ , Ruelle & Kesselring et al. 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.72; 5.75, 5.57 (generator column-GC; calculated-group contribution method, estimated-TSA and K_{OW} , Doucette & Andren 1987)

5.72; 5.75, 5.85, 6.14, 5.81, 5.68 (generator column-GC; calculated- π const., HPLC-RT correlation, calculated-MW, calculated-MCI χ , calculated-TSA and K_{OW} , Doucette & Andren 1988b)

5.72 (HPLC-RT correlation, Gobas et al. 1988,)

5.72 (recommended, Sangster 1993)

4.67 (calculated-UNIFAC, Chen et al. 1993)

5.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

5.43 (guppy, lipid weight-based, Gobas et al. 1989)

4.19; 5.43 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)

3.825, 4.365 (calculated-MCI χ , K_{OW} , Lu et al. 1999)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

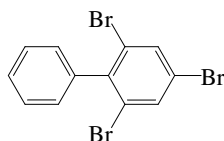
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$\log k_1 = 3.35$ d^{-1} (guppy, Gobas et al. 1989)

$\log k_2 = -0.91$ d^{-1} (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

4.1.4.7 2,4,6-Tribromobiphenyl



Common Name: 2,4,6-Tribromobiphenyl

Synonym: PBB-30

Chemical Name: 2,4,6-tribromobiphenyl

CAS Registry No: 59080-33-0

Molecular Formula: $C_{12}H_7Br_3$

Molecular Weight: 390.896

Melting Point ($^{\circ}C$):

64 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

208.3 (Ruelle & Kesselring 1997)

254.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.414 (mp at $64^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.016 (generator column-GC, Gobas et al. 1988)

0.0131 (quoted, Chessells et al. 1992)

0.054 (calculated-MCI χ , Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.03 (HPLC-RT correlation, Gobas et al. 1988, 1989)

6.03; 4.78 (quoted; calculated-UNIFAC, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

5.06 (guppy, lipid weight-based, Gobas et al. 1989)

3.97; 5.06 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)

4.408, 4.645 (calculated-MCI χ , K_{ow} , Lu et al. 1999)

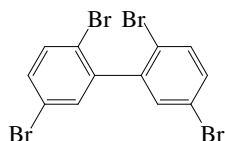
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$\log k_1 = 3.05 d^{-1}$; $\log k_2 = -0.83 d^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

4.1.4.8 2,2',5,5'-Tetrabromobiphenyl

Common Name: 2,2',5,5'-Tetrabromobiphenyl

Synonym: PBB-52

Chemical Name: 2,2',5,5'-tetrabromobiphenyl

CAS Registry No: 59080-37-4

Molecular Formula: $C_{12}H_6Br_4$

Molecular Weight: 469.792

Melting Point ($^{\circ}C$):

144 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

224.4 (Ruelle & Kesselring 1997)

277.8 (calculated-Le Bas at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.068 (mp at $144^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00429 (generator column-GC, Gobas et al. 1988)

0.0545 (quoted, Chessells et al. 1992)

0.00409 (calculated-AQUAFAC, Myrdal et al. 1995)

0.00246 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.50 (HPLC-RT correlation, Gobas et al. 1988,)

4.88 (calculated-UNIFAC group contribution, Chen et al. 1993)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

6.16 (guppy, lipid weight-based, Gobas et al. 1989)

4.62; 6.16 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)

5.097; 6.16 (calculated-MCI χ , K_{ow} , Lu et al. 1999)

Sorption Partition Coefficient, $\log K_{oc}$:

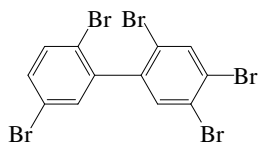
Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$\log k_1 = 2.96 d^{-1}$; $\log k_2 = -2.02 d^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

4.1.4.9 2,2',4,5,5'-Pentabromobiphenyl



Common Name: 2,2',4,5,5'-Pentabromobiphenyl

Synonym:

Chemical Name: 2,2',4,5,5'-pentabromobiphenyl

CAS Registry No: 6788-96-4

Molecular Formula: $C_{12}H_5Br_5$

Molecular Weight: 548.688

Melting Point ($^{\circ}C$):

157 (Dickhut et al. 1994; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

301.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

45.44 (Doucette & Andren 1988)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0507 (mp at $157^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations.):

1.032×10^{-4} , 4.42×10^{-4} , 9.82×10^{-4} (4.9 , 25 , $40^{\circ}C$, generator column-GC/ECD, Doucette & Andren 1988a)

$S/(mol/L) = 1.52 \times 10^{-10} \exp(0.063 \cdot t/^{\circ}C)$ (generator column-GC, temp range $4-40^{\circ}C$, Doucette & Andren 1988a)

$\log x = -2374/(T/K) - 2.373$, temp range $4-40^{\circ}C$ (generator column-GC, Doucette & Andren 1988a)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

77.10 (generator column-GC Doucette & Andren 1987)

77.10; 8.76 (generator column-GC; HPLC-RT correlation, Doucette & Andren 1988b)

7.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

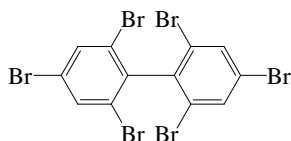
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.1.4.10 2,2',4,4',6,6'-Hexabromobiphenyl



Common Name: 2,2',4,4',6,6'-Hexabromobiphenyl

Synonym: 2,2',4,4',6,6'-HBB

Chemical Name: 2,2',4,4',6,6'-hexabromobiphenyl

CAS Registry No: 59261-08-4

Molecular Formula: $C_{12}H_4Br_6$

Molecular Weight: 627.584

Melting Point ($^{\circ}C$):

176 (Gobas et al. 1988; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

256.6 (Ruelle & Kesselring 1997)

324.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.033 (mp at $176^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.23×10^{-4} (generator column-GC, Gobas et al. 1988)

0.0210 (lit. mean, Chessells et al. 1992)

1.04×10^{-4} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

8.033×10^{-6} (for hexabrominated biphenyl, GC-RT correlation, Watanabe & Tatsukawa 1989)

4.52×10^{-10} (quoted, Pijnenburg et al. 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.50 (for hexabrominated biphenyl, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

7.20 (HPLC-RT correlation, Gobas et al. 1987, 1989)

7.20; 5.09 (quoted; calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

5.85 (guppy, lipid weight-based, Gobas et al. 1989)

4.26 (calculated- K_{ow} , Chessells et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

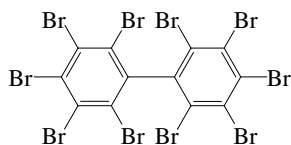
Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$\log k_1 = 2.51 d^{-1}$; $\log k_2 = -2.15 d^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

4.1.4.11 Decabromobiphenyl



Common Name: Decabromobiphenyl

Synonym: PBB-209

Chemical Name:

CAS Registry No: 13654-09-6

Molecular Formula: $C_{12}Br_{10}$

Molecular Weight: 943.168

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

417.6 (calculated-Le Bas method at normal boiling point)

Heat of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$):

$> 1.33 \times 10^{-9}$ (GC-RT correlation, Watanabe & Tatsukawa 1989)

$< 7.4 \times 10^{-4}$ (quoted, Pijnenburg et al. 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.58; 12.63, 9.36 (generator column-GC; calculated-group contribution method, estimated-TSA and K_{ow} , Doucette & Andren 1987)

8.58; 10.42, 13.87, 8.46, 8.69, 7.10 (generator column-GC; calculated- π const., HPLC-RT correlation, calculated-MW, calculated-MCI χ , calculated-TSA and K_{ow} , Doucette & Andren 1988b)

8.60 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

4.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 4.2.1
Summary of physical properties of polynuclear aromatic hydrocarbons (PAHs)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p.°C	b.p.°C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol	
							MW/ρ at 20°C	Le Bas
Indan	496-11-7	C ₉ H ₁₀	118.175	-51.38	177.97	1	123.0	143.7
Naphthalene	91-20-3	C ₁₀ H ₈	128.171	80.26	217.9	0.287	125.0	147.6
1-Methyl-	90-12-0	C ₁₁ H ₁₀	142.197	-30.43	244.7	1	139.4	169.8
2-Methyl-	91-57-6	C ₁₁ H ₁₀	142.197	34.6	241.1	0.805	141.4	169.8
1,2-Dimethyl-	573-98-8	C ₁₂ H ₁₂	156.223	0.8	266.5	1		192.0
1,3-Dimethyl-	575-41-7	C ₁₂ H ₁₂	156.223	-6	263	1	154.0	192.0
1,4-Dimethyl-	571-58-4	C ₁₂ H ₁₂	156.223	7.6	268	1	153.7	192.0
1,5-Dimethyl-	571-61-9	C ₁₂ H ₁₂	156.223	82	265	0.276		192.0
2,3-Dimethyl-	581-40-8	C ₁₂ H ₁₂	156.223	105	268	0.164	155.8	192.0
2,6-Dimethyl-	581-42-0	C ₁₂ H ₁₂	156.223	112	262	0.140	155.8	192.0
1-Ethyl-	1127-76-0	C ₁₂ H ₁₂	156.223	-10.9	258.6	1	155.0	192.0
2-Ethyl-	939-27-5	C ₁₂ H ₁₂	156.223	-7.4	258	1	157.4	192.0
1,4,5-Trimethyl-	2131-41-1	C ₁₃ H ₁₄	170.250	63	285	0.424		214.2
Biphenyl	92-52-4	C ₁₂ H ₁₀	154.207	68.93	256.1	0.371	148.3	184.6
4-Methyl-	644-08-6	C ₁₃ H ₁₂	168.234	49.5	267.5	0.575		206.8
4,4'-Dimethyl-	613-33-2	C ₁₄ H ₁₄	182.261	125	295	0.104		229.0
Diphenylmethane	101-81-5	C ₁₃ H ₁₂	168.234	25.4	265	0.991	167.2	206.8
Bibenzyl	103-29-7	C ₁₄ H ₁₄	182.261	52.5	284	0.537		229.0
<i>trans</i> -Stilbene	103-30-0	C ₁₄ H ₁₂	180.245	124.2	307	0.106	185.7	221.6
Acenaphthylene	208-96-8	C ₁₂ H ₈	150.192	91.8	280	0.221		165.7
Acenaphthene	83-32-9	C ₁₂ H ₁₀	154.207	93.4	279	0.213	126.2	173.1
Fluorene	86-73-7	C ₁₃ H ₁₀	166.218	114.77	295	0.132		187.9
1-Methylfluorene	1730-37-6	C ₁₄ H ₁₂	180.245	87	318	0.246		210.1
Phenanthrene	85-01-8	C ₁₄ H ₁₀	178.229	99.24	340	0.187		199.2
1-Methyl-	832-69-9	C ₁₅ H ₁₂	192.256	123	354	0.109		221.4
Anthracene	120-12-7	C ₁₄ H ₁₀	178.229	215.76	339.9	0.0134		196.7
2-Methyl-	613-12-7	C ₁₅ H ₁₂	192.256	209	359	0.0157		218.9
9-Methyl-	779-02-2	C ₁₅ H ₁₂	192.256	81.5		0.279		218.9
9,10-Dimethyl-	781-43-1	C ₁₆ H ₁₄	206.282	183.6	360	0.0278		241.1

(Continued)

TABLE 4.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol	
							MW/ρ at 20°C	Le Bas
Pyrene	129-00-0	C ₁₆ H ₁₀	202.250	150.62	404	0.0585		213.8
Fluoranthene	206-44-0	C ₁₆ H ₁₀	202.250	110.19	384	0.146		217.3
Benzo[<i>a</i>]fluorene	238-84-6	C ₁₇ H ₁₂	216.227	189.5	405	0.0243		239.5
Benzo[<i>b</i>]fluorene	243-17-4	C ₁₇ H ₁₂	216.227	212	401	0.0146		239.5
Chrysene	218-01-9	C ₁₈ H ₁₂	228.288	255.5	448	0.00548	179.2	250.8
Triphenylene	217-59-4	C ₁₈ H ₁₂	228.288	197.8	425	0.0202		250.8
<i>o</i> -Terphenyl	84-15-1	C ₁₈ H ₁₄	230.304	56.2	332	0.494		273.2
<i>m</i> -Terphenyl	92-06-8	C ₁₈ H ₁₄	230.304	87	363	0.246	192.1	273.2
<i>p</i> -Terphenyl	92-94-4	C ₁₈ H ₁₄	230.304	213.9	376	0.0140		273.2
Naphthacene	92-24-0	C ₁₈ H ₁₂	228.288	357	sublim	0.00055		250.8
Benz[<i>a</i>]anthracene	56-55-3	C ₁₈ H ₁₂	228.288	160.5	438	0.0468		248.3
Benzo[<i>b</i>]fluoranthene	205-99-2	C ₂₀ H ₁₂	252.309	168	481	0.0395		268.9
Benzo[<i>j</i>]fluoranthene	205-82-3	C ₂₀ H ₁₂	252.309	166	480	0.0414		268.9
Benzo[<i>k</i>]fluoranthene	207-08-9	C ₂₀ H ₁₂	252.309	217	480	0.0131		268.9
Benzo[<i>a</i>]pyrene	50-32-8	C ₂₀ H ₁₂	252.309	181.1	495	0.0294		262.9
Benzo[<i>e</i>]pyrene	192-97-2	C ₂₀ H ₁₂	252.309	181.4	311	0.0292		262.9
Perylene	198-55-0	C ₂₀ H ₁₂	252.309	277.76	503	0.00331		262.9
7,12-DMBA	57-97-6	C ₂₀ H ₁₆	256.341	122.5		0.111		292.7
9,10-DMBA	56-56-35	C ₂₀ H ₁₆	256.341	122		0.112		292.7
3-MCA	56-49-5	C ₂₁ H ₁₆	268.352	180		0.0301	209.6	296.0
Benzo[ghi]perylene	191-24-2	C ₂₂ H ₁₂	276.330	272.5		0.00373		277.5
Indeno[1,2,3- <i>c,d</i>]pyrene	193-39-5	C ₂₂ H ₁₂	276.330	162		0.0453		283.5
Dibenz[<i>a,c</i>]anthracene	215-58-7	C ₂₂ H ₁₄	278.346	205		0.0171		299.9
Dibenz[<i>a,h</i>]anthracene	53-70-3	C ₂₂ H ₁₄	278.346	269.5	524	0.00399		299.9
Dibenz[<i>a,j</i>]anthracene	224-41-9	C ₂₂ H ₁₄	278.346	197.5		0.0203		299.9
Pentacene	135-48-8	C ₂₂ H ₁₄	278.346	> 300 dec				299.9
Coronene	191-07-1	C ₂₄ H ₁₂	300.352	437.4	525	0.00009		292.1
2,4",5-Trichloro- <i>p</i> -terphenyl	61576-93-0	C ₁₈ H ₁₁ Cl ₃	333.639	92		0.220		335.9
2,4,4",6-Tetrachloro- <i>p</i> -terphenyl		C ₁₈ H ₁₀ Cl ₄	368.084	114		0.134		356.8
1-Chloronaphthalene	90-13-1	C ₁₀ H ₇ Cl	162.616	-2.5	259	1	136.2	168.5
2-Chloronaphthalene	91-58-7	C ₁₀ H ₇ Cl	162.616	58	256	0.474		168.5
1,2-Dichloronaphthalene	2050-69-3	C ₁₀ H ₆ Cl ₂	197.061	36	296.5	0.780		189.4
1,4-Dichloronaphthalene	1825-31-6	C ₁₀ H ₆ Cl ₂	197.061	67.5	288	0.383		189.4
1,8-Dichloronaphthalene	2050-74-0	C ₁₀ H ₆ Cl ₂	197.061	89	sublim	0.236		189.4

2,3-Dichloronaphthalene	2050–75–1	C ₁₀ H ₆ Cl ₂	197.061	120		0.117		189.4
2,7-Dichloronaphthalene	2198–77–8	C ₁₀ H ₆ Cl ₂	197.061	115		0.131		189.4
1,2,3-Trichloronaphthalene	50402–52–3	C ₁₀ H ₅ Cl ₃	231.506	81–84		0.273		210.3
1,3,7-Trichloronaphthalene	55720–37–1	C ₁₀ H ₅ Cl ₃	231.506	113	274	0.137		210.3
1,2,3,4-Tetrachloronaphthalene	20020–02–4	C ₁₀ H ₄ Cl ₄	265.951	199		0.0196		231.2
1,2,3,5-Tetrachloronaphthalene	53555–63–8	C ₁₀ H ₄ Cl ₄	265.951	141		0.0728		231.2
1,3,5,7-Tetrachloronaphthalene	53555–64–9	C ₁₀ H ₄ Cl ₄	265.951	179		0.0308		231.2
1,3,5,8-Tetrachloronaphthalene	31604–28–1	C ₁₀ H ₄ Cl ₄	265.951	131		0.0912		231.2
1,2,3,4,6-Pentachloronaphthalene	67922–25–2	C ₁₀ H ₃ Cl ₅	300.396	147		0.0635		252.1
1,2,3,5,7-Pentachloronaphthalene	53555–65–0	C ₁₀ H ₃ Cl ₅	300.396	171	313	0.0369		252.1
1,2,3,5,8-Pentachloronaphthalene	150224–24–1	C ₁₀ H ₃ Cl ₅	300.396	174–176		0.0340		252.1
1,2,3,4,5,7-Hexachloronaphthalene	67927–67–4	C ₁₀ H ₂ Cl ₆	334.842	194	331	0.0220		273.0
1,2,3,4,6,7-Hexachloronaphthalene	103426–96–6	C ₁₀ H ₂ Cl ₆	334.842	205–206		0.0340		273.0
1,2,3,5,6,7-Hexachloronaphthalene	103426–97–7	C ₁₀ H ₂ Cl ₆	334.842	234–235		0.00880		273.0
1,2,3,5,7,8-Hexachloronaphthalene	103426–94–4	C ₁₀ H ₂ Cl ₆	334.842	148–149		0.0614		273.0
1,2,3,4,5,6,7-Heptachloro-	58863–14–2	C ₁₀ HCl ₇	369.287					293.9
1,2,3,4,5,6,8-Heptachloro-	58863–15–3	C ₁₀ HCl ₇	369.287	194	348	0.0220		293.9
Octachloronaphthalene	2234–13–1	C ₁₀ Cl ₈	403.731	197.5	365	0.0203		314.8
1-Bromonaphthalene	90–11–9	C ₁₀ H ₇ Br	207.067	6.1	281	1	140.0	170.9
2-Bromonaphthalene	580–13–1	C ₁₀ H ₇ Br	207.067	55.9	281.5	0.498		170.9
1,4-Dibromonaphthalene	83–53–4	C ₁₀ H ₆ Br ₂	285.963	83	310	0.270		194.2
2,3-Dibromonaphthalene	13214–70–5	C ₁₀ H ₆ Br ₂	285.963	140		0.0744		194.2
4-Bromobiphenyl	92–66–0	C ₁₂ H ₉ Br	233.103	91.5	310	0.223		207.9
4,4'-Dibromobiphenyl	92–86–4	C ₁₂ H ₈ Br ₂	312.000	164	357.5	0.0433		231.2
2,4,6-Tribromobiphenyl	59080–33–0	C ₁₂ H ₇ Br ₃	390.896	64		0.414		254.5
2,2',5,5'-Tetrabromobiphenyl	59080–37–4	C ₁₂ H ₆ Br ₄	469.792	144		0.0680		277.8
2,2',4,5,5'-Pentabromobiphenyl	6788–96–4	C ₁₂ H ₅ Br ₅	548.688	157		0.0507		301.1
2,2',4,4',6,6'-Hexabromobiphenyl	59261–08–4	C ₁₂ H ₄ Br ₆	627.584	176		0.0330		324.4
Decabromobiphenyl	13654–09–6	C ₁₂ Br ₁₀	943.168					417.6

Note:

3-MCA	3-Methylcholanthrene
7,12-DMBA	7,12-Dimethylbenz[<i>a</i>]anthracene
9,10-DMBA	9,10-Dimethylbenz[<i>a</i>]anthracene

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

TABLE 4.2.2

Summary of selected physical-chemical properties of polynuclear aromatic hydrocarbons (PAHs) at 25°C

Compound	Selected properties		Solubility			Henry's law constant	
	Vapor pressure					H/(Pa·m³/mol)	
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mmol/m³)	C _L /(mmol/m³)	log K _{OW}	calculated P/C
Indan	197	197	100	846.2	846.2	3.33	232.8
Naphthalene	10.4	36.24	31	241.9	842.7	3.37	43.00
1-Methyl-	8.84	8.84	28	196.9	196.9	3.87	44.89
2-Methyl-	9.0	11.2	25	175.8	218.4	3.86	51.19
1,2-Dimethyl-	0.87	0.87				4.31	
1,3-Dimethyl-			8	51.21	51.21	4.42	
1,4-Dimethyl-	2.27	2.27	11.4	72.97	72.97	4.37	31.11
1,5-Dimethyl-			3.1	19.84	71.90	4.38	
2,3-Dimethyl-	1.0	6.10	2.5	16.00	97.58	4.40	62.49
2,6-Dimethyl-	1.4	10.0	1.7	10.88	77.73	4.31	128.7
1-Ethyl-	2.51	2.51	10.1	64.65	64.65	4.40	38.82
2-Ethyl-	4.0	4.0	8.0	51.21	51.21	4.38	78.11
1,4,5-Trimethyl-	0.681	1.61	2.1	12.33	29.09	5.00	55.21
Biphenyl	1.3	3.50	7.0	45.39	122.4	3.90	28.64
4-Methyl-			4.05	24.07	41.87	4.63	
4,4'-Dimethyl-			0.175	0.960	9.232	5.09	
Diphenylmethane	0.0885	0.0893	16	95.10	95.10	4.14	0.931
Bibenzyl	0.406	0.756	4.37	23.98	44.65	4.70	16.93
<i>trans</i> -Stilbene	0.065	0.613	0.29	1.609	15.18	4.81	40.40
Acenaphthylene	0.9	4.14	16.1	107.2	485.0	4.00	8.396
Acenaphthene	0.3	1.41	3.80	24.64	115.7	3.92	12.17
Fluorene	0.09	0.682	1.90	11.43	85.60	4.18	7.873
1-Methyl-			1.09	6.047	24.58	4.97	
Phenanthrene	0.02	0.107	1.10	6.172	33.00	4.57	3.240
1-Methyl-			0.27	1.404	12.88	5.14	
Anthracene	0.001	0.0746	0.045	0.252	18.84	4.54	3.961
2-Methyl-			0.03	0.156	9.939	5.15	
9-Methyl-	0.00224	0.00803	0.261	1.358	4.866	5.07	1.650
9,10-Dimethyl-	1.53 × 10 ⁻⁴	5.50 × 10 ⁻³	0.056	0.271	9.765	5.25	0.564
Pyrene	0.0006	0.0119	0.132	0.652	12.89	5.18	0.919
Fluoranthene	0.00123	8.42 × 10 ⁻³	0.26	1.286	8.805	5.22	0.957
Benzo[<i>a</i>]fluorene			0.045	0.208	8.564	5.40	

Benzo[<i>b</i>]fluorene			0.002	0.00925	0.634	5.75	
Chrysene	5.70×10^{-7}	1.07×10^{-4}	0.002	0.00876	1.599	5.60	0.065
Triphenylene	2.30×10^{-9}	1.21×10^{-4}	0.043	0.188	9.325	5.49	0.012
<i>p</i> -Terphenyl	4.86×10^{-9}	3.47×10^{-4}	0.0180	0.0782	5.583	6.03	0.062
Naphthacene	7.30×10^{-9}	1.33×10^{-5}	0.0006	0.00263	4.779	5.76	2.77×10^{-3}
Benz[<i>a</i>]anthracene	2.80×10^{-5}	5.98×10^{-4}	0.011	0.0482	1.030	5.91	0.581
Benzo[<i>b</i>]fluoranthene			0.0015	0.00595	0.150	5.80	
Benzo[<i>j</i>]fluoranthene			0.0025	0.0099	0.239		
Benzo[<i>k</i>]fluoranthene	5.20×10^{-8}	3.97×10^{-9}	0.0008	0.00317	0.242	6.00	0.016
Benzo[<i>a</i>]pyrene	7.00×10^{-7}	2.38×10^{-5}	0.0038	0.0151	0.512	6.04	0.046
Benzo[<i>e</i>]pyrene	7.40×10^{-7}	2.53×10^{-5}	0.004	0.0159	0.543		0.047
Perylene	1.40×10^{-8}	4.23×10^{-9}	0.0004	0.00159	0.479	6.25	8.83×10^{-3}
7,12-DMBA	3.84×10^{-8}	3.45×10^{-7}	0.0500	0.195	1.757	6.00	1.97×10^{-4}
9,10-DMBA	3.73×10^{-7}	3.33×10^{-9}	0.0435	0.170	1.543	6.00	2.20×10^{-3}
3-MCA	1.03×10^{-9}	3.42×10^{-5}	0.0019	0.00708	0.235	6.42	0.145
Benzo[<i>ghi</i>]perylene		2.25×10^{-5}	0.00026	0.000941	0.252	6.50	
Indeno[1,2,3- <i>c,d</i>]pyrene							
Dibenz[<i>a,c</i>]anthracene	1.30×10^{-9}	7.84×10^{-8}	0.0016	0.00575	0.336		2.26×10^{-4}
Dibenz[<i>a,h</i>]anthracene	3.70×10^{-10}	9.27×10^{-8}	0.0006	0.00216	0.540	6.75	1.72×10^{-4}
Dibenz[<i>a,j</i>]anthracene			0.012	0.0431	2.210		
Pentacene	1.0×10^{-10}						
Coronene	2.0×10^{-10}	2.22×10^{-9}	0.00014	0.000466	5.179	6.75	4.29×10^{-4}

Abbreviations:

3-MCA	3-Methylcholanthrene
7,12-DMBA	7,12-Dimethylbenz[<i>a</i>]anthracene
9,10-DMBA	9,10-Dimethylbenz[<i>a</i>]anthracene

TABLE 4.2.3

Suggested half-life classes of polynuclear aromatic hydrocarbons (PAHs) in various environment compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Indan	2	4	6	7
Naphthalene	2	4	6	7
1-Methyl-	2	4	6	7
2,3-Dimethyl-	2	4	6	7
1-Ethyl-	2	4	6	7
1,4,5-Trimethyl-	2	4	6	7
Biphenyl	3	4	5	6
Acenaphthene	3	5	7	8
Fluorene	3	5	7	8
Phenanthrene	3	5	7	8
Anthracene	3	5	7	8
Pyrene	4	6	8	9
Fluoranthene	4	6	8	9
Chrysene	4	6	8	9
Benz[<i>a</i>]anthracene	4	6	8	9
Benzo[<i>k</i>]fluoranthene	4	6	8	9
Benzo[<i>a</i>]pyrene	4	6	8	9
Perylene	4	6	8	9
Dibenz[<i>a,h</i>]anthracene	4	6	8	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,00
9	55000 (~ 6 years)	> 30,000

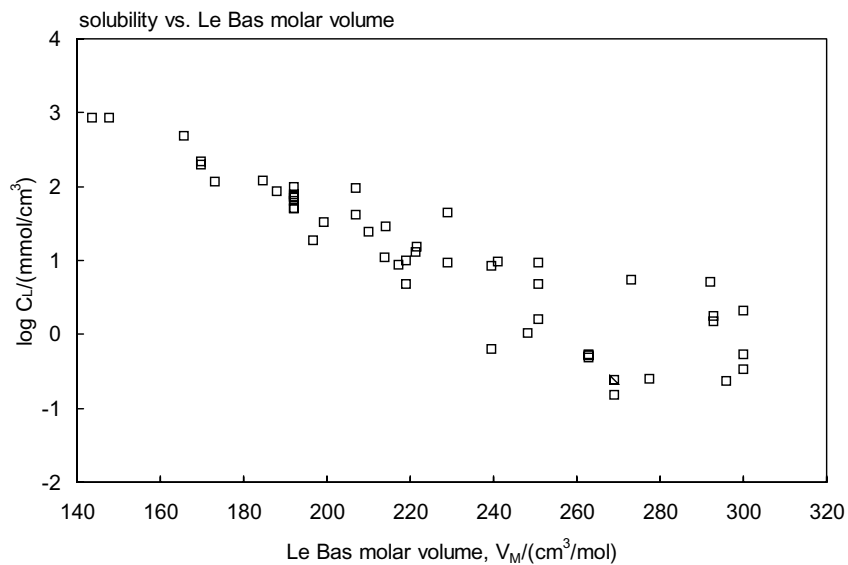


FIGURE 4.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polynuclear aromatic hydrocarbons.

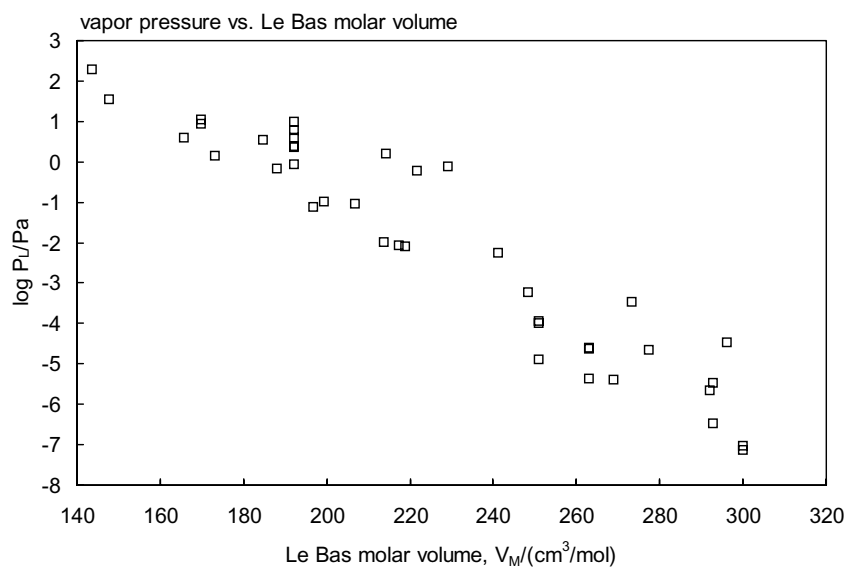


FIGURE 4.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polynuclear aromatic hydrocarbons.

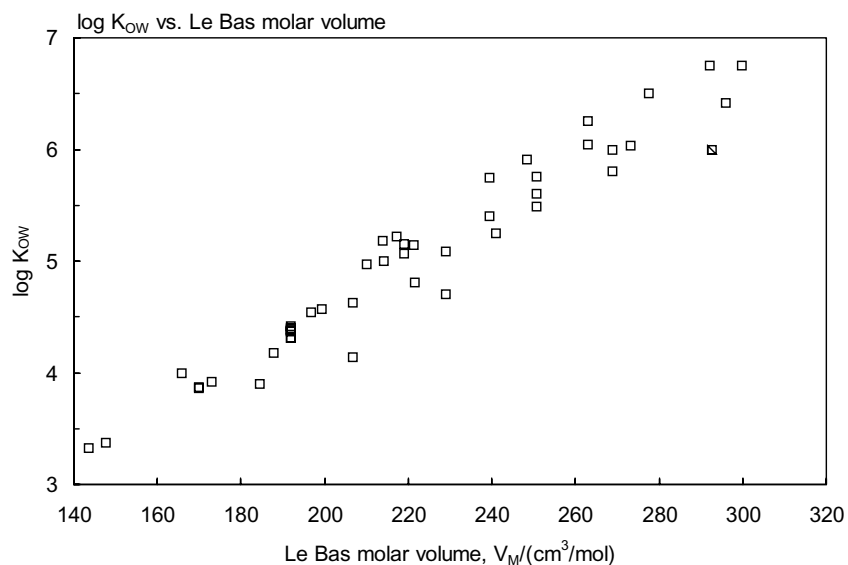


FIGURE 4.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polynuclear aromatic hydrocarbons.

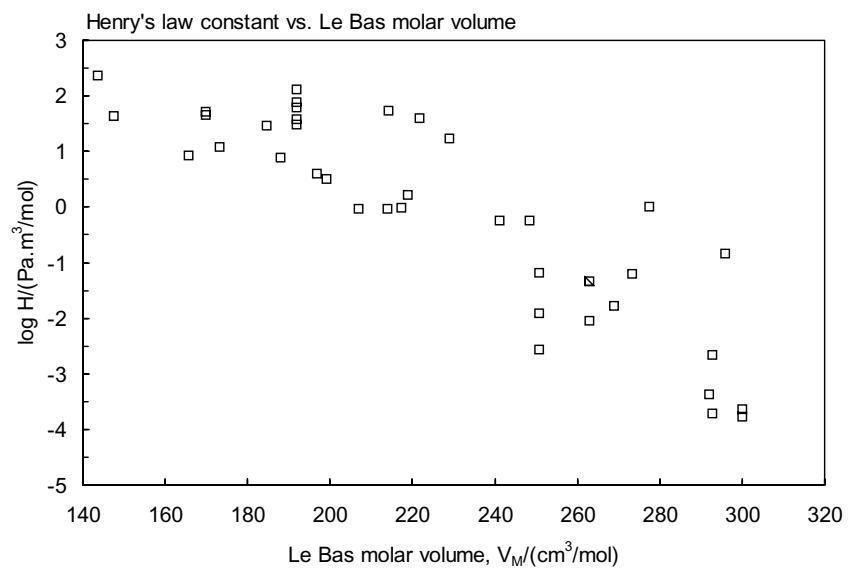


FIGURE 4.2.4 Henry's law constant versus Le Bas molar volume for polynuclear aromatic hydrocarbons.

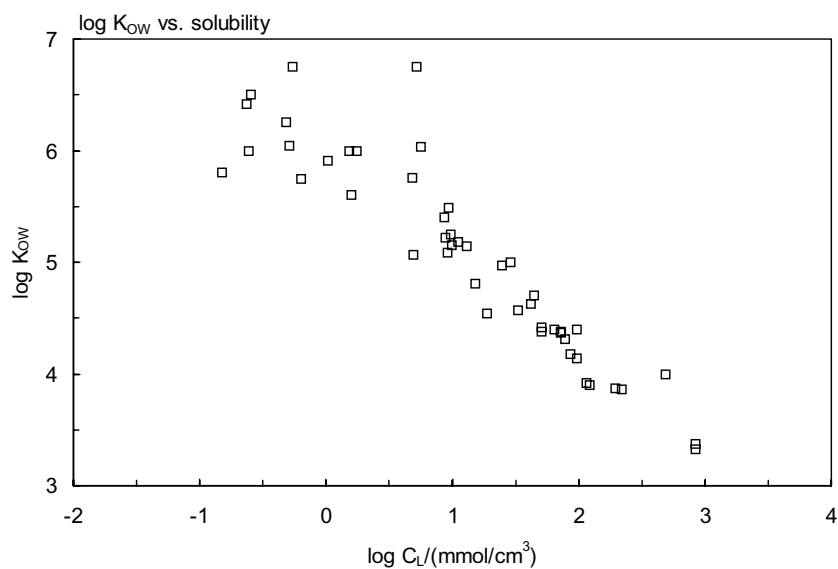


FIGURE 4.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polynuclear aromatic hydrocarbons.

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5 Halogenated Aliphatic Hydrocarbons

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	Fluoroethane	
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	1,2-Difluoroethane	
	1,1,1-Trifluoroethane	
	1,1,2-Trifluoroethane	
	1,1,2,2-Tetrafluoroethane	
	1,1,1,2-Tetrafluoroethane	
	Pentafluoroethane	
	Hexafluoroethane	
	1-Chloro-2-fluoroethane	
	1-Chloro-1,1-difluoroethane	
	1-Chloro-1,1,2-trifluoroethane	
	1-Chloro-1,2,2,2-tetrafluoroethane	
	1-Chloropentafluoroethane	

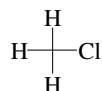
1,1-Dichloro-1-fluoroethane
1,2-Dichloro-1,1-difluoroethane
1,1-Dichlorotrifluoroethane
1,2-Dichloro-1,1,2,2-tetrafluoroethane
1,1-Dichloro-1,2,2,2-tetrafluoroethane
1,1,1-Trichloro-2,2,2-trifluoroethane
1,1,2-Trichloro-1,2,2-trifluoroethane
1,1-Difluorotetrachloroethane
1,1,2,2-Tetrachloro-1,2-difluoroethane
2-Fluoropropane
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1,1,1,3,3-Pentafluoropropane
1,1,1,2,2-Pentafluoropropane
1,1,1,2,3,3-Hexafluoropropane
1,1,1,3,3,3-Hexafluoropropane
1,1,1,2,3,3,3-Heptafluoropropane
Octafluoropropane
Trichlorotrifluoropropane
1-Chloro-2,2,2-trifluoropropane
Perfluorobutane
Perfluorocyclobutane
Perfluoropentane
Perfluorocyclopentane
Perfluoro-2-methylcyclopentane
Perfluoro-3-methylcyclopentane
Perfluorocyclohexane
Perfluorohexane
Fluoroethene
1,1-Difluoroethene
Tetrafluoroethene
Chlorotrifluoroethene
1,2-Dichloro-1,2-difluoroethene
1,1-Dichloro-2,2-difluoroethene
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5.1 LIST OF CHEMICALS AND DATA COMPILATIONS

5.1.1 CHLOROALKANES AND CHLOROALKENES

5.1.1.1 Chloromethane (Methyl chloride)



Common Name: Chloromethane

Synonym: methyl chloride, monochloromethane

Chemical Name: chloromethane

CAS Registry No: 74-87-3

Molecular Formula: CH₃Cl

Molecular Weight: 50.488

Melting Point (°C):

−97.7 (Lide 2003)

Boiling Point (°C):

−24.09 (Lide 2003)

Density (g/cm³ at 20°C):

0.9159 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

0.9214, 0.9111 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

55.0 (calculated-density, Wang et al. 1992)

50.6, 48.8, 54.3, 50.4 (exptl., Tyn and Calus method, Schroeder method, Le Bas method, Reid et al. 1987)

50.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

19.06, 21.45 (at 25°C, at normal boiling point, Dreisbach 1961)

18.92, 21.40 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.43 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

7400 (30°C at 1 atm, McGovern 1943)

5346 (gravitational method, Glew & Moelwyn-Hughes 1953)

6450 (20°C, Dean 1973)

7250 (20°C under 101.3 kPa pressure of CH₃Cl, McConnell et al. 1975; Pearson & McConnell 1975)

6270, 5380 (20, 25°C literature average at 760 mmHg, Dilling 1977)

5325* (summary of literature data, temp range 5–80°C, Horvath 1982)

4800 (Dean 1985)

6480 (30°C, quoted, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

98048* (248.9 K, static-manometer, measured range 191.4–248.9 K, Messerly & Aston 1940)

101325* (−24.0°C, summary of literature data, temp range −99.58 to 24.0°C, Stull 1947)

559860 (interpolated from graph, temp range −50 to 60°C, McGovern 1943)

100800 (Glew & Moelwyn-Hughes 1953)

574500 (calculated-Antoine eq., Dreisbach 1959; 1961)

log (P/mmHg) = 6.99445 − 902.451/(243.63 + t/°C); temp range −80 to 3°C (Antoine eq. for liquid state, Dreisbach 1959; 1961)

$\log (P/\text{mmHg}) = 6.99445 - 902.451/(243.60 + t/^{\circ}\text{C})$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

1081* (29.43°C, concentration ratio, measured range 29.43–40.59°C, Swain & Thornton 1962)

539300 (20–25°C, calculated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 5375.3/(T/K)] + 7.546207$; temp range –99 to 137.5°C (Antoine eq., Weast 1972–73)

567900, 576300 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/\text{mmHg}) = 6.98762 - 899.739/(242.921 + t/^{\circ}\text{C})$; temp range –69.2 to –23°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log (P/\text{mmHg}) = 6.09349 - 948.582/(249.336 + t/^{\circ}\text{C})$; temp range –75.2 to 5°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

574600 (selected lit., Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.16533 - 920.86/(245.58 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P/\text{mmHg}) = 7.09349 - 948.58/(249.34 + t/^{\circ}\text{C})$; temp range –77 to –5°C (Antoine eq., Dean 1985, 1992)

572800 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.11935 - 902.451/(-29.55 + T/K)$; temp range 180–266 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.04835 - 869.887/(-33.773 + T/K)$; temp range 247–310 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.94638 - 1448.913/(47.966 + T/K)$; temp range 308–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.94022 - 1447.601/(48.385 + T/K)$; temp range 368–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 25.7264 - 1.7503 \times 10^3/(T/K) - 6.7151 \cdot \log (T/K) - 1.2956 \times 10^{-9} \cdot (T/K) + 4.4341 \times 10^{-6} \cdot (T/K)^2$; temp range 175–416 K (vapor pressure eq., Yaws 1994)

498820 (293.15 K, selected summary of literature data, temp range 175.44–293.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

953*, 957 (distribution ratio, measured range 4–80°C; calculated-P/C, Glew & Moelwyn-Hughes 1953)

$\log \{H/(\text{mmHg} \cdot \text{L/mol})\} = 71.005 - 21.656 \cdot \log (T/K) - 4043.9/(T/K)$; temp range 277.24–353.23 K (Glew & Moelwyn-Hughes 1953)

1010 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

744, 892 (exptl. as per McConnell et al. 1975, calculated-P/C, Neely 1976)

739 (20°C, Pearson & McConnell 1975)

942 (calculated- C_A/C_W , Dilling 1977)

875 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

$\log (k_H/\text{atm}) = 6.93 - 1248.11/(T/K)$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)

951, 950 (calculated-P/C, recommended, Mackay & Shiu 1981)

894* (EPICS-GC/FID, measured range 10.3–34.6°C, Gossett 1987)

$\ln [H/(\text{atm m}^3/\text{mol})] = 9.358 - 4215/(T/K)$, temp range: 10.3–34.6°C (EPICS measurements, Gossett 1987)

669 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

867 (computed value, Yaws et al. 1991)

363, 834 (0, 22°C, distilled water, headspace-GC, Elliot & Rowland 1993)

386 (0°C, gas stripping-GC, Moore et al. 1995)

392, 465, 533 (0, 3.0, 6.0°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

$\ln K_{AW} = 9.17 - 2982/(T/K)$, seawater of salinity of 30.4‰, temp range: 0–6°C (Moore et al. 1995)

668 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

743 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{AW} = 3.899 - 1292/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.91 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)

0.91 (shake flask, Log P Database, Hansch & Leo 1987)

0.89, 0.936 (calculated-MO, calculated- π substituent const., Bodor et al. 1989)

0.91 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

1.39 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

0.505 (microorganism-water, calculated from K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

0.633 (calculated- K_{OW} , Mabey et al. 1982)

0.778 (selected, Jury et al. 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: half-life of 27–28 min for initial concentration of 1 mg/L in an open container stirred at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation $t_{1/2}(\text{exptl.}) = 27.6$ min, $t_{1/2}(\text{calc}) = 0.599$ min, 14.9 min from water (Dilling 1977)

$t_{1/2} \sim 2.4$ h from water (estimated, Thomas 1982);

$t_{1/2} \sim 120$ d from soil (estimated, Jury et al. 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:

$k_{OH} = 4.7 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, bimolecular rate constant (Yung et al. 1975)

$k_{OH} = 8.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, bimolecular rate constant with a lifetime $\tau = 0.37$ yr in the troposphere (Cox et al. 1976)

$k_{OH}^* = (4.29 \pm 0.21) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 250–350 K, with a tropospheric lifetime of 1.19 yr (flash photolysis-resonance fluorescence, Davis et al. 1976)

$k_{OH}^* = (4.29 \pm 0.21) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K with lifetime $\tau = 1.19$ yr, measured range 250–350 K (flash photolysis-resonance fluorescence, Davis et al. 1976; quoted, Altshuller 1980)

$k_{OH} = (3.6 \pm 0.8) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH}^* = (4.4 \pm 0.5) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.4 K, measured range 298–423 K and the calculated $t_{1/2} \sim 0.2$ yr in lower troposphere (flash photolysis-RF, Perry et al. 1976)

$k_{OH} = 24.7 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 297 K (flash photolysis-resonance absorption, Paraskevopoulos et al. 1981)

$k_{OH} = 5.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 231 d, loss of 0.4% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH}^* = 3.95 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 293 K, measured range 247–483 K (discharge-flow resonance fluorescence, Jeong & Kaufman, 1982)

$k_{OH}(\text{calc}) = 2.4 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $0.05 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{OH}^* = 4.36 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH}^* = 4.9 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–800 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)

$k_{NO_3} = 9.8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1991)

Hydrolysis: $k = 6.8 \times 10^{-5} \text{ h}^{-1}$ with hydrolytic $t_{1/2} = 417$ d at pH 7 and 25°C (Radding et al. 1977; Mabey & Mill 1978; quoted, Callahan et al. 1979; Mabey et al. 1982);

hydrolysis $k = 2.3710^{-8} \text{ h}^{-1}$ with $t_{1/2} 0.93$ yr (Mabey & Mill 1978)

$t_{1/2} = 7000$ h, based on neutral and base catalyzed hydrolysis rate constants at 25°C extrapolated from data obtained at higher temperatures (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 168\text{--}672$ h, based on unacclimated aerobic aqueous screening test data for dichloromethane from experiments utilizing selected domestic waste water inoculum (Tabak et al. 1981; quoted, Howard et al. 1991) and activated sludge inoculum (Klecka 1982; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (Darnall et al. 1976);
tropospheric lifetime of 1.19 yr due to reaction with OH radical (Davis et al. 1976);
estimated residence time to be about 2 yr for the reaction with OH radical in troposphere (Singh et al. 1979);
lifetime $\tau = 1.19$ yr for reaction with OH radical (Altshuller 1980)
residence time of 231 d, loss of 0.4% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
estimated residence time in troposphere to be 1 yr (Lyman 1982);
 $t_{1/2} = 1472\text{--}14717$ h, based on photooxidation half-life in air from measured rate constants for reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);
estimated tropospheric lifetimes of 1.3 yr, and 1.54 yr by rigorous calculation (Nimitz & Skaggs 1992).
lifetime for reaction with OH radicals, $\tau = 11.7$ yr for Polar region, $\tau = 2.2$ yr for Middle region and $\tau = 0.8$ yr for Tropical region in the Northern hemisphere; $\tau = 0.9$ yr for Tropical, $\tau = 3.6$ yr for Middle and $\tau = 12.3$ yr for Polar region in the Southern hemisphere; $\tau = 1.4$ yr in the Global atmosphere, based on data from 1981–1996 (Khalil & Rasmussen 1999a)
Surface water: $t_{1/2} = 168\text{--}672$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).
Ground water: $t_{1/2} = 336\text{--}1344$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $t_{1/2} > 50$ d (Ryan et al. 1988); estimated $t_{1/2} = 120$ d for volatilization from soil (Jury et al. 1990);
 $t_{1/2} = 168\text{--}672$ h, based on estimated aerobic biodegradation half-life (Howard et al. 1991).
Biota: $t_{1/2} > 50$ d, subject to plant uptake from soil via volatilization (Ryan et al. 1988).

TABLE 5.1.1.1.1

Reported aqueous solubilities and Henry's law constants of chloromethane (methyl chloride) at various temperatures

$$S/(\text{wt}\%) = 1.4019 - 6.3562 \times 10^{-2} \cdot (t/^{\circ}\text{C}) + 1.71977 \times 10^{-3} \cdot (t/^{\circ}\text{C})^2 - 2.8262 \times 10^{-5} \cdot (t/^{\circ}\text{C})^3 + 2.5268 \times 10^{-7} \cdot (t/^{\circ}\text{C})^4 - 9.3470 \times 10^{-10} \cdot (t/^{\circ}\text{C})^5 \quad (1)$$

Aqueous solubility		Henry's law constant					
Horvath 1982		Glew & Moelwyn-Hughes 1953		Swain & Thornton 1962		Gossett 1987	
summary of literature data		concentration ratio		concentration ratio		EPICS-GC	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
5	14019	4.09	437	29.44	1081	10.3	396.2
10	9113	10.17	568	29.44	1085	17.5	591.7
20	6274	15.06	681	29.44	1073	24.8	893.7
25	5325	20.03	816	29.43	1080	34.6	1256.4
30	4579	25.01	957	29.43	1084		
40	3490	39.91	1475	40.34	1465	ln H = A - B/(T/K) H/(atm m ³ /mol)	
50	2742	49.78	1860	40.35	1459		
60	2228	59.99	2260	40.35	1460	A	8.637
70	1891	70.06	2746	40.59	1791	B	4128
80	1609	80.08	3173				
		25.0	956				
eq.1	S/wt%	log H = A - B·log (T/K) - C/(T/K) P/(mmHg·L/mol)					
		A	59.096				
		B	21.656				
		C	4043.9				

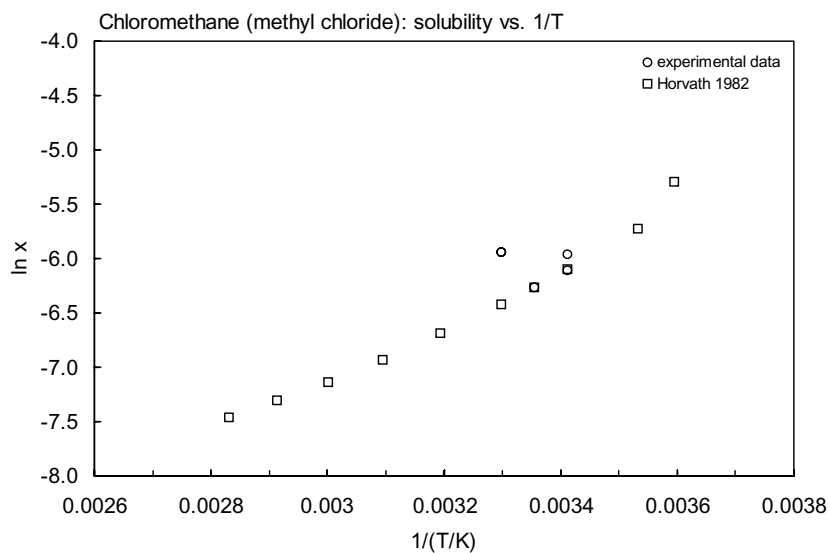


FIGURE 5.1.1.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for chloromethane.

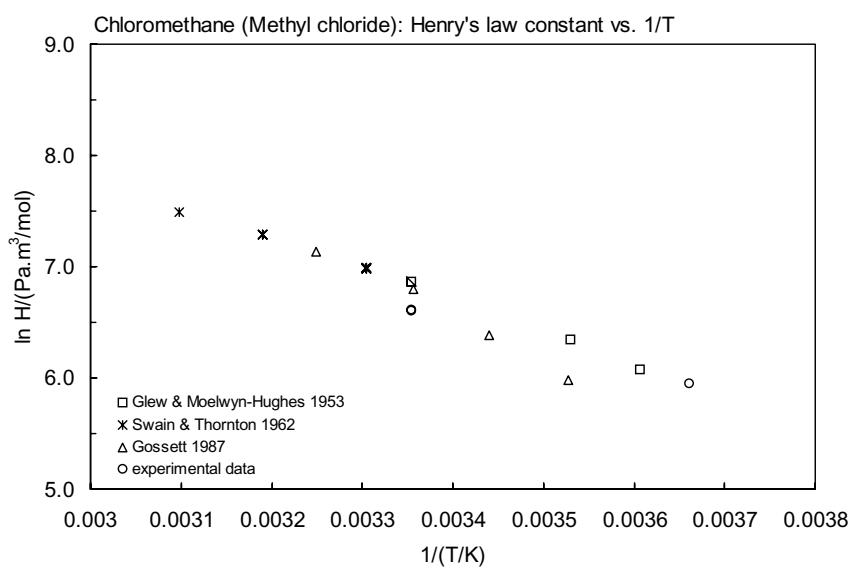


FIGURE 5.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for chloromethane.

TABLE 5.1.1.1.2

Reported vapor pressures of chloromethane (methyl chloride) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot \log (T/K) + D \cdot (T/K)$	(5)		

Messerly & Aston 1940				Stull 1947	
static-manometer				summary of literature data	
T/K	P/Pa	T/K	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
191.424	3509	248.998	101521	-	
191.378	3498	248.943	98048	-99.58	666.6
194.556	4474			-92.4	1333
199.272	6338	eq. 5	P/mmHg	-84.8	2666
206.324	10320	A	31.07167	-76.0	5333
213.539	16343	B	1822.60	-70.4	7999
213.526	16328	C	9.287119	-63.0	13332
222.999	28384	C	0.00555556	-51.2	26664
230.184	41739			-38.0	53329
237.125	59004	mp/K	175.44	-24.0	101325
242.845	77224	bp/K	248.94		
246.441	90805	$\Delta H_v/(\text{kJ mol}^{-1}) = 0.945$		mp/ $^{\circ}\text{C}$	-97.7

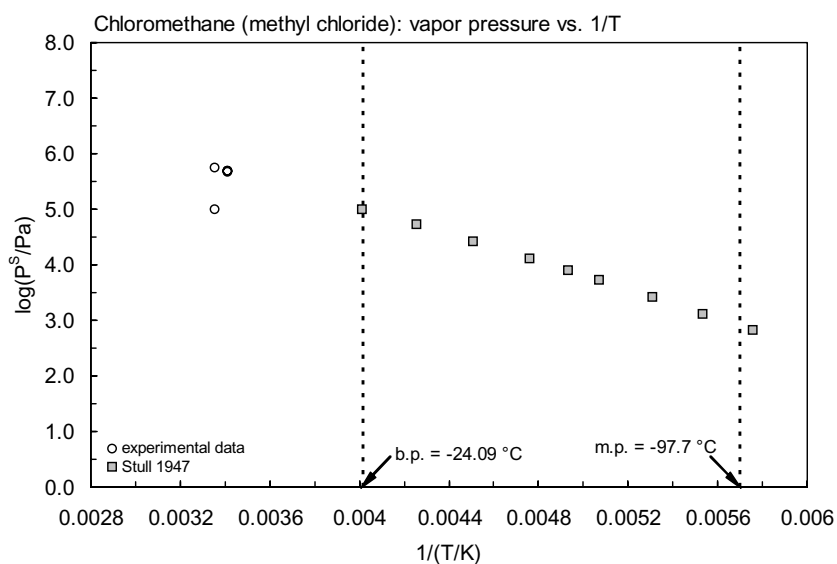
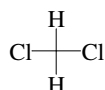


FIGURE 5.1.1.1.3 Logarithm of vapor pressure versus reciprocal temperature for chloromethane.

5.1.1.2 Dichloromethane



Common Name: Dichloromethane

Synonym: methylene chloride, methylene dichloride, methane dichloride, methylene bichloride

Chemical Name: dichloromethane

CAS Registry No: 75-09-2

Molecular Formula: CH_2Cl_2

Molecular Weight: 84.933

Melting Point ($^{\circ}\text{C}$):

-95.2 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

40 (Lide 2003)

Density (g/cm^3 at 20°C):

1.3255, 1.3163 (20°C , 25°C , Dreisbach 1959; 1961)

1.3266 (Horvath 1982; Weast 1982–83)

1.3256, 1.131678 (20°C , 25°C , Riddick et al. 1986)

Molar Volume (cm^3/mol):

64.0 (calculated-density, Wang et al. 1992)

71.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

28.56, 28.98 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

1.435 (calculated, Dreisbach 1959; 1961)

1.472 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

20000* (20°C , volumetric method, Rex 1906)

19910 (Seidell 1940)

13200 (25°C , data presented between 0 – 50°C in graph, McGovern 1943)

34480 (shake flask-residue volume method, Booth & Everson 1948)

13200 (20°C , McConnell et al. 1975; Pearson & McConnell 1975)

20000* (Archer & Sterns 1977; Andelman 1978; measured range 0 – 30°C , quoted, Horvath 1982)

22700, 19400 (1.5, 20°C , literature average, Dilling 1977)

13700 (shake flask-titration/turbidity, Coca et al. 1980)

13030* (summary of literature data, Horvath 1982)

13000 (selected, Thomas 1982; Riddick et al. 1986; Howard 1990)

16700 (Verschueren 1983; selected, Valsaraj 1988)

19020 (calculated-UNIFAC activity coeff., Banerjee 1985)

17200* (26.8°C , shake flask-GC/TC, measured range 0 – 35.7°C , Stephenson 1992)

19260, 19830, 19500, 19500 (20, 30, 35, 40°C , infinite dilution activity coeff. γ° -GC, Tse et al. 1992)

18080, 19995, 20880, 21850 (20, 30, 35, 40°C , infinite dilution activity coeff. γ° -UNIFAC, Tse et al. 1992)

20080, 18800, 18880 (10, 20, 30°C , activity coeff. γ° -differential pressure transducer, Wright et al. 1992)

18650 (gas stripping-GC, Li et al. 1993)

20340 (20°C , limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

46510, 68170 (20°C , 30°C , Rex 1906)

57120 (interpolated from graph, temp range -40 to 110°C , McGovern 1943)

- 57480* (Antoine eq. regression, temp range -70 to 40.7°C , Stull 1947)
 58100 (calculated-Antoine eq., Dreisbach 1959; 1961)
 $\log(P/\text{mmHg}) = 7.07138 - 1134.6/(231.0 + t/^{\circ}\text{C})$; temp range -28 to 121°C (Antoine eq. for liquid state, Dreisbach 1955)
 49704* (21.199°C , temp range -9.03 to 39.429°C , Boublik 1960; quoted, Boublik et al. 1984)
 70530* (29.993°C , temp range 29.993 – 39.993°C , Mueller & Ignatowski 1960)
 $\log(P/\text{mmHg}) = 7.0803 - 1138.91/(231.45 + t/^{\circ}\text{C})$; temp range -28 to 73°C (Antoine eq. for liquid state, Dreisbach 1961)
 57390 (calculated-Antoine eq., temp range -70 to 40.7°C , Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 7572.3/(T/\text{K})] + 8.18330$; temp range -70 to 40.7°C (Antoine eq., Weast 1972–73)
 58275, 57270 (calculated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 9.72567 - 2979.516/(395.553 + t/^{\circ}\text{C})$; temp range 30 – 40°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 48200 (20°C , McConnell et al. 1975; Pearson & McConnell 1975)
 21065, 57062 (1.5 , 25°C , Dow Chemicals data, Dilling 1977)
 57950, 57980 (calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.96841 - 1014.441/(216.227 + t/^{\circ}\text{C})$; temp range 30 – 40°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.18791 - 1127.232/(229.764 + t/^{\circ}\text{C})$; temp range -9.05 to 38.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 47990 (selected, Daniels et al. 1985)
 $\log(P/\text{mmHg}) = 7.4092 - 1325.9/(252.6 + t/^{\circ}\text{C})$; temp range -40 to 40°C (Antoine eq., Dean 1985, 1992)
 58100 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.07622 - 1070.07/(223.24 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 57990 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_1/\text{kPa}) = 6.18649 - 1126.53/(-43.46 + T/\text{K})$; temp range 264 – 312 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_1/\text{kPa}) = 6.88926 - 1545.323/(3.375 + T/\text{K})$; temp range 311 – 383 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_1/\text{kPa}) = 5.87285 - 861.817/(-94.102 + T/\text{K})$; temp range 379 – 455 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P_1/\text{kPa}) = 5.20540 - 449.586/(-193.701 + T/\text{K})$; temp range 450 – 510 K (Antoine eq., Stephenson & Malanowski 1987)
 47660, 71000, 85640, 102540 (20 , 30 , 35 , 40°C , quoted from DIPPR, Tse et al. 1992)
 $\log(P/\text{mmHg}) = 32.5069 - 2.5166 \times 10^3/(T/\text{K}) - 8.8015 \cdot \log(T/\text{K}) + 1.2934 \times 10^{-10} \cdot (T/\text{K}) + 3.3194 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 178 – 510 K (vapor pressure eq., Yaws 1994)
 57844 (selected summary of literature data, temp range 178.25 – 338.15 K, Xiang 2002)
 70486 (30°C , vapor-liquid equilibrium study, Pathare et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 231.3 (calculated as $1/K_{\text{AW}} C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
 301.0 (McConnell et al. 1975; Pearson & McConnell 1975)
 322.3 (calculated, Neely 1976)
 292, 271.5 (exptl., calculated- $C_{\text{A}}/C_{\text{W}}$, Dilling 1977)
 111.3 (20°C , calculated- P/C , Kavanaugh & Trussell 1980)
 $\log(k_{\text{H}}/\text{atm}) = 7.92 - 1821.84/(T/\text{K})$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)
 295 (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
 295* (24.9°C equilibrium cell-concn ratio-GC/FID, measured range 1.9 – 24.9°C Leighton & Calo 1981)
 $\ln(k_{\text{H}}/\text{atm}) = 17.42 - 3645/(T/\text{K})$; temp range 1.9 – 24.9°C (equilibrium cell-concn ratio measurements, Leighton & Calo 1981)
 205.7 (calculated- P/C , Mabey et al. 1982)
 303.9 (calculated- P/C , Thomas 1982)
 229.1 (20°C , EPICS-GC, Lincoff & Gossett 1983)
 227.9 (20°C , EPICS-GC, Lincoff & Gossett 1984)

- 199.6 (20°C, batch air stripping-GC, Lincoff & Gossett 1984)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 8.200 - 4191/(T/K)$; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.035 - 4472/(T/K)$; temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)
 222.0 (EPICS-GC, Gossett 1987)
 173.0* (20°C, EPICS-GC/FID, measured range 9.6–34.6°C, Gossett 1987)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.843 - 5612/(T/K)$; temp range: 9.6–34.6°C (EPICS measurements, Gossett 1987)
 187.7 (20°C, EPICS, Yurteri et al. 1987)
 323 (gas stripping-GC, Warner et al. 1987)
 300* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm-m}^3/\text{mol})] = 8.483 - 4268/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 451.1 (calculated-QSAR, Nirmalakhandan & Speece 1988)
 202.6 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 254.4 (calculated-P/C, Suntio et al. 1988)
 251 (computed value, Yaws et al. 1991)
 213, 314, 375, 456 (20, 30, 35, 40°C, infinite dilution activity coeff. γ° -GC, Tse et al. 1992)
 128, 209, 308 (10, 20, 30°C, activity coeff. γ° -differential pressure transducer, Wright et al. 1992)
 266 (γ° from gas stripping-GC, Li et al. 1993)
 16.72, 26.04 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 197 (20°C, inert gas stripping-GC, Hovorka & Dohnal 1997)
 244.1 (modified EPICS method-GC, Ryu & Park 1999)
 260; 221; 211 (EPICS-GC; quoted lit.; calculated-P/C, David et al. 2000)
 220 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 4.561 - 1644/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 1.25 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
 1.51 (Hansch & Leo 1979)
 1.22 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
 1.25 (HPLC- k' correlation, Tomlinson & Hafkenscheid 1986)
 1.25 (recommended, Sangster 1989)
 1.35* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
 1.25 (recommended, Hansch et al. 1995)
 1.25 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 2.27 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 0.699 (calculated as per Lyman et al. 1982, Howard 1990)
 0.778 (microorganism-water, calculated from K_{OW} , Mabey et al. 1982)
 0.600 (calculated-MCI χ , Koch 1983)
 0.362 (selected, Daniels et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.944 (calculated- K_{OW} , Mabey et al. 1982)
 1.440 (calculated- MCI χ , Koch 1983; quoted, Bahnick & Doucette 1988)
 1.000 (selected, Daniels et al. 1985)
 1.390 (calculated-MCI χ , Bahnick & Doucette 1988)

Sorption Partition Coefficient, $\log K_{OM}$:

- 1.44, 1.23 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, and Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2}(\text{calc}) = 2.23$ min (Mackay & Wolkoff 1973; quoted, Dilling et al. 1975; Callahan et al. 1979);
 $t_{1/2}(\text{calc}) = 20.7$ min (Mackay & Leinonen 1975; quoted, Dilling 1977; Callahan et al. 1979);
 $t_{1/2}(\text{exptl}) = (21 \pm 3)$ min for 1 ppm in water at 25°C when stirred at 200 rpm in water (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);
 evaporation $t_{1/2}(\text{exptl}) = (18.3\text{--}25.2)$ min, $t_{1/2}(\text{calc}) = 2.23$ and 20.7 min at 25°C and $t_{1/2}(\text{exptl.}) = 34.9$ min, $t_{1/2} = 24.5$ min at 1.5°C (Dilling 1977)
 $t_{1/2} \sim 3.0$ h from water (estimated, Thomas 1982);
 $t_{1/2} \sim 100$ d from soil (estimated, Jury et al. 1990).
- Photolysis: estimated photodecomposition $t_{1/2} > 250$ h from a simulated environmental sunlight exposure (> 290 nm at $27 \pm 1^\circ\text{C}$) study (Dilling et al. 1976; quoted, Callahan et al. 1979);
 photodegradation $t_{1/2} = 30\text{--}120$ d (Darnall et al. 1976; quoted, Daniels et al. 1985);
 photocatalyzed mineralization by the presence of TiO_2 with a rate of 1.6 ppm/min per gram of catalyst (Ollis 1985).
- Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
 $k_{\text{OH}} = 1.24 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K corresponding to a lifetime of 0.30 yr (relative rate method, Cox et al. 1976; quoted, Callahan et al. 1979)
 $k_{\text{OH}}^* = (1.16 \pm 0.05) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K with lifetime of 0.39 yr, measured range 245–375 K (flash photolysis-resonance fluorescence, Davis et al. 1976)
 $k_{\text{OH}} = 1.55 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow-LMR, Howard & Evenson 1976a)
 $k_{\text{OH}} = (14.5 \pm 2.0) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.5 K and the calculated tropospheric half-life of ~ 0.05 yr in lower troposphere (flash photolysis-RF, Perry et al. 1976)
 $k_{\text{OH}} = 1.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 77 d, loss of 1.3% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
 $k_{\text{OH}}^* = 1.53 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K, measured range 251–455 K (discharge flow-resonance fluorescence, Jeong & Karfman 1982)
 $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $0.2 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)
 $k \leq 0.1 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with O_3 in water as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)
 photooxidation $t_{1/2} = 458\text{--}4584$ h based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)
 $k = 4.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ with reference to CH_3CCl_3 (Buxton et al. 1988; quoted, Haag & Yao 1992)
 $k_{\text{OH}} = 1.42 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 9.6 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)
 $k_{\text{OH}}^* = 1.42 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)
 $k_{\text{OH}}^* = 1.76 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 298–775 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)
 $k = (9 \pm 6) \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)
- Hydrolysis: a minimum hydrolysis $t_{1/2} = 18$ months was estimated from aqueous reactivity experiments (Dilling et al. 1975; quoted, Callahan et al. 1979; Howard 1990);
 rate constant $k = 3.2 \times 10^{-11} \text{ s}^{-1}$ with a maximum $t_{1/2} = 704$ yr for hydrolysis at pH 7 and 25°C was reported from the extrapolated experimental data obtained at 100–150°C (Radding et al. 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)
 $t_{1/2} = 260000$ d in natural waters at pH 7 (Capel & Larson 1995)
- Biodegradation: completely biodegradable under aerobic conditions with sewage seed or activated sludge between 6 h to 7 d (Rittman & McCarty 1980; Davis et al. 1981; Tabak et al. 1981; Klecka 1982; Stover & Kincannon 1983; quoted, Howard 1990)
 $t_{1/2}(\text{aq. aerobic}) = 168\text{--}672$ h based on unacclimated aerobic screening test data (Kawasaki 1980; Tabak et al. 1981; quoted, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688$ h based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).
 $t_{1/2}(\text{aerobic}) = 7$ d, $t_{1/2}(\text{anaerobic}) = 28$ d in natural waters (Capel & Larson 1995)
- Biotransformation:
 Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 33$ wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 2.4$ –24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976)

lifetime of 4.4 yr in troposphere for the reaction with OH radical (Altshuller 1980)

estimated disappearance time to be 12 h to 1.0 year in simulated troposphere chamber (Dilling & Goersch 1979; quoted, Lyman 1982)

residence time of 77 d, loss of 1.3% in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

estimated residence time in troposphere to be 160–250 d (Lyman 1982);

$t_{1/2} = 458$ –4584 h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991)

Surface water: estimated $t_{1/2} = 33$ –38 d in various locations in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

biodegradation $t_{1/2}$ (aerobic) = 100 d, $t_{1/2}$ (anaerobic) = 400 d, hydrolysis $t_{1/2} = 3800$ d at pH 7 in natural waters (Capel & Larson 1995)

$t_{1/2} = 1$ –1.2 d for the first days up to 4 d and 2.71–2.80 d for a period of up to 14 d for disappearance from water calculated from a pseudo first order equation of mesocosms experiment (Merlin et al. 1992)

Ground water: estimated for the first days up to 4 d and $t_{1/2} = 2.71$ –2.80 d for a period of up to 14 d of 10 yr in the ground water of The Netherlands (Zoeteman et al. 1981)

$t_{1/2} = 336$ –1344 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 10$ –50 d (Ryan et al. 1988);

volatilization $t_{1/2} \sim 100$ d from soil (Jury et al. 1990);

biodegradation $t_{1/2}$ (aerobic) = 1.3 d (0.16 ppm, conc of dichloromethane), $t_{1/2} = 9.4$ d (0.5 ppm), $t_{1/2} = 191.4$ d (5 ppm), all in sandy loam soil; $t_{1/2} = 54.8$ d in sand (0.5 ppm); $t_{1/2} = 12.7$ d (0.5 ppm) in sandy clay loam soil; $t_{1/2} = 7.2$ d (0.5 ppm) in clay with 50 d lag and $t_{1/2}$ (anaerobic) = 21.5 d (5 ppm) with 70 d lag (Davis & Madsen 1991);

$t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} = 10$ –50 d, subject to plant uptake in soil via volatilization (Ryan et al. 1988);

$t_{1/2} = 0.4$ –0.5 d to eliminate from small fish (McCarty et al. 1992).

TABLE 5.1.1.2.1

Reported aqueous solubilities of dichloromethane at various temperatures

$$S/(\text{wt}\%) = 1.961 - 4.4883 \times 10^{-2} \cdot (t/^\circ\text{C}) + 8.6617 \times 10^{-4} \cdot (t/^\circ\text{C})^2 + 4.9463 \times 10^{-6} \cdot (t/^\circ\text{C})^3 \quad (1)$$

1.

Rex 1906		Andelman 1978		Horvath 1982		Stephenson 1992	
volumetric method				summary of literature data		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	23630	0	23100	0	19610	0	20300
10	21220	10	20800	10	15938	9.2	19200
20	20000	20	19600	20	13702	17.3	18000
30	19690	25	20000	25	13030	26.8	17200
		30	19000	30	12605	35.7	17700
				40	12350		
				50	12640		
				eq.1	S/wt%		

TABLE 5.1.1.2.1 (Continued)

2.

Tse et al. 1992		Wright et al. 1992	
activity coefficient -GC		activity coefficient	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	19260	10	20080
30	19830	20	18880
35	19500	30	18880
40	19500		

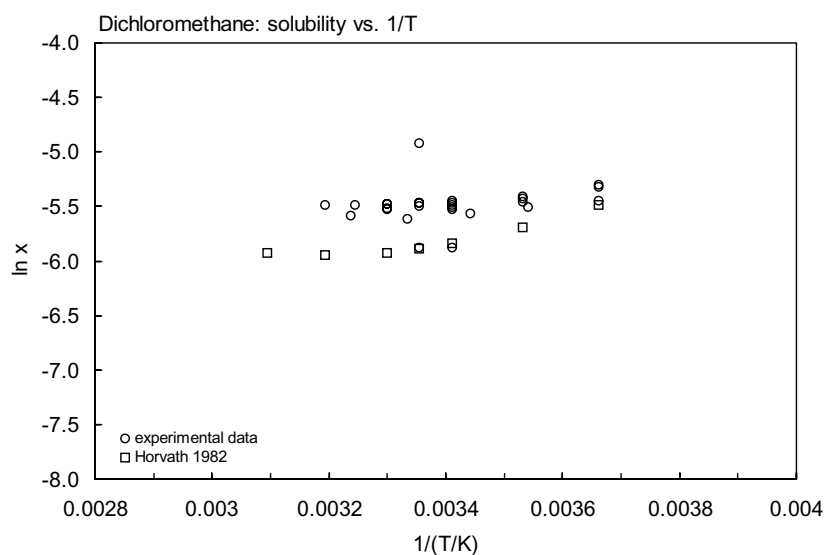


FIGURE 5.1.1.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.2

Reported vapor pressures of dichloromethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		Mueller & Ignatowski 1960		Boublik 1960, thesis	
summary of literature data				in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-70.0	133.3	29.993	70530	-9.03	12046
-52.1	666.6	34.993	85175	-5.45	14549
-43.3	1333	38.993	98070	-1.322	17921
-33.4	2666	39.993	102117	2.228	21314
-22.3	5333			6.230	25780
-15.7	7999			9.457	29923
-6.30	13332			13.289	35493

(Continued)

TABLE 5.1.1.2.2 (Continued)

Stull 1947		Mueller & Ignatowski 1960		Boublik 1960, thesis in Boublik et al. 1984	
summary of literature data					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
8.0	26664			16.693	41470
24.1	53329			21.199	49704
40.7	101325			26.393	61295
				32.337	77123
mp/°C	-96.7			39.429	96484
				eq. 2	P/kPa
				A	6.18791
				B	127.232
				C	229.764
				bp	39.767

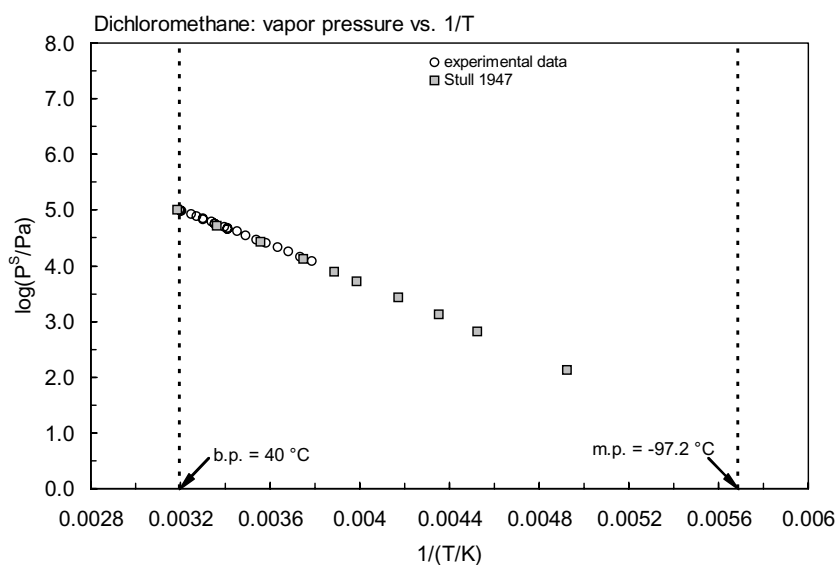


FIGURE 5.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.3
Reported Henry’s law constants of dichloromethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/atm) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		
Leighton & Calo 1981		Gossett 1987	
equilibrium cell-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.9	112	9.6	116.5
13.5	203	17.5	132.7
15.7	222	24.8	221.9
22.0	286.5	34.6	330.3
24.9	295		
25	295.3		
		eq. 4	H/(atm m³/mol)
		A	6.653
eq. 3	k _H /atm	B	4215
A	17.42		
B	3645		
		eq. 4	H/(atm m³/mol)
		A	8.483
		B	4268
		Wright et al. 1992	
		activity coefficient	

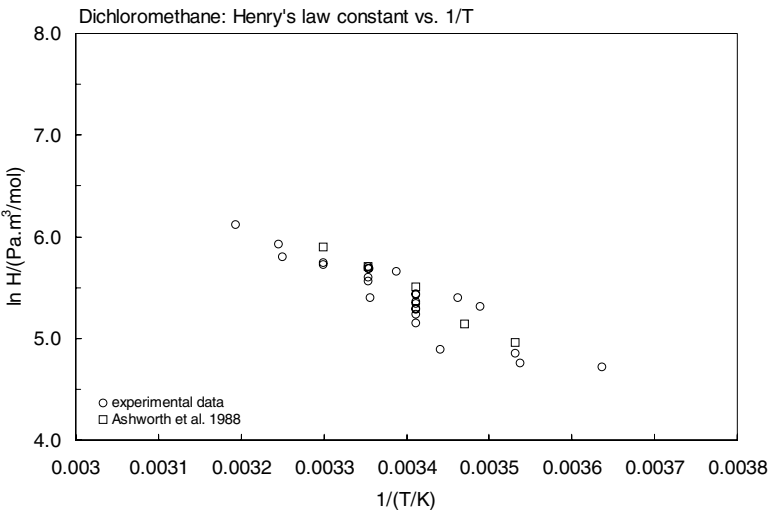


FIGURE 5.1.1.2.3 Logarithm of Henry’s law constant versus reciprocal temperature for dichloromethane.

TABLE 5.1.1.2.4
Reported octanol-water partition coefficients of dichloromethane
at various temperatures

Bhatia & Sandler 1995	
relative GC-RT technique	
t/°C	log K _{OW}
25	1.35
35	1.34
50	1.37
enthalpy of transfer	
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$	
$\log K_{\text{OW}} = A - \Delta H/2.303RT$	
A	1.0195
ΔH	-20.2

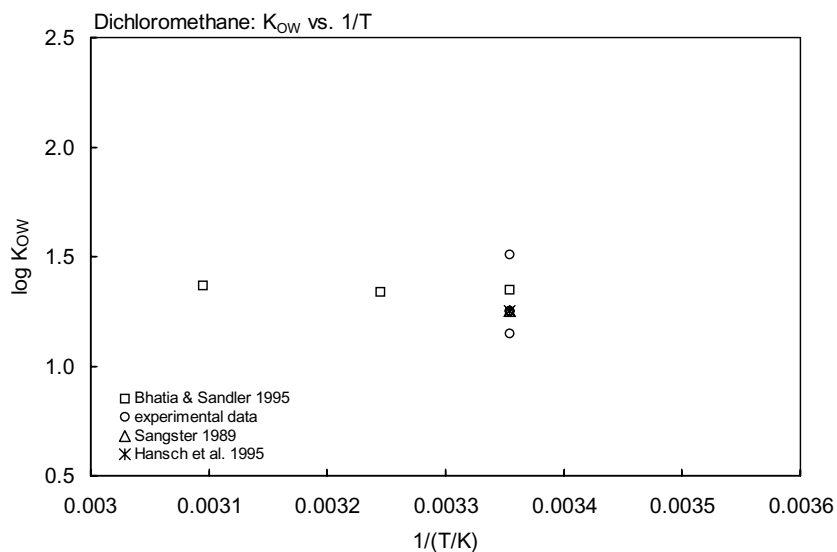
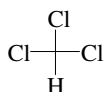


FIGURE 5.1.1.2.4 Logarithm of K_{OW} versus reciprocal temperature for dichloromethane.

5.1.1.3 Trichloromethane (Chloroform)



Common Name: Trichloromethane

Synonym: chloroform, trichloromethaneq

Chemical Name: trichloromethane

CAS Registry No: 67-66-3

Molecular Formula: CHCl_3

Molecular Weight: 119.378

Melting Point ($^{\circ}\text{C}$):

−63.41 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

61.17 (Lide 2003)

Density (g/cm^3 at 20°C):

1.4832 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

1.49845, 1.48911, 1.47970 (15, 20, 25°C , Riddick et al. 1986)

Molar Volume (cm^3/mol):

80.0 (calculated-density, Mailhot 1987; Wang et al. 1992)

92.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

33.35, 29.37 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol)

8.80 (calculated, Dreisbach 1959)

9.54 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

8220, 7760 (20°C , 30°C , volumetric method, Rex 1906)

8520, 7710 (15, 30°C , shake flask-interferometer, Gross & Saylor 1931)

8000 (Wright & Schaffer 1932)

7361 (Seidell 1940)

7700 (Seidell 1941)

7900 (data presented from 0 – 50°C in graph, McGovern 1943)

13320 (shake flask-residue volume method, Booth & Everson 1948)

8000 (20°C , Stephen & Stephen 1963)

8150 (20°C , Riddick & Bunger 1970)

8200 (20°C , Pearson & McConnell 1975)

8000 (20°C , Neely 1976; Verschueren 1977)

10300, 7840 (1.5, 25°C , selected, Dilling 1977)

7230 (shake flask-LSC, Banerjee et al. 1980)

11900 (shake flask-titration/turbidity, Coca et al. 1980)

7360 (shake flask-LSC, Veith et al. 1980)

7920* (summary of literature data, temp range 0 – 60°C , Horvath 1982)

2525 (30°C , headspace-GC, McNally & Grob 1984)

7190 (calculated-UNIFAC activity coeff., Banerjee 1985)

8200 (shake flask-radiometric method, Lo et al. 1986)

8150 (20°C , selected, Riddick et al. 1986)

8080, 7435, 7290 (20, 35, 50°C , infinite dilution activity coeff. γ^{∞} -GC, Barr & Newsham 1987)

8670 (23 – 24°C , shake flask-GC, Broholm et al. 1992)

8200*, 7900 (19.6°C , 29.5°C , shake flask-GC/TC, measured range 0 – 59.2°C , Stephenson 1992)

7280, 8118, 8558, 9011 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞ -UNIFAC, Tse et al. 1992)
 8108, 7030, 7694 (20, 35, 50°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 7345 (gas stripping-GC, Li et al. 1993)
 8098 (20°C, activity coeff. by inert air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

21115, 31990 (20°C, 30°C, Rex 1906)
 39345* (35.0°C, vapor-liquid equilibrium, measured range 35.0–60.0°C, Scatchard & Raymond 1938)
 26660 (interpolated from graph, temp range –30 to 170°C, McGovern 1943)
 25700* (interpolated-Antoine eq. regression, temp range –58.0 to 61.3°C, Stull 1947)
 26310 (calculated-Antoine eq., Dreisbach 1959)
 $\log(P/\text{mmHg}) = 6.90328 - 1163.0/(227.0 + t/^\circ\text{C})$; temp range –15 to 90°C (Antoine eq. for liquid state, Dreisbach 1959)
 $\log(P/\text{mmHg}) = 6.93708 - 1171.2/(227.0 + t/^\circ\text{C})$; temp range –13 to 97°C (Antoine eq. for liquid state, Dreisbach 1961)
 25780* (24.598°C, temp range –10.356 to 60.319°C, Boublik & Aim 1972; quoted, Boublik et al 1984)
 23080 (interpolated from Antoine eq., temp range –58 to 254°C, Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 7500.5/(T/K)] + 7.735083$; temp range –58 to 254°C (Antoine eq., Weast 1972–73)
 26240, 18950 (calculated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 6.85465 - 1170.966/(226.252 + t/^\circ\text{C})$; temp range (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 6.4934 - 959.444/(196.03 + t/^\circ\text{C})$; temp range (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 26217, 26104 (static method-differential pressure gauge, Bissell & Williamson 1975)
 20000 (20°C, Pearson & McConnell 1975)
 25590 (literature average, Dilling 1977)
 21330 (20°C, Verschueren 1983)
 26220, 32080 (calculated-Antoine eq., Boublik et al. 1984)
 21330 (20°C, quoted, McNally & Grob 1984)
 $\log(P/\text{mmHg}) = 6.4934 - 929.44/(196.03 + t/^\circ\text{C})$; temp range –36 to 61°C (Antoine eq., Dean 1985, 1992)
 25970 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.96288 - 1106.94/(218.552 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 26220 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.07853 - 1170.42/(-46.98 + T/K)$; temp range 262–334 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.38327 - 948.979/(-61.73 + T/K)$; temp range 227–269 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.11152 - 1173.606/(-48.54 + T/K)$; temp range 333–416 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.89882 - 2879.244/(-161.978 + T/K)$; temp range 410–481 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 4.58922 - 181.802/(-325.74 + T/K)$; temp range 479–523 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 56.6178 - 3.2462 \times 10^3/(T/K) - 18.7 \cdot \log(T/K) + 9.515 \times 10^{-3} \cdot (T/K) + 1.1553 \times 10^{-12} \cdot (T/K)^2$; temp range 210–536 K (vapor pressure eq., Yaws 1994)
 26182 (selected summary of literature data, temp range 209.64–368.15 K, Xiang 2002)
 32408 (30°C, vapor-liquid equilibrium VLE data, Pathare et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

314.1 (20°C, Dilling et al. 1975)
 440.8 (calculated as $1/K_{AW}$, C_W/C_A , Hine & Mookerjee 1975)
 283.4 (20°C, McConnell et al. 1975; Pearson & McConell 1975)
 310 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

- $\log(k_H/\text{atm}) = 9.10 - 2103.09/(T/K)$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)
 373* (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
 $\ln(k_H/\text{atm}) = 18.97 - 4046/(T/K)$; temp range 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
 292.0 (20°C, calculated-P/C, Mabey et al. 1982; Mills et al. 1982)
 536.9 (batch stripping-GC, Munz & Roberts 1982; Roberts & Dändliker 1983; Roberts et al. 1985)
 432.2 (calculated-UNIFAC activity coeff., Arbuckle 1983)
 $\ln K_{AW} = 10.63 - 3649/(T/K)$; measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith et al. 1983)
 298 (calculated-P/C, Jury et al. 1984; Jury et al. 1990)
 337.4; 308 (20°C, EPICS-GC; batch air stripping-headspace GC, Lincoff & Gossett 1984)
 $\ln[H/(\text{atm m}^3/\text{mol})] = 8.553 - 4180/(T/K)$; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)
 $\ln[H/(\text{atm m}^3/\text{mol})] = 8.956 - 4322/(T/K)$, temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)
 304; 314; 486, 365 (20°C, batch air stripping-GC; calculated-P/C; quoted lit. values, Nicholson et al. 1984)
 334, 294, 314 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)
 $\ln[H/(\text{atm m}^3/\text{mol})] = 11.90 - 5200/(T/K)$; temp range 10–30°C (air stripping-GC, Nicholson et al. 1984)
 343.4 (adsorption isotherm, Urano & Murata 1985)
 372* (EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)
 $\ln[H/(\text{atm m}^3/\text{mol})] = 9.843 - 4612/(T/K)$; temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)
 334 (EPICS-GC, Munz & Roberts 1987)
 $\log K_{AW} = 4.990 - 1729/(T/K)$, temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)
 343 (gas stripping-GC, Warner et al. 1987)
 427; 387; 372; 374; 399 (EPICS-GC; calculated-P/C; EPICS; direct concn ratio; calculated-UNIFAC activity coefficient, Ashworth et al. 1988)
 427* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 11.41 - 5030/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 294 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 318 (calculated-P/C, Suntio et al. 1988; Mackay & Shiu 1990)
 411 (computed value, Yaws et al. 1991)
 199.3* (26.5°C, tap water, EPICS-GC, measured range 26.5–47.2°C, Tancrede & Yanagisawa 1990)
 $\log K_{AW} = 9.154 - 3051/(T/K)$; temp range 26.5–47.2°C (EPICS measurements, Tancrede & Yanagisawa 1990)
 306, 592, 1046 (20, 35, 50°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 362 (activity coefficient γ^∞ from gas stripping-GC, Li et al. 1993)
 514, 513 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 379* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)
 177, 444 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
 $\ln K_{AW} = -4142/(T/K) + 0.00588 \cdot Z + 12.012$; with Z salinity of 0–35.5‰ and temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)
 212, 341 (10, 20°C, gas stripping-GC, Moore et al. 1995)
 126, 214, 352 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
 $\ln K_{AW} = 11.17 - 3840/(T/K)$; seawater of salinity of 30.4‰, temp range: 0–20°C (Moore et al. 1995)
 261, 451 (15, 25°C, vapor liquid equilibrium-GC, Turner et al. 1996)
 $K_{AW} = 0.0394 + 0.00486 \cdot (T/K)$; temp range 0–60°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)
 312 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)
 331.2 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 370.8 (modified EPICS method-GC, Ryu & Park 1999)
 411; 260 (EPICS-GC; calculated-P/C, David et al. 2000)
 307 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 5.343 - 1830/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)
 704.5 (37°C, equilibrium headspace-GC, Batterman et al. 2002)
 408* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
 $\ln K_{AW} = 10.96 - 3821.3/(T/K)$; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:

- 1.97 (Hansch & Anderson 1967)
- 1.97 (shake flask-UV, Hansch et al. 1968; Leo et al. 1971; Hansch et al. 1975)
- 1.94 (Hansch & Leo 1979)
- 1.90 (shake flask-LSC, Banerjee et al. 1980)
- 1.90 (shake flask-LSC, Veith et al. 1980)
- 1.81 (HPLC- k' correlation, McDuffie 1981)
- 2.15 (HPLC- k' correlation, Wells et al. 1981)
- 1.91 (calculated-UNIFAC activity coeff., Arbuckle 1983)
- 1.90 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
- 2.14, 2.13, 2.03 (HPLC- k' correlation, Tomlinson & Hafkenscheid 1986)
- 1.66 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
- 1.97 (recommended, Sangster 1989)
- 2.00* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
- 1.86* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 2.80 (equilibrium head-space-GC, Abraham et al. 2001)
- 2.55; 2.53 (equilibrium headspace-GC; calculated- K_{OW}/K_{AW} , Batterman et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 0.92 (calculate- K_{OW} , Veith et al. 1979; quoted, Veith et al. 1980)
- 0.78 (bluegill sunfish, Barrows et al. 1980; Bysshe 1982)
- 0.78 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982; quoted, Davies & Dobbs 1984; Suntio et al. 1988; Isnard & Lambert 1988; Saito et al. 1992)
- 0.63 (calculated- K_{OW} , Mackay 1982)
- 1.41 (microorganisms-water, calculated from K_{OW} , Mabey et al. 1982)
- 0.97 (calculated-MCI χ , Koch 1983)
- 0.78 (bluegill sunfish, LSC, Davies & Dobbs 1984)
- 2.84 (green algae, Mailhot 1987)
- 2.84 (*Selenastrum capricornutum*, Mailhot 1987)
- 0.52–1.01; 0.204–0.40; 0.46–0.49; 0.552–0.57 (rainbow trout; bluegill sunfish; large mouth bass; catfish, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 1.64 (calculated- K_{OW} , Mabey et al. 1982)
- 1.65 (calculated-MCI χ , Koch 1983)
- 2.15 (wastewater solids with correlation to K_{OW} , Dobbs et al. 1989)
- 1.44 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
- 1.98 (20°C, weathered shale, mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 2.79 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 1.85, 1.92 (20°C, calculated- K_{OW} , Grathwohl 1990)
- 1.53 (soil, Howard 1990)
- 1.46 (selected, Jury et al. 1990)
- 1.57; 1.46; 1.54 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 1.63, 1.65, 1.63, 1.66, 1.69, 1.65, 1.70 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)

Sorption Partition Coefficient, $\log K_{OM}$:

- 1.65, 1.40 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: calculated $t_{1/2} = 1.4$ min (Mackay & Wolkoff 1973);

primary transport process from the aquatic environment with $t_{1/2} = 21$ –26 min at pH 7 and 25°C stirred at 200 rpm in an open container (Dilling et al. 1975)

evaporation rate $k(\text{exptl}) = 13.2 \times 10^{-5} \text{ g cm}^{-2} \text{ s}^{-1}$ to still air (Chiou & Freed 1977; Chiou et al. 1980)

evaporation $t_{1/2}(\text{exptl}) = (8.5\text{--}25.7)$ min, $t_{1/2}(\text{calc}) = 1.46, 2.37$ min at 20–25°C, $t_{1/2}(\text{exptl}) = 34.6$ min at 1.5°C (Dilling 1977)

$t_{1/2} = 3$ –5.6 h for different laboratory studies of evaporation from water with moderate mixing conditions (Smith et al. 1980; Rathbun & Tai 1981; Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2} = 1.2$ d in Rhine River and $t_{1/2} = 31$ d in a lake in Rhine Basin. (Zoeteman et al. 1980).

$t_{1/2} \sim 3.7$ h from water (estimated, Thomas 1982);

$t_{1/2} = 29$ min–11.3 d from rivers and streams, calculated using published O_2 reaeration values; and $t_{1/2}(\text{calc}) = 31.2$ h from rivers and streams, calculated using estimated O_2 reaeration rate constant (Kaczmar et al. 1984);

predicted $t_{1/2} = 36$ h in a river, $t_{1/2} = 40$ h in a pond and $t_{1/2} = 9$ –10 d in a lake (USEPA 1984; quoted, Howard 1990);

$t_{1/2} = 4$ h at 20°C was predicted from a model river of 1 m deep at flowing speed of 1 m/s with a wind velocity of 3 m/s and its Henry's law constant (Smith et al. 1980; quoted, Howard 1990);

Photolysis: not important only by UV in the stratosphere (Robbins 1976);

probably not significant in aquatic systems (Callahan et al. 1979);

photocatalyzed mineralization by the presence of TiO_2 with a rate of $4.4 \text{ ppm min}^{-1} \text{ g}^{-1}$ of catalyst (Ollis 1985).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = 1.01 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{\text{OH}}^* = 1.14 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K with lifetime of 0.56 yr, measured range 245–375 K (flash photolysis-resonance fluorescence, Davis et al. 1976; quoted, Altshuller 1980)

troposphere with $t_{1/2} = 0.19$ –0.32 yr due to reaction with OH radical (Callahan et al. 1979)

$k_{\text{OH}} = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 116 d, loss of 0.9% in 1d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}}^* = 1.01 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 249–487 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1982)

$k_{\text{OH}} = 6.6 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ of estimated at 300 K (Lyman 1982)

$t_{1/2} = 78.5$ –3140 yr from the rate constant for the reaction with OH radical (estimated, Dorfman & Adams 1973)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $0.7 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical both at 25°C (Mabey et al. 1982)

$k \leq 0.1 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

photooxidation $t_{1/2} = 26$ –260 d, based on measured data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k = 4.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ with reference to CH_3CCl_3 (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{\text{OH}} = 1.03 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.8 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}}^* = 1.03 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–775 K (laser photolysis/laser induced fluorescence technique, Taylor et al. 1989)

$k = (5.4 \pm 3.0) \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

$k_{\text{OH}}^* = 1.03 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis: first-order rate constant $k = 0.045 \text{ mo}^{-1}$ with $t_{1/2} \sim 15$ months (Dilling et al. 1975; quoted, Callahan et al. 1979);

$k = 6.9 \times 10^{-12} \text{ s}^{-1}$ (Radding 1976);

hydrolysis rate constant $k = 6.9 \times 10^{-12} \text{ s}^{-1}$ with $t_{1/2} = 3500$ yr at 25°C and pH 7 (Mabey & Mill 1978)

no hydrolysis in acidic aqueous solutions, and rate constant in alkaline aqueous solution, $k = 0.23 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C, and $k = 2.5 \times 10^{-9} \text{ M}^{-1} \text{ h}^{-1}$ at 25°C in neutral aqueous solutions (Mabey & Mill 1978; Mabey et al. 1982; Mills et al. 1982);

probably not a significant fate process with $t_{1/2} = 3500$ yr, based on reported rate constant $k = 6.9 \times 10^{-12} \text{ s}^{-1}$ at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Haque et al. 1980).

Biodegradation: very slow by BOD bottle experiments (Pearson & McConnell 1975);

$t_{1/2}$ (aq. aerobic) = 4 wk to 6 months by unacclimated screening tests (Kawasaki 1980; Flathman & Dahlgran 1982; quoted, Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 1–4 wk by unacclimated anaerobic screening tests (Bouwer et al. 1981; Bouwer & McCarty 1983; quoted, Howard et al. 1991);

$k = 0.5 \text{ d}^{-1}$ (Tabak et al. 1981; Mills et al. 1982).

Bioaccumulation: weak to moderate bioaccumulation; no evidence of biomagnification of trichloromethane in marine food chain (Callahan et al. 1979).

Bioconcentration, Uptake(k_1) and Elimination(k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 23$ wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 2.4$ –24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

residence time of 1.7 yr in troposphere, based on one compartment nonsteady state model (Singh et al. 1978; quoted, Lyman 1982);

residence time of 116 d, loss of 0.9% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

estimated residence time in N. troposphere to be 100 d (Lyman 1982);

$t_{1/2} = 623$ –6231 h, based on photooxidation half-life in air from measured reaction data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

tropospheric lifetime ~ 0.17 yr (estimated, Nimitz & Skaggs 1992)

lifetime for reaction with OH radicals, $\tau = 3.0$ yr for Polar region, $\tau = 0.6$ yr for Middle region and $\tau = 0.2$ yr for Tropical region in the Northern hemisphere; $\tau = 0.3$ yr for Tropical, $\tau = 1.0$ yr for Middle and $\tau = 3.2$ yr for Polar region in the Southern hemisphere; $\tau = 0.5$ yr in the Global atmosphere, based on data from 1985–1996 (Khalil & Rasmussen 1999b)

Surface water: not important for aqueous phase (Dilling et al. 1975);

$t_{1/2} = 1.0$ –31 d in various location in the Netherlands in case of a first order reduction process (estimated, Zoeteman et al. 1980)

$t_{1/2} = 672$ –4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344$ –43200 h, based on unacclimated aqueous aerobic biodegradation and grab sample data of aerobic soil from a ground water aquifer (Wilson et al. 1983; quoted, Howard et al. 1991).

Soil: $t_{1/2} = 10$ –50 d (Ryan et al. 1988);

$t_{1/2} = 100$ d, estimated volatilization loss from soil (Jury et al. 1990)

disappearance $t_{1/2} = 4.1$ d was calculated from first order kinetic for volatilization loss from soil mixtures (Anderson et al. 1991);

$t_{1/2} = 672$ –4320 h, based on estimated aqueous aerobic biodegradation (Howard et al. 1991).

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{1/2} = 10$ –50 d, subject plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.3.1

Reported aqueous solubilities of trichloromethane at various temperatures

$$S/(\text{wt}\%) = 0.995 - 1.0531 \times 10^{-2} \cdot t/^{\circ}\text{C} + 7.9819 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 6.6431 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

1.

Rex 1906		Gross & Saylor 1931		Horvath 1982		Barr & Newsham 1987	
volumetric method		shake flask-IR		summary of literature data		activity coefficient	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	8220	15	8520	0	9905	20	8080
30	7760	30	7710	10	8983	35	7435
				20	8216	50	7290
				25	7920		
				30	7689		
				40	7440		
				50	7511		
				60	7940		
				eq.1	S/wt%		

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
shake flask-GC		activity coefficient		activity coefficient	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	10200	20	7280	20	8108
9.5	9300	30	8118	35	7030
19.6	8200	35	8558	50	7694
29.5	7900	40	9011		
39.3	7400				
49.2	7700				
59.2	7900				

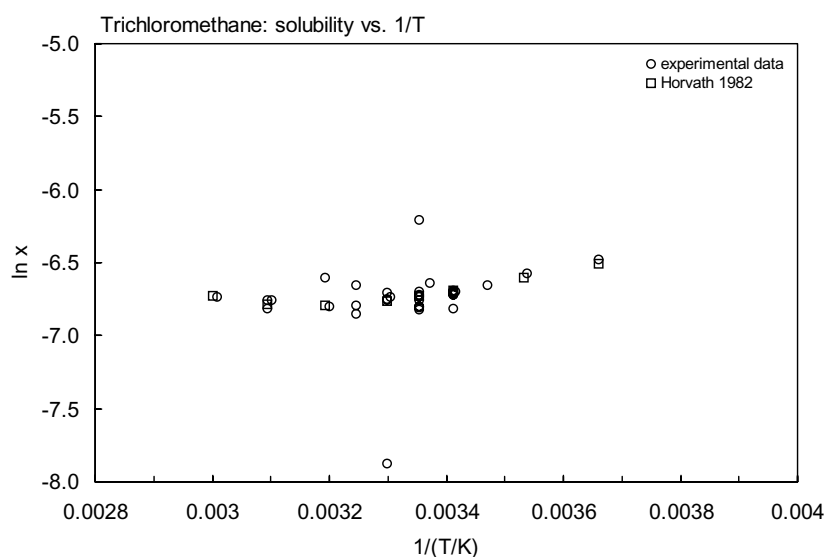
FIGURE 5.1.1.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for trichloromethane.

TABLE 5.1.1.3.2
Reported vapor pressures of trichloromethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Scatchard & Raymond 1938	Stull 1947	Boublik & Aim 1972					
vapor-liquid equilibrium	summary of literature data	in Boublik et al 1984					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
35.0	39345	−58.0	133.3	−10.356	4524	46.583	61295
40.0	48023	−39.1	666.6	−2.610	6967	53.070	77125
45.0	57800	−29.7	1333	2.882	9306	60.319	98412
50.0	69218	−19.0	2666	8.010	12046		
55.0	82372	−7.10	5333	11.927	14549	bp/°C	61.203
60.0	97342	0.50	7999	16.417	17921	Antoine eq	P/kPa
		10.4	13332	20.240	21314	eq. 2	6.07945
		25.9	26664	24.598	25780	A	1170.902
		42.7	53329	28.118	29923	B	226.224
		61.3	101325	32.289	35493	C	
				36.223	41470		
		mp/°C	−65.3	40.913	49704		

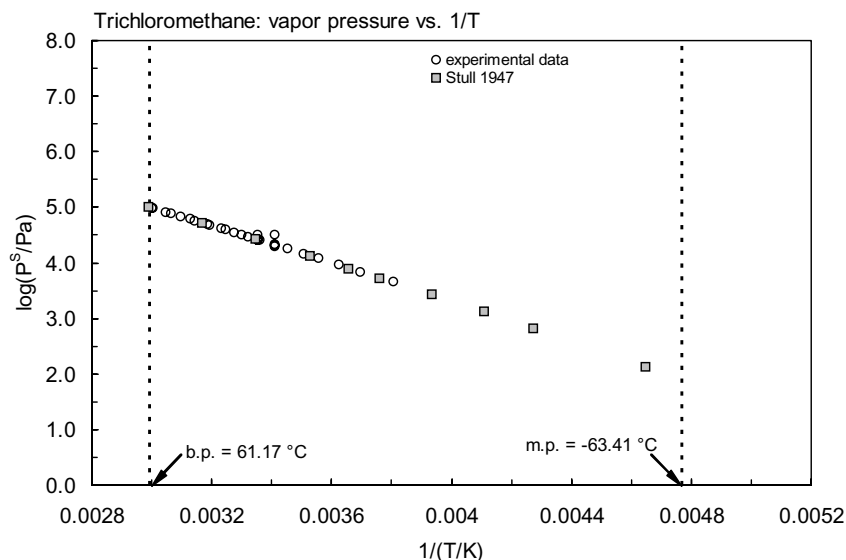


FIGURE 5.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for trichloromethane.

TABLE 5.1.1.3.3

Reported Henry's law constants of trichloromethane at various temperatures and temperature dependence equations

$$\begin{array}{llll} \ln K_{AW} = A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) = A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) = A - B/(T/K) & (3) & & \\ \ln H = A - B/(T/K) & (4) & \log H = A - B/(T/K) & (4a) \\ K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 & (5) & & \end{array}$$

1.

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancrede & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
1.90	125.7	9.6	152	10	174	26.5	199.3
13.5	234.7	17.5	249.3	15	236	27.4	274.9
15.7	267.6	24.8	371.9	20	336	28.9	401.8
17.1	282.7	34.6	570.5	25	427	28.9	276.2
22.0	354.7			30	561	29.7	226.6
24.9	373.5	eq. 4	H/(atm m ³ /mol)			29.9	277.2
25	373	A	9.843	eq. 4	H/(atm m ³ /mol)	33.3	382.2
		B	4612	A	11.41	35.6	693.1
eq. 3	k _H /atm			B	5030	38.3	517.9
A	18.97					40	624.8
B	4046					44.7	951.2
						45	925.8
						47.2	1145
						eq. 1	K _{AW}
						A	9.154
						B	3051

2.

Wright et al. 1992		Dewulf et al. 1995		Moore 1995		Görgényi et al. 2002	
activity coefficient		EPICS-GC		gas stripping-GC		EPICS-SPME method	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
20	306	2	116	10	212	2	108
35	592	6	135.1	20	341	6	151.3
50	1046	10	165.7			10	181.3
		18.2	276.1	In sea water 30.4‰ NaCl		16	297.8
		25	379.3	0	126	25	407.5
				10	214	35	526.5
				20	352	40	769.9
Bhatia & Sandler 1995		eq. 1	K _{AW}			50	1120
activity coefficient		A	12.012			60	1497
35	514	B	4142				
50	513						
				Turner et al. 1996			
				vapor liquid equilibrium-GC		eq. 1	K _{AW}
				15	261	A	10.96
				25	451	B	3821.3

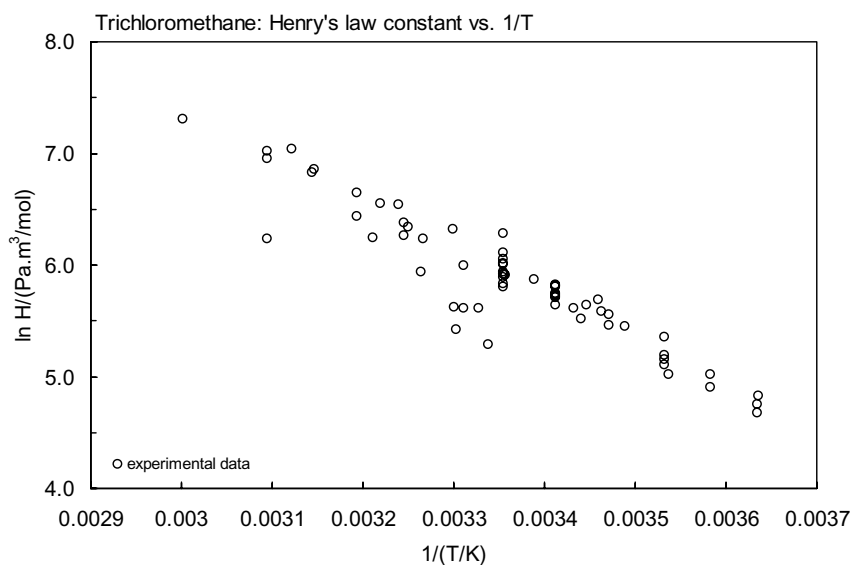


FIGURE 5.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for trichloromethane.

TABLE 5.1.1.3.4
Reported octanol-water partition coefficients of trichloromethane at various temperatures

Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		EPICS-GC	
t/°C	log K _{OW}	t/°C	log K _{OW}
25	2.00	2.2	1.83
35	2.01	6.0	1.815
50	2.00	10.0	1.90
		14.1	1.87
enthalpy of transfer		18.7	1.92
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$		24.8	1.86
$\log K_{OW} = A - \Delta H/2.303RT$		change in enthalpy:	
A	1.0195	$\Delta H_{OW}/(\text{kJ mol}^{-1}) = 4.2$	
ΔH	-20.2	(-4.4 to 12.8)	
		enthalpy of transfer	
		$\Delta H_{oct}/(\text{kJ mol}^{-1}) = 0.7$	
		(-7.9 to 9.3)	

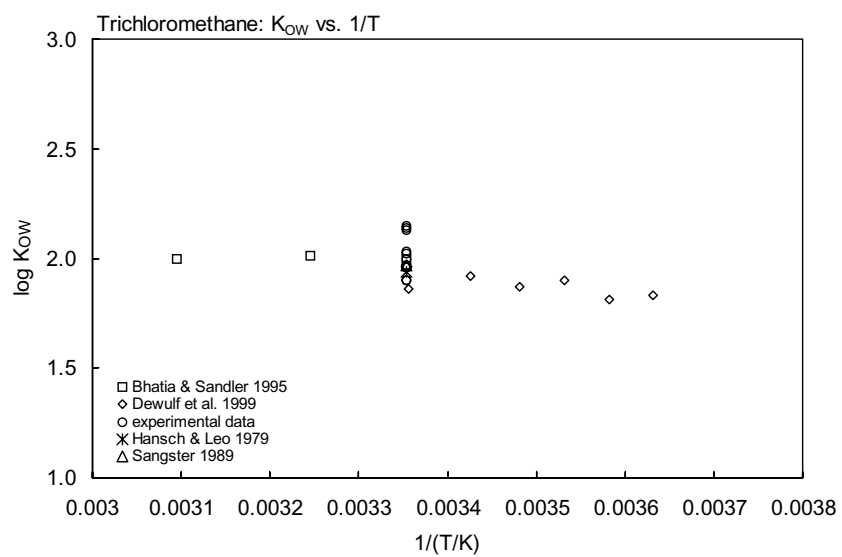
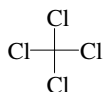


FIGURE 5.1.1.3.4 Logarithm of K_{OW} versus reciprocal temperature for trichloromethane.

5.1.1.4 Tetrachloromethane (Carbon tetrachloride)



Common Name: Carbon tetrachloride

Synonym: tetrachloromethane, methane tetrachloride, perchloromethane, benzinofom

Chemical Name: tetrachloromethane

CAS Registry No: 56-23-5

Molecular Formula: CCl_4

Molecular Weight: 153.823

Melting Point ($^{\circ}\text{C}$):

-22.62 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

76.8 (Lide 2003)

Density (g/cm^3 at 20°C):

1.594 (McGovern 1943; Dreisbach 1959, 1961; Weast 1982–83; Horvath 1982; Riddick et al. 1986)

1.6037, 1.59402, 1.58436 (15, 20, 25°C , Riddick et al. 1986)

Molar Volume (cm^3/mol):

113.2 (calculated-Le Bas method at normal boiling point)

96.0 (calculated-density, Wang et al. 1992)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.41, 29.96 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

0.775 (calculated, Dreisbach 1959)

0.581 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

800, 850 (20°C , 30°C , volumetric method, Rex 1906)

770 (shake flask-interferometer, Gross 1929a,b)

770, 810 (15, 30°C , shake flask-interferometer, Gross & Saylor 1931)

780 (Seidell 1941)

800 (data presented in graph, temp range 0 – 70°C , McGovern 1943; Dilling 1977)

770 (15°C , Jones et al. 1957)

785 (20°C , McConnell et al. 1975; Pearson & McConnell 1975)

778 (20°C , recommended, Sørensen & Arit 1979)

800* (measured range 20 – 30°C , Andelman 1978)

757 (shake flask-LSC, Banerjee et al. 1980)

700 (shake flask-titration/turbidity, Coca et al. 1980)

793.4* (summary of literature data, Horvath 1982)

831 (calculated-UNIFAC activity coeff., Arbuckle 1983)

753 (calculated-UNIFAC activity coeff., Banerjee 1985)

800 (shake flask-radiometric method, Lo et al. 1986)

770 (selected, Riddick et al. 1986)

780 (23 – 24°C , shake flask-GC, Broholm et al. 1992)

600*, 720 (20.5 , 31.0°C , shake flask-GC/TC, measured range 0 – 75°C , Stephenson 1992)

930, 873, 950, 982 (20 , 30 , 35 , 40°C , infinite dilution activity coeff. γ° -GC, Tse et al. 1992)

756, 896, 972, 1052 (20 , 30 , 35 , 40°C , infinite dilution activity coeff. γ° -UNIFAC, Tse et al. 1992)

700, 652, 652 (20 , 30 , 40°C , activity coeff. γ° -differential pressure transducer, Wright et al. 1992)

701, 702 (20°C , calculated-activity coefficients, Wright et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

17170, 18810 (20°C, 30°C, Rex 1906)

11372* (19.8°C, manometry, measured range 19.8–76.4°C, Smyth & Engel 1929)

15200 (extrapolated-Antoine eq., vapor-liquid equilibrium VLE data, measured range 30–70°C, Scatchard et al. 1939; quoted, Bissell & Williamson 1975)

$\log(P/\text{mmHg}) = 6.68148 - 1045.022/(T/K) - 99.577/(T/K)^2$; temp range 30–70°C (VLE data, Scatchard et al. 1939)

14530 (interpolated from graph, temp range –20 to 170°C, McGovern 1943)

14340* (interpolated from Antoine eq. regression, temp range –50 to 76.7°C, Stull 1947)

15200 (McGlashan et al. 1954)

15100 (Moelwyn-Hughes & Missen 1957)

15360 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/\text{mmHg}) = 6.93390 - 1242.43/(230.0 + t/^\circ\text{C})$; temp range –15 to 138°C (Antoine eq. for liquid state, Dreisbach 1959)

15372* (25.2°C, temp range 14.06–76.84°C, Boublik 1960; quoted, Boublik et al. 1984)

$\log(P/\text{mmHg}) = 6.94369 - 1221.1/(224.0 + t/^\circ\text{C})$; temp range –1 to 113°C (Antoine eq. for liquid state, Dreisbach 1961)

15220* (twin ebulliometer, measured range 20–77°C, Hildenbrand & McDonald 1959)

15230 (Marsh 1968; quoted, Bissell & Williamson 1975)

13200 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 7628.8/(T/K)] + 7.586045$; temp range –50 to 276°C (Antoine eq., Weast 1972–73)

15250, 15240 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/\text{mmHg}) = 6.9218 - 1235.172/(228.957 + t/^\circ\text{C})$; temp range 19.9–77.7°C (Antoine eq. from reported exptl. data of Hildenbrand & McDonald 1959, Boublik et al. 1973)

$\log(P/\text{mmHg}) = 6.87926 - 1212.021/(226.409 + t/^\circ\text{C})$; temp range 14.06–76.04°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

15195, 15184 (static method-differential pressure gauge, Bissell & Williamson 1975)

12000 (20°C, Pearson & McConnell 1975)

15230 (calculated-Antoine eq., Boublik et al. 1984)

15370, 15300 (25.2°C, quoted exptl., calculated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.04073 - 1231.791/(228.51 + t/^\circ\text{C})$; temp range 19.9–77.7°C (Antoine eq. from reported exptl. data of Hildenbrand & McDonald 1959, Boublik et al. 1984)

$\log(P/\text{kPa}) = 5.94824 - 1177.609/(222.028 + t/^\circ\text{C})$; temp range 40–65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.00535 - 1212.676/(226.483 + t/^\circ\text{C})$; temp range 14.06–76.04°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

15170 (Daubert & Danner 1985)

$\log(P/\text{mmHg}) = 6.87926 - 1212.021/(226.41 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Dean 1985, 1992)

15360 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.10455 - 1265.632/(232.148 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

15210 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 8.214 - 2027/(T/K)$; temp range 208–225 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 7.946 - 1975.3/(T/K)$, temp range 226–248 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.99114 - 1202.9/(-48.01 + T/K)$; temp range 262–249 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.97092 - 1195.9034/(-48.217 + T/K)$; temp range 349–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.22882 - 1392.458/(-19.19 + T/K)$; temp range 412–497 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 31.9407 - 2.6614 \times 10^3/(T/K) - 8.5763 \cdot \log(T/K) - 6.7136 \times 10^{-10} \cdot (T/K) + 2.9732 \times 10^{-6} \cdot (T/K)^2$; temp range 250–556 K (vapor pressure eq., Yaws 1994)

15320 (selected summary of literature data, temp range 250.33–398.15 K, Xiang 2002)

18826 (30°C, vapor-liquid equilibrium study, Pathare et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 2912 (calculated as $1/K_{\text{AW}} C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
 152.8 (calculated-bond method, Hine & Mookerjee 1975)
 2216 (20°C , McConnell et al. 1975; Pearson & McConnell 1975)
 2776 (gas stripping-GC, Mackay et al. 1979)
 2350 (20°C , calculated-P/C, Kavanaugh & Trussell 1980, 1983)
 $\log (H/\text{atm}) = 10.06 - 2038.25/(T/K)$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)
 2797* (equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)
 $\ln (k_{\text{H}}/\text{atm}) = 22.22 - 4438/(T/K)$; temp range $1.0\text{--}27.2^\circ\text{C}$ (equilibrium cell-concn ratio, Leighton & Calo 1981)
 2160 (calculated-P/C, Mackay & Shiu 1981)
 2330 (20°C , calculated-P/C, Mabey et al. 1982)
 2454 (20°C , batch stripping, Munz & Roberts 1982)
 2418 (20°C , calculated-UNIFAC activity coeff., Arbuckle 1983)
 3081 (20°C , EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
 $\ln K_{\text{AW}} = 9.77 - 2918/(T/K)$; measured range $5\text{--}33^\circ\text{C}$ (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)
 $\ln K_{\text{AW}} = 11.27 - 3230/(T/K)$; measured range $5\text{--}33^\circ\text{C}$ (seawater, multiply equilibrium-GC, Hunter-Smith 1983)
 3060 (adsorption isotherm, Urano & Murata 1985)
 2369 (20°C , multiple equilibration, Munz & Roberts 1986)
 3080* (EPICS-GC/FID, Gossett 1987)
 2367* (20°C , EPICS-GC/FID, measured range $10.0\text{--}34.6^\circ\text{C}$, Gossett 1987)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 11.29 - 4411/(T/K)$; temp range $10.0\text{--}34.6^\circ\text{C}$ (EPICS measurements, Gossett 1987)
 2266 (20°C , calculated-P/C, McKone 1987)
 3027 (EPICS-GC, Munz & Roberts 1987)
 $\log K_{\text{AW}} = 5.853 - 1718/(T/K)$; temp range $10\text{--}30^\circ\text{C}$ (EPICS-GC measurements, Munz & Roberts 1987)
 2900 (calculated-P/C, Warner et al. 1987)
 228 (20°C , EPICS-GC, Yurteri et al. 1987)
 2989* (EPICS-GC, measured range $10\text{--}30^\circ\text{C}$, Ashworth et al. 1988)
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 9.739 - 3951/(T/K)$; temp range $10\text{--}30^\circ\text{C}$ (EPICS measurements, Ashworth et al. 1988)
 2330 ($20\text{--}25^\circ\text{C}$ and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 2980 (computed value, Yaws et al. 1991)
 2990 (EPICS-GC, Tancréde et al. 1992)
 2875* (tap water, EPICS-GC, measured range $25\text{--}47.2^\circ\text{C}$, Tancréde & Yanagisawa 1990)
 $\log K_{\text{AW}} = 5.569 - 1639/(T/K)$; temp range: $25\text{--}47.2^\circ\text{C}$ (EPICS measurements, Tancréde & Yanagisawa 1990)
 2067, 3415, 3871, 4580 ($20, 30, 35, 40^\circ\text{C}$, infinite dilution activity coeff. $\gamma\text{-GC}$, Tse et al. 1992)
 2646, 4392, 6624 ($20, 35, 50^\circ\text{C}$, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 3133* (27.6°C , EPICS-GC, measured range $27.6\text{--}45^\circ\text{C}$, Hansen et al. 1993)
 $\ln [H/(\text{kPa}\cdot\text{m}^3/\text{mol})] = -3553/(T/K) + 13.0$; temp range $27\text{--}45^\circ\text{C}$ (EPICS measurements, Hansen et al. 1993)
 4.04, 6.0 ($35, 50^\circ\text{C}$, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 2598* (EPICS-GC/FID, measured range $2.0\text{--}25^\circ\text{C}$, Dewulf et al. 1995)
 1341, 3370 ($6.0, 25^\circ\text{C}$, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
 $\ln K_{\text{AW}} = -4073/(T/K) + 0.00814\cdot Z + 13.772$; with Z salinity $0\text{--}35.5\text{‰}$, temp range: $2\text{--}35^\circ\text{C}$ (EPICS-GC/FID, Dewulf et al. 1995)
 2352 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)
 2612 (modified EPICS method-GC, Ryu & Park 1999)
 2313 (20°C , selected from reported experimental determined values, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 5.736 - 1689/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 2.64 (Leo et al. 1971)
 2.62 (shake flask-GC, Chiou et al. 1977)
 2.83 (shake flask, Hansch & Leo 1979, 1987)

- 2.73 (shake flask-LSC, Banerjee et al. 1980)
- 2.73 (shake flask-LSC, Veith et al. 1980)
- 2.94 (HPLC- k' correlation, McDuffie 1981)
- 2.81, 290 (calculated from UNIFAC activity coeff. with octanol and water mutual solubility considered, not considered, Arbuckle 1983)
- 2.83 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
- 2.03 (HPLC correlation, Eadsforth 1986)
- 2.73 (HPLC- k' correlation, Tomlinson & Hafkenscheid 1986)
- 2.38 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
- 2.83 (recommended, Sangster 1989)
- 2.83 (recommended, Hansch et al. 1995)
- 2.73* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
- 2.38* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 2.79 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 1.24 (rainbow trout, Neely et al. 1974; Veith et al. 1979)
- 1.25 (trout muscle, calculated-ratio of rate const. k_1/k_2 , Neely et al. 1974)
- 1.48 (bluegill sunfish, Barrows et al. 1980; Veith et al. 1980; Veith & Kosian 1982)
- 2.32 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.72 (rainbow trout, Veith & Kosian 1982)
- 2.68 (activated sludge, Freitag et al. 1984)
- 2.48 (*alga chlorella fusca*-LSC, Geyer et al. 1984)
- 2.68, 2.48, < 1.0 (activated sludge, *Chlorella fusca*, golden ide, Freitag et al. 1985)
- 2.06 (calculated- K_{OW} , $S_{OCTANOL}$, and mp, Banerjee & Baughman 1991)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 2.04 (calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.64 (calculated- K_{OW} , Mabey et al. 1982)
- 1.85 (calculated-MCI χ , Koch 1983)
- 1.70 (calculated-MCI χ , Bahnick & Doucette 1988)
- 1.26, 1.34, 1.70, 1.96, 2.07 (DTMA-clay, TTMA-clay, HTMA-clay, BDHA-clay, DDPA-clay, Smith et al. 1990)
- 1.69 (80% DTMA-clay at 20°C, Smith & Jaffé 1991)
- 2.16; 1.70; 2.06 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43, weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 2.20, 2.24, 2.24, 2.25, 2.28, 2.27, 2.33 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)%o
- 1.80, 1.80, 1.78 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
- 2.01, 2.00, 2.02 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Sorption Partition Coefficient, $\log K_{OM}$:

- 1.55 (calculated-MCI χ , Sabljic 1984)
- 1.89, 1.72 (Florida peat, OC 57.1%; Michigan muck, OC 53.1%, batch equilibrium-sorption equilibrium, Rutherford & Chiou 1992; Rutherford et al. 1992)
- 0.243, 1.866 (cellulose, extracted peat, Rutherford et al. 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2} = 29$ min was determined in an open container with initial concentration of 1 mg/L when stirred at 100 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982; Verschueren 1983);
- Evaporation $t_{1/2}(\text{exptl}) = 28.8$ min, $t_{1/2}(\text{calc}) = 0.2$ min, 25.5 min from water (Dilling 1977);

ratio of evaporation rate constant to that of oxygen reaeration: 0.47 as measured value compared to 0.43 as predicted (Smith et al. 1980);

$k < 2.4 \times 10^8 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, estimated rate constant for the reaction with OH radical at 300 K (Lyman 1982);
 $t_{1/2} \sim 3.7 \text{ h}$ from a model river of 1 m deep for water flowing at 1 m/s with wind speed of 3 m/s and Henry's law constant (Thomas 1982; Lyman et al. 1982; quoted, Howard 1990).

Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 0.18 ppm/min per gram of catalyst (Ollis 1985).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} < 1.25 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Cox et al. 1976)

$k_{\text{OH}} = 1 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$ bimolecular reaction rate, with a reported tropospheric lifetime of greater than 330 yr (Cox et al. 1976; quoted, Callahan et al. 1979)

$k_{\text{OH}} < 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (discharge flow-LMR, Howard & Evenson 1976a)

$k_{\text{OH}} < 1.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time $> 11600 \text{ d}$, loss $\approx 0.0\%$ in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}}(\text{calc}) \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

photooxidation half-life in air: $1.6 \times 10^4 \text{--}1.6 \times 10^5 \text{ h}$, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k < 2 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

$k_{\text{OH}} < 5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis: hydrolysis rate constant $k = 4.8 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 7000 \text{ yr}$ (1 ppm), $t_{1/2} = 7 \text{ yr}$ (1000 ppm) at 25°C and pH 7 (Mabey & Mill 1978)

calculated first-order $t_{1/2} = 7000 \text{ yr}$, based on reported rate constant $k = 4.8 \times 10^{-7} \text{ mol}^{-1} \text{ s}^{-1}$ for 1 mg/L concentration at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Howard 1990; Howard et al. 1991)

$t_{1/2} = 2,600,000 \text{ d}$ at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 4320\text{--}8640 \text{ h}$, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 168\text{--}672 \text{ h}$, based on unacclimated anaerobic screening test data (Bouwer & McCarty 1983; quoted, Howard et al. 1991) and acclimated anaerobic sediment/aquifer grab sample data (Parsons et al. 1985; quoted, Howard et al. 1991).

$t_{1/2}(\text{aerobic}) = 170 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 7 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria in water (Mabey et al. 1982).

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 4.05 \text{ h}^{-1}$; $k_2 = 0.229 \text{ h}^{-1}$ (trout muscle, Neely et al. 1974; quoted, Thomann 1989)

$k_1 = 4.05 \text{ mL g}^{-1} \text{ h}^{-1}$ (10°C , trout gill, Neely 1979)

$k_1 = 4.10 \text{ h}^{-1}$; $k_2 = 0.25 \text{ h}^{-1}$ (trout, Hawker & Connell 1985)

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 10 \text{ wk}$, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} > 10 \text{ d}$ for the reaction with OH radical in air (Darnall et al. 1976);

estimated residence time in troposphere, $> 330 \text{ yr}$ (CEQ 1975);

estimated residence time of 100 yr in troposphere (Singh et al. 1979);

residence time $> 11600 \text{ d}$, loss $\approx 0.0\%$ in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

estimated residence time of 4–20 yr in troposphere (Lyman 1982);

$t_{1/2} = 30\text{--}50 \text{ yr}$ residence time in the troposphere (Howard 1990);

$t_{1/2} = 1.6 \times 10^4 \text{--}1.6 \times 10^5 \text{ h}$, based on photooxidation half-life in air from measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: estimated $t_{1/2} = 0.4\text{--}56 \text{ d}$ in various locations in the Netherlands in case of a first order reduction process; $t_{1/2} \sim 3\text{--}30 \text{ d}$ in rivers and $t_{1/2} = 3\text{--}300 \text{ d}$ in lakes (Zoeteman et al. 1980);

$t_{1/2} = 4320\text{--}8640 \text{ h}$, based on estimated aqueous aerobic biodegradation (Howard et al. 1991).

$t_{1/2}(\text{aerobic}) = 170 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 7 \text{ d}$ in natural waters (Capel & Larson 1995)

Ground water: estimated $t_{1/2} \sim 3\text{--}300$ d (Zoeteman et al. 1980; quoted, Howard 1990);

$t_{1/2} = 168\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life and acclimated anaerobic sediment/aquifer grab sample data (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 4320\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{calc}) = 50$ d in soil mixtures from first-order kinetic (Anderson et al. 1991).

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 5.1.1.4.1

Reported aqueous solubilities of tetrachloromethane at various temperatures

$$S/(\text{wt}\%) = 9.7842 \times 10^{-2} - 1.4942 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 3.5854 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 2.2775 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

1.

Rex 1906		Gross & Saylor 1931		Andelman 1978		Horvath 1982	
volumetric method		shake flask-IR				summary of literature data	
t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$
20	800	15	770	20	793	0	978.4
30	850	30	810	25	800	10	682.6
				30	814	20	804.8
						25	793.4
						30	791.3
						40	808.6
						50	843.0
						60	880.7
						70	908.1
						eq. 1	S/wt%

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
shake flask-GC		activity coefficient		activity coefficient	
t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$	t/ $^{\circ}\text{C}$	S/g·m $^{-3}$
0	890	20	930	20	700
10	630	30	873	30	652
20.5	600	35	950	40	652
31.0	720	40	982		
41.3	680				
52.5	780				
64.0	960				
75.0	1150				

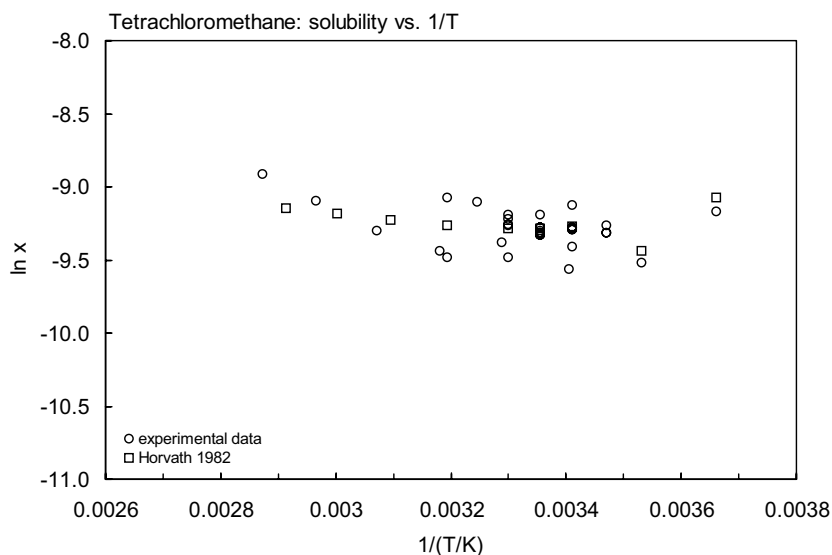


FIGURE 5.1.1.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.2

Reported vapor pressures of tetrachloromethane at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)						
log P = A – B/(T/K) – C·log (T/K)		(4)						
Smyth & Engel 1929		Stull 1947		Hildenbrand & McDonald 1959		Boublik 1960, thesis		
static-manometer		summary of literature data		twin ebulliometer system		in Boublik et al. 1984		
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	
19.2	11732	–50.0	133.3	19.88	12079	14.06	9120	
32.4	20798	–30.0	666.6	30.93	25211	16.66	10426	
41.2	29704	–19.6	1333	56.16	51605	18.46	11876	
50.0	41597	–8.20	2666	75.28	96965	21.71	13159	
60.8	60368	4.30	5333	76.16	99645	25.2	15372	
68.7	78180	12.3	7999	76.87	101729	29.13	18252	
76.4	101325	23.0	13332	77.71	104369	33.45	21891	
		38.3	26664	76.73	101325	36.98	25264	
bp/°C	76.4	57.8	53329			42.07	30864	
		76.7	101325			47.21	37543	
					ΔH _v /(kJ mol ^{–1}) = 32.41			
					at 25°C	52.36	45367	
						58.61	56448	
					eq. 2	P/mmHg	64.78	69487
					A	6.89406	71.43	86053
					B	1219.58	76.84	99256
			C	227.16				
						bp/°C	76.714	
						eq. 2	P/kPa	
						A	6.00535	
						B	1212.676	
						C	226.483	

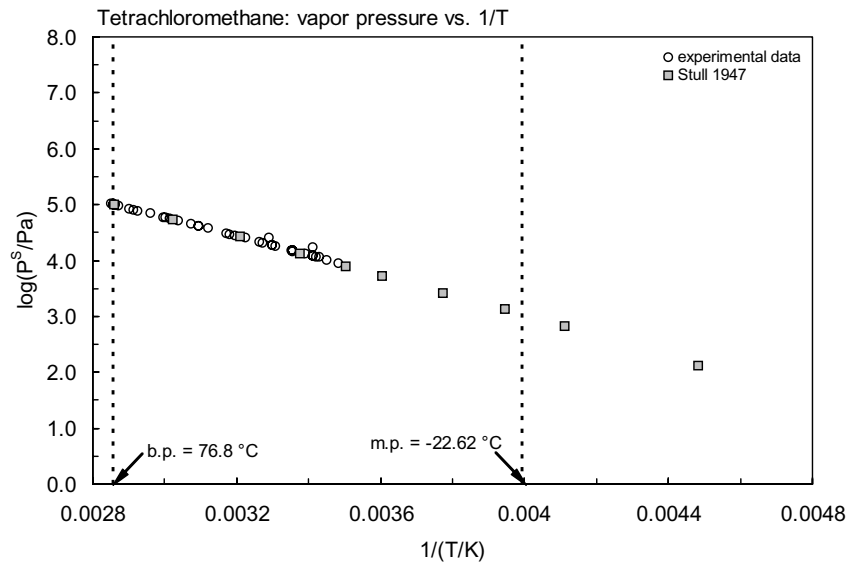


FIGURE 5.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.3
Reported Henry’s law constants of tetrachloromethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$
 $\ln (1/K_{AW}) = A - B/(T/K)$
 $\ln (k_H/\text{atm}) = A - B/(T/K)$
 $\ln H = A - B/(T/K)$
 $K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$

(1)

(2)

(3)

(4)

(5)

$\log K_{AW} = A - B/(T/K)$
 $\log (1/K_{AW}) = A - B/(T/K)$
 $\log H = A - B/(T/K)$

(1a)

(2a)

(4a)

1.

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancrede & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.0	751.6	10.0	1337.5	10	1500	25	2875
1.3	752.2	17.5	2138	15	1935	26.5	2666
11.0	1312	24.8	3080	20	2351	27.4	3248
13.0	1568	34.6	4661	25	2989	28.9	3315
21.0	2335			30	3830	28.9	3466
22.0	2406	eq. 4	H/(atm m³/mol)			29.7	3525
27.1	2866	A	11.29	eq. 4	H/(atm m³/mol)	29.9	3527
25	2797	B	4411	A	9.739	33.3	4713
				B	3951	35.6	4390
eq. 3	k _H /atm					38.3	5334
A	22.22					40	5546
B	4438					44.7	5416
						45	6993
						47.2	7484
						eq. 1	K _{AW}
						A	5.569
						B	1639

(Continued)

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TABLE 5.1.1.4.3 (Continued)

2.

Tse et al. 1992		Wright et al. 1992		Hansen et al. 1993		Dewulf et al. 1995	
activity coefficient		activity coefficient		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
20	2067	20	2646	27.6	3133	2.0	835
30	3415	35	4550	35.0	4550	6.0	912
35	3871	50	6624	45.0	6343	10.0	1055
40	4580					18.2	1926
				eq. 4	H/(kPa m³/mol)	25.0	2598
				A	13.0		
				B	3553	eq. 1	K _{AW}
						A	13.722
						B	4073

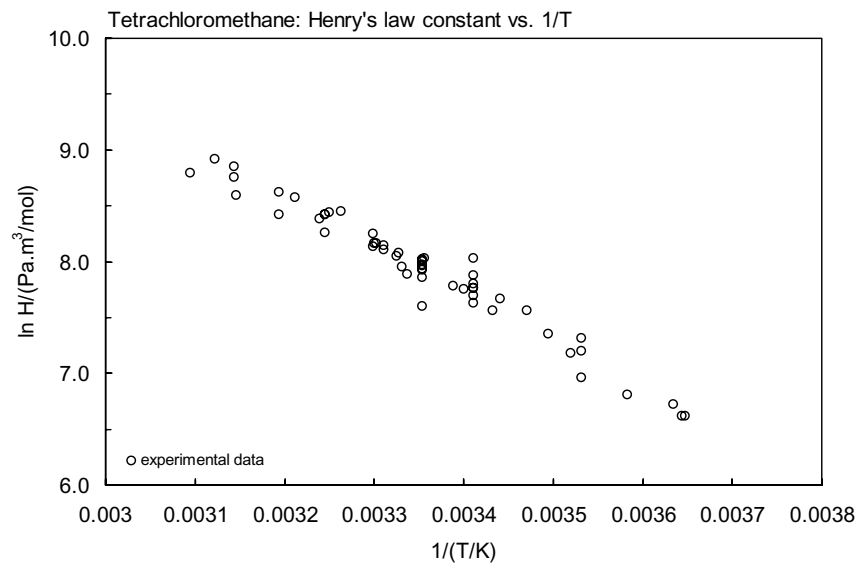


FIGURE 5.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for tetrachloromethane.

TABLE 5.1.1.4.4

Reported octanol-water partition coefficients of tetrachloromethane at various temperatures

Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		EPICS-GC	
t/°C	log K _{OW}	t/°C	log K _{OW}
25	2.73	2.2	2.39
35	2.74	6.0	2.38
50	2.73	10.0	2.50
		14.1	2.44
		18.7	2.47
		24.8	2.38

change in enthalpy:
 $\Delta H_{OW}/(\text{kJ mol}^{-1}) = 1.3$
 (−12.1 to 14.6)

enthalpy of transfer
 $\Delta H_{oct}/(\text{kJ mol}^{-1}) = -0.5$
 (−13.9 to 12.8)

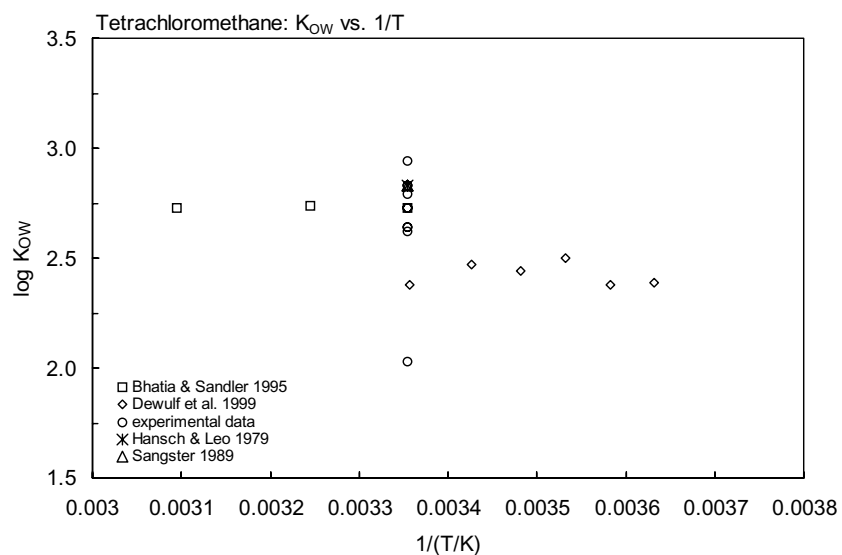


FIGURE 5.1.1.4.4 Logarithm of K_{OW} versus reciprocal temperature for tetrachloromethane.

5.1.1.5 Chloroethane (Ethyl chloride)



Common Name: Ethyl chloride

Synonym: chloroethane, monochloroethane

Chemical Name: chloroethane, ethyl chloride, monochloroethane, hydrochloric ether, muriatic ether

CAS Registry No: 75-00-3

Molecular Formula: C_2H_5Cl , CH_3CH_2Cl

Molecular Weight: 64.514

Melting Point ($^{\circ}C$):

-138.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

12.30 (McGovern 1943; Weast 1982–83; Dean 1985; Howard 1990; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8978 (Weast 1982–83)

0.92390, 0.8960, 0.88981 (0, 20, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

72.0 (calculated-density, Wang et al. 1992)

72.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.8, 24.652 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.45 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5735 ($12.5^{\circ}C$, shake flask, Fühner 1924)

7580 (Seidell 1940)

4500 ($0^{\circ}C$, McGovern 1943; Dean 1985)

5710 ($20^{\circ}C$, Neely 1976)

5700 ($20^{\circ}C$, selected, Dilling 1977)

5678* ($20^{\circ}C$, summary of literature data, Horvath 1982)

5740 ($20^{\circ}C$, Verschuere 1977, 1983)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

136630 (data presented in graph, temp range -50 to $\sim 105^{\circ}C$, McGovern 1943)

187000* (extrapolated-Antoine eq. regression, summary of literature data, Stull 1947)

101436* ($12.51^{\circ}C$, static method-Hg manometer, measured range -55.88 to $12.51^{\circ}C$, Gordon & Giauque 1948)

160000 (calculated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.94914 - 1012.77/(236.47 + t/^{\circ}C)$; temp range -50 to $70^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

$\log (P/mmHg) = 6.94914 - 1012.77/(236.67 + t/^{\circ}C)$, pressure range of 10 to 1500 mmHg, (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log (P/mmHg) = [-0.2185 \times 6310.6/(T/K)] + 7.660205$; temp range -89.8 to $180.5^{\circ}C$ (Antoine eq., Weast 1972–73)

160000 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 6.98647 - 1030.007/(238.612 + t/^{\circ}C)$; temp range -55.94 to $12.5^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

149400 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.11833 - 1033.161/(236.956 + t/^{\circ}C)$; temp range -55.94 to $12.5^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.98647 - 1030.01/(238.61 + t/^{\circ}\text{C})$; temp range -56 to 12.2°C (Antoine eq., Dean 1985, 1992)
 159880 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.09088 - 1020.63/(237.57 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 160000 (calculated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.07404 - 1012.771/(-36.48 + T/\text{K})$; temp range 207 – 305 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.14258 - 1053.998/(-30.686 + T/\text{K})$; temp range 285 – 344 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.4495 - 1248.788/(-3.798 + T/\text{K})$; temp range: 334 – 413 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.70739 - 1465.734/(29.696 + T/\text{K})$; temp range 403 – 460 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 28.3448 - 2.0788 \times 10^3/(T/\text{K}) - 7.5387 \cdot \log (T/\text{K}) - 1.6384 \times 10^{-11} \cdot (T/\text{K}) + 4.055 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 137 – 460 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

860 (calculated as $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
 1140 (calculated, Dilling 1977)
 1145 (calculated-P/C, Mackay & Shiu 1981, 1990)
 1125* (24.8°C , EPICS-GC/FID, measured range 10.3 – 34.6°C , Gossett 1987)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 5.974 - 3120/(T/\text{K})$; temp range: 10.3 – 34.6°C (EPICS measurements, Gossett 1987)
 1226* (EPICS-GC/FID, measured range 10 – 30°C , Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 4.265 - 2580/(T/\text{K})$; temp range 10 – 30°C (EPICS measurements, Ashworth et al. 1988)
 1270 (calculated-QSAR, Nirmalakhandan & Speece 1988)
 942 (20 – 25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 701 (computed value, Yaws et al. 1991)
 1019 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 3.406 - 1110/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.54 (Leo et al. 1971)
 1.39 (calculated- π substituent const., Hansch et al. 1968; Hansch & Leo 1979)
 1.43 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1987)
 1.43 (recommended, Sangster 1989, 1993)
 1.43 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.86, 0.67 (estimated- K_{OW} , S, Lyman et al. 1982; quoted, Howard et al. 1990)
 0.99 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.16, 1.52 (estimated- K_{OW} , S, Lyman et al. 1982; quoted, Howard 1990)
 1.17 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 1.40 (soil, selected, Jury et al. 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental $t_{1/2} = 21$ min for 1 mg/L to evaporate from aqueous solution stirred at 200 rpm in an open container of depth 65 mm at 25°C (Dilling et al. 1975);
 Evaporation $t_{1/2}(\text{exptl}) = 23.1$ min, $t_{1/2}(\text{calc}) = 0.5$ min, 16.7 min from water (Dilling 1977);
 volatilization $t_{1/2} = 2.5$ h from a model river of 1 m deep, based on Henry's law constant (Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2} = 5.6, 1.1,$ and 4.5 d from representative pond, river and lake were estimated based on oxygen reaeration ratio of 0.645 (Mabey et al. 1982; quoted, Howard 1990);

$t_{1/2} = 30$ d for volatilization loss from soil (Jury et al. 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = (3.9 \pm 0.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K and the calculated lifetime of about 2.6×10^8 s or 30 d (discharge flow-laser magnetic resonance, Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980)

$k_{OH} = (2.37 \pm 0.32) \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $(3.94 \pm 0.53) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (flash photolysis-resonance fluorescence, Paraskevopoulos et al. 1978)

$k_{OH} = 2.3 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, estimated at 300 K (Lyman 1982)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{O_3} = 2.0 \times 10^{-23} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–323 K (quoted, Atkinson & Carter 1984) photooxidation half-life of 160–1604 h, based on measured rate constants for the reaction with OH radical in air (Atkinson 1985; quoted, Howard 1990; Howard et al. 1991)

$k_{OH} = 3.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}^* = (4.08 \pm 0.31) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294.8 K, measured range 294.8–788.7 K (laser photolysis/laser induced fluorescence, Kasner et al. 1990)

Hydrolysis: $k = 2.0 \times 10^{-7} \text{ s}^{-1}$ was estimated for reaction at pH 7 and 25°C with a maximum $t_{1/2} = 40$ d (Radding et al. 1977; quoted, Callahan et al. 1979; Mabey et al. 1982);

$k = 2.10 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 38$ day at 25°C and pH 7 (Mabey & Mill 1978)

estimated $t_{1/2} = 38$ d at 25°C was based on an exptl $t_{1/2} = 1.68$ h at 100°C with ethanol and HCl being the hydrolysis product (Mabey & Mill 1978; quoted, Haque et al. 1980; Howard 1990; Howard et al. 1991);

$k = 4.5 \times 10^{-5} \text{ h}^{-1}$ at pH 7 and 25°C with a calculated $t_{1/2} = 1.8$ yr (Jeffers et al. 1989; quoted, Ellington 1989); abiotic hydrolysis or dehydrohalogenation $t_{1/2} = 1.3$ month (Olsen & Davis 1990).

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 168\text{--}672$ h, based on aqueous aerobic screening test data for 1-chloropropane and 1-chlorobutane (Gerhold & Malaney 1966; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}2688$ h, based on estimated unacclimated aqueous aerobic half-life (Howard et al. 1991)

$k = 0.02 \text{ yr}^{-1}$ with $t_{1/2} = 10$ d and $k = 0.001 \text{ yr}^{-1}$ with $t_{1/2} = 700$ d (Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetime of about 2.6×10^8 s or 30 d (Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980);

$t_{1/2} = 160\text{--}1604$ h, based on photooxidation half-life in air from measured rate constants for the gas phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 0.04 yr (Nimitz & Skaggs 1992).

Surface water: $t_{1/2} = 168\text{--}672$ h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 336\text{--}1344$ h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 10\text{--}50$ d (Ryan et al. 1988);

$t_{1/2} = 30$ d, volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 168\text{--}672$ h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} = 10\text{--}50$ d, subject to plant uptake by soil through volatilization (Ryan et al. 1988).

TABLE 5.1.1.5.1
Reported aqueous solubilities and vapor pressures of chloroethane at various temperatures

$S/(wt\%) = 0.5842 - 1.6863 \times 10^{-3} \cdot (t/^{\circ}C) + 9.3949 \times 10^{-5} \cdot (t/^{\circ}C)^2 - 2.5316 \times 10^{-6} \cdot (t/^{\circ}C)^3$ (1)

Aqueous solubility		Vapor pressure			
Horvath 1982		Stull 1947		Gordon & Giauque 1948	
summary of literature data		summary of literature data		static method-Hg manometer	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
0	5842	−89.8	133.3	−55.88	2993
10	5742	−73.9	666.6	−43.64	6726
20	5678	−65.8	1333	−35.44	10992
eq. 1	S/wt%	−56.8	2666	−28.085	16549
		−47.0	5333	−19.99	25119
		−40.6	7999	−13.48	34379
		−32.0	13332	−7.64	44878
		−18.6	26664	−1.878	57621
		−3.90	53329	3.448	17859
		12.4	101325	6.481	81100
				10.48	94708
				12.51	101436
				mp/K =	134.80
		bp/K =	285.37		
				log P = A − B/(T/K) − C·(T/K) + D·(T/K) ²	
				P/cmHg	
				A	10.54417
				B	1777.378
				C	0.0115789
				D	1.06734 × 10 ⁵
				ΔH _{fus} /(kJ mol ^{−1}) = 4.452	
				ΔH _v /(kJ mol ^{−1}) = 24.65	
				at 285.37 K	

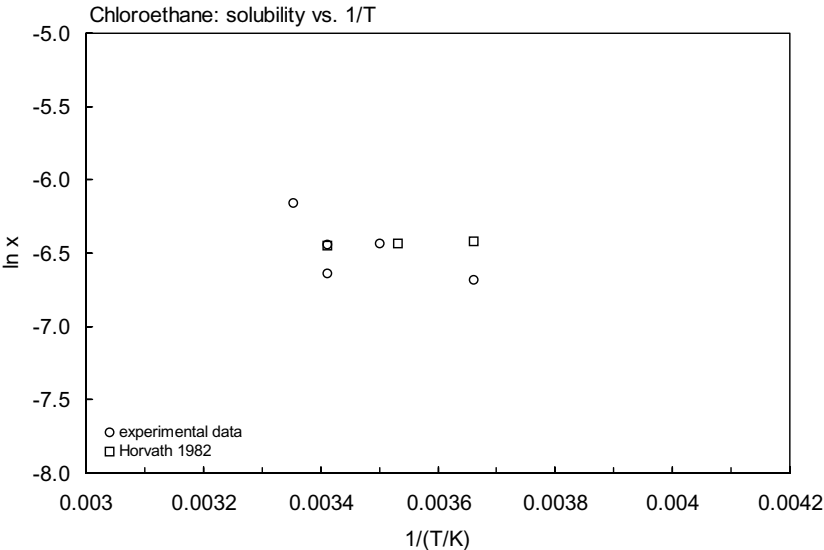


FIGURE 5.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for chloroethane.

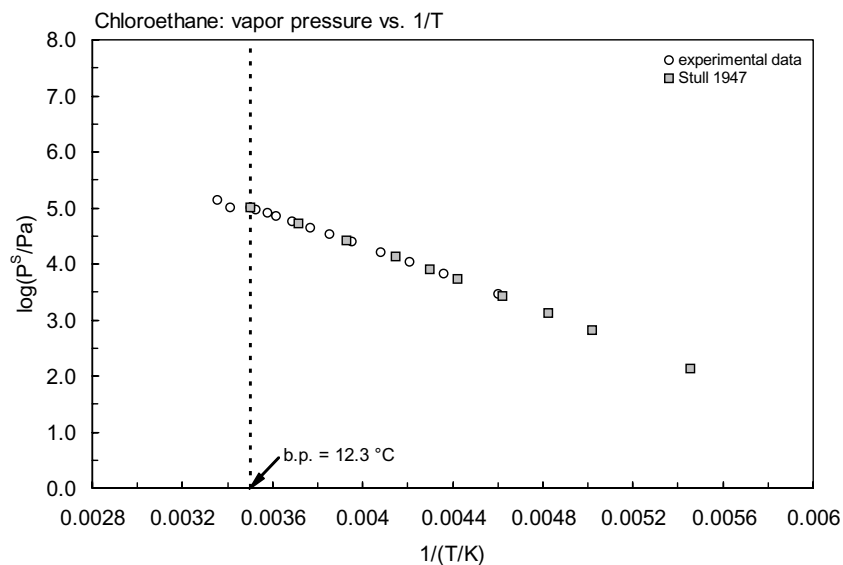


FIGURE 5.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for chloroethane.

TABLE 5.1.1.5.2
Reported Henry’s law constants of chloroethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Gossett 1987			Ashworth et al. 1988		
EPICS-GC			EPICS-GC		
t/°C	H/(Pa m ³ /mol)		t/°C	H/(Pa m ³ /mol)	
10.3	660		10	769	
17.5	857.2		15	970.7	
24.8	1125		20	1115	
34.6	1571		25	1226	
			30	1449	
eq. 4a	H/(atm m ³ /mol)		eq. 4a	H/(atm m ³ /mol)	
A	7.385		A	4.265	
B	3286		B	2580	

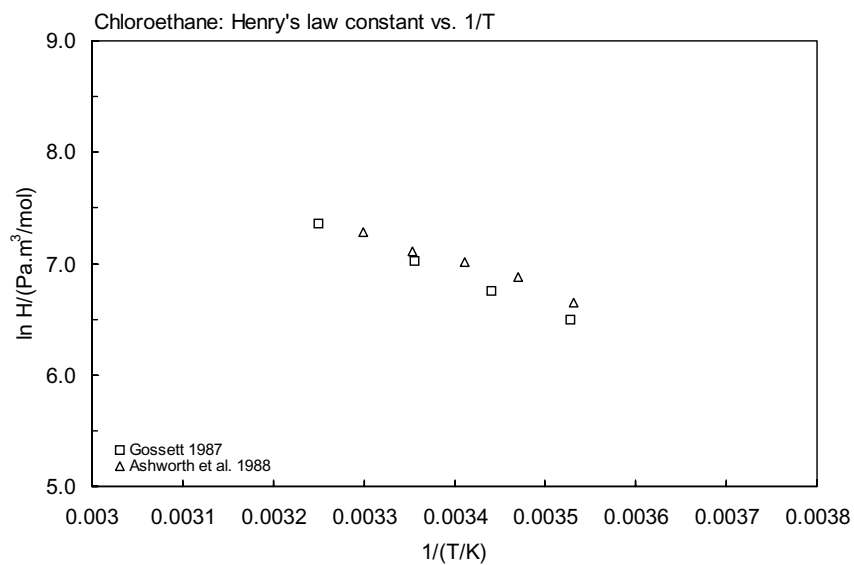


FIGURE 5.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for chloroethane.

5.1.1.6 1,1-Dichloroethane



Common Name: 1,1-Dichloroethane

Synonym: ethylidene chloride, ethylidene dichloride

Chemical Name: 1,1-dichloroethane

CAS Registry No: 75-34-3

Molecular Formula: $C_2H_4Cl_2$, CH_3CHCl_2

Molecular Weight: 98.959

Melting Point ($^{\circ}C$):

−96.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

57.3 (Weast 1982–83, Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1757 (Dreisbach 1961; Horvath 1982; Weast 1982–83; Dean 1985)

1.1755, 1.1679 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

84.0 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

93.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

30.62, 28.6 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.87 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5500* ($20^{\circ}C$, volumetric method, measured range 0 – $30^{\circ}C$, Rex 1906)

5060 (shake flask-interferometer, Gross 1929; quoted, Horvath 1982)

5555 (volumetric method, Wright & Schaffer 1932)

5060* ($20^{\circ}C$, shake flask, measured range 0 – $50^{\circ}C$, Van Arkel & Vles 1936)

5060 (Seidell 1941)

4800* (shake flask, measured range 10 – $70^{\circ}C$, Walraevens et al. 1974)

$\log [S/(mol/L)] = 2070/(T/K) - 15.116 + 0.0230 \cdot (T/K)$, temp range 10 – $70^{\circ}C$, Walraevens et al. 1974

5100 (literature average, Dilling 1977, 1982)

4767* (summary of literature data, temp range 0 – $80^{\circ}C$, Horvath 1982)

4834 ($30^{\circ}C$, headspace-GC analysis, McNally & Grob 1983)

4589 ($30^{\circ}C$, headspace-GC analysis, McNally & Grob 1984)

5030 ($20^{\circ}C$, selected, Riddick et al. 1986)

5090, 4910, 5090 (20 , 35 , $50^{\circ}C$, infinite dilution activity coeff. γ^{∞} -GC, Barr & Newsham 1987)

4842, 4984 (predicted-MCI χ and polarizability, Nirmalakhandan & Speece 1988)

5240, 5317, 5406 (20 , 30 , $40^{\circ}C$, infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)

6560, 7300, 8085 (20 , 30 , $40^{\circ}C$, infinite dilution activity coeff. γ^{∞} -UNIFAC, Tse et al. 1992)

4998, 4434, 5236 (20 , 35 , $45^{\circ}C$, activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)

5196* ($20^{\circ}C$, activity coeff. by inert air stripping-GC, measured range 10 – $50^{\circ}C$, Hovorka & Dohnal 1997)

5040* (recommended, temp range 0 – $50^{\circ}C$, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 9.4136 - 5.7249 \times 10^{-2} \cdot (T/K) + 9.17839 \times 10^{-5} \cdot (T/K)^2$, temp range 273 – $323 K$ (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

24300, 37000 ($20^{\circ}C$, $30^{\circ}C$, Rex 1906)

- 30000* (Antoine eq. regression, temp range -60.7 to 57.4°C, Stull 1947)
 22001* (17.62°C, static-Hg manometer, measured range -38.76 to 17.62°C, Li & Pitzer 1956)
 30400 (calculated-Antoine eq., Dreisbach 1961)
 $\log (P/\text{mmHg}) = 6/9853 - 1171.42/(228.12 + t/^\circ\text{C})$; temp range -15 to 82°C (Antoine eq. for liquid state, Dreisbach 1961)
 26000 (calculated-Antoine eq., Weast 1972-73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 7288.0/(T/K)] + 7.629952$; temp range -60.7 to 261.5°C (Antoine eq., Weast 1972-73)
 30260 (calculated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 6.97702 - 1174.022/(229.06 + t/^\circ\text{C})$; temp range -38.8 to 17.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 30260 (Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.10983 - 1177.636/(229.409 + t/^\circ\text{C})$; temp range -38.8 to 17.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 6.9971 - 1174.02/(229.08 + t/^\circ\text{C})$; temp range -39 to 16°C (Antoine eq., Dean 1985, 1992)
 30360 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.16780 - 1201.05/(231.27 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 30360 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.1102 - 1171.42/(-45.03 + T/K)$; temp range 258-365 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.14443 - 1216.12/(-36.569 + T/K)$; temp range 323-535 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.22839 - 1288.092/(-24.381 + T/K)$; temp range 363-535 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 24440, 37240 54990 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
 $\log (P/\text{mmHg}) = 33.380 - 2.6102 \times 10^3/(T/K) - 9.1336 \cdot \log (T/K) - 2.8838 \times 10^{-11} \cdot (T/K) + 3.7323 \times 10^{-6} \cdot (T/K)^2$; temp range 176-523 K (vapor pressure eq., Yaws 1994)
 $\log (P/\text{kPa}) = 6.110022 - 1171.420/(T/K - 45.03)$ (from database of CData 1991, Hovorka & Dohnal 1997)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 595 (calculated-1/K_{AW} (C_W/C_A) reported as exptl., Hine & Mookerjee 1975)
 595 (calculated-P/C, Dilling 1977)
 $\log (k_H/\text{atm}) = 8.87 - 1902.37/(T/K)$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)
 569* (EPICS-GC/FID, measured range 9.6-34.6°C, Gossett 1987)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.637 - 4128/(T/K)$; temp range 9.6-34.6°C (EPICS measurements, Gossett 1987)
 552 (gas stripping-GC, Warner et al. 1987)
 633* (EPICS-GC/FID, measured range 10-30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 5.484 - 3137/(T/K)$; temp range 10-30°C (EPICS measurements, Ashworth et al. 1988)
 436 (20-25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 584 (calculated-P/C, Mackay & Shiu 1990)
 595 (computed value, Yaws et al. 1991)
 436 (20°C, quoted from Gossett 1987, Tse et al. 1992)
 466, 709, 1034 (20, 30, 40°C, infinite dilution activity coeff. γ -GC, Tse et al. 1992)
 477, 995, 1226 (20, 35, 45°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 588, 1125, 1844 (25, 35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 511* (EPICS-GC/FID, measured range 2.0-25°C, Dewulf et al. 1995)
 246, 627 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
 $\ln K_{AW} = -3975/(T/K) + 0.00768 \cdot Z + 11.727$; with Z salinity 0-35.5‰, temp range: 2-35°C, (EPICS-GC/FID, Dewulf et al. 1995)
 526 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 466* (20°C, equilibrium air stripping-GC, measured range 10-50°C, Hovorka & Dohnal 1997)
 500 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
 $\log K_{AW} = 4.416 - 1498/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

592* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
 $\ln K_{AW} = 10.09 - 3447.7/(T/K)$; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 1.79 (shake flask-GC, Hansch et al. 1975, Hansch & Leo 1987)
- 1.92 (Hansch & Leo 1979)
- 1.79 (recommended, Sangster 1993)
- 1.89 (calculated-activity coefficients, Tse & Sandler 1994)
- 1.82* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
- 1.79 (recommended, Hansch et al. 1995)
- 1.75* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 2.41 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 1.20 (estimated-S, Lyman et al. 1982)
- 1.28 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 1.60 (estimated-S, Lyman et al. 1982)
- 1.48 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.66 (soil, selected, Jury et al. 1990)
- 1.43, 1.46, 1.43, 1.48, 1.50, 1.49, 1.55 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental $t_{1/2} = 22$ min for initial concentration of 1.0 mg/L when stirred at 200 rpm in water at approx. 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);
 Evaporation $t_{1/2}(\text{exptl}) = 32.2$ min, $t_{1/2}(\text{calc}) = 0.98$ min, 21.2 min from water (Dilling 1977);
 $t_{1/2} = 6\text{--}9$ d in a typical pond, $t_{1/2} = 5\text{--}8$ d in a typical lake, and $t_{1/2} = 24\text{--}32$ h in a typical river (Smith et al. 1980; quoted, Howard 1990);
 ratio of rate of evaporation to that of oxygen reaeration: measured value of 0.57 compared to that predicted value of 0.47 (Smith et al. 1980);
 $t_{1/2} = 45$ d for the volatilization loss from soil (Jury et al. 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.6 \pm 0.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-laser magnetic resonance, Howard & Evenson 1976b; quoted, Callahan et al. 1979; Altshuller 1980; Howard 1990)

$k_{OH} = 2.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 44 d, loss of 2.3% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{OH} < 1.6 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with OH radical at 300 K (Lyman 1982)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $1.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical both at 25°C (Mabey et al. 1982; quoted, Ma et al. 1990)

photooxidation $t_{1/2} = 247\text{--}2468$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis: $k = 1.15 \times 10^{-7} \text{ M}^{-1} \text{ h}^{-1}$ for neutral process by analogy to dichloromethane (Mabey et al. 1982);

$k = 1.29 \times 10^{-6} \text{ h}^{-1}$ at pH 7 and 25°C with calculated $t_{1/2} = 61$ yr (Jeffers et al. 1989; quoted, Ellington 1989).

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 768\text{--}3696$ h, based on estimated methane acclimated soil grab sample data (Henson et al. 1989; quoted, Howard et al. 1991) and sub-soil grab sample data from a ground water aquifer

(Wilson et al. 1983; quoted, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 3072\text{--}14784$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} > 60$ d (Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetime of 1.5 months based on reaction with OH radical (Callahan et al. 1979; Altshuller 1980; Howard 1990);

residence time of 44 d, loss of 2.3% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 247\text{--}2468$ h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991); estimated tropospheric lifetime of 0.02 yr (Nimitz & Skaggs 1992).

Surface water: $t_{1/2} = 768\text{--}3696$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 1344\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life and sub-soil grab sample data from a groundwater aquifer (Wilson et al. 1983; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 10\text{--}50$ d (Ryan et al. 1988);

$t_{1/2} = 768\text{--}3696$ h, based on methane acclimated soil grab sample data (Henson et al. 1989; quoted, Howard et al. 1991) and sub-soil grab sample data from a groundwater aquifer (Wilson et al. 1983; quoted, Howard et al. 1991);

$t_{1/2} = 45$ d, volatilization loss from soil (Jury et al. 1990).

Biota: $t_{1/2} < 2$ d of elimination from whole body of bluegill sunfish (USEPA 1980; quoted, Howard 1990);

$t_{1/2} = 10\text{--}50$ d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.6.1

Reported aqueous solubilities of 1,1-dichloroethane at various temperatures

$$S/(\text{wt}\%) = 0.5826 - 7.8236 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 1.5268 \times 10^{-4} \cdot (t/^{\circ}\text{C})^2 - 3.6609 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 9.4136 - 5.7249 \times 10^{-2} \cdot (T/\text{K}) + 9.17839 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Rex 1906		Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982	
volumetric method		shake flask		shake flask-GC		summary of literature data	
t/ $^{\circ}\text{C}$	S/g·m ⁻³	t/ $^{\circ}\text{C}$	S/g·m ⁻³	t/ $^{\circ}\text{C}$	S/g·m ⁻³	t/ $^{\circ}\text{C}$	S/g·m ⁻³
0	6560	0	5940	10	5030	0	5826
10	5950	20	5060	20	4830	10	5193
20	5500	35	4820	25	4800	20	4843
30	5400	50	5190	30	4810	25	4766
				40	4960	30	4754
				50	5280	40	4905
				60	5790	50	5274
				70	8520	60	5838
				80	7510	70	6575
						80	7465
						eq.1	S/wt%

(Continued)

TABLE 5.1.1.6.1 (Continued)

2.

Barr & Newsham 1987		Wright et al. 1992		Hovorka & Dohnal 1997		Horvath & Getzen 1999a	
infinite dilution activity coeff.		activity coefficient		activity coefficient		recommended, IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	5090	20	4998	10	5627	0	6240
35	4910	35	4434	20	5196	5	5910
50	5090	45	5236	30	5236	10	5620
				35	5266	15	5380
				40	5395	20	5190
				45	5576	25	5040
				50	5812	30	4930
						35	4880
						40	4870
						45	4900
						50	4980
						eq. 2	S/wt%
						temp range 273–323 K	

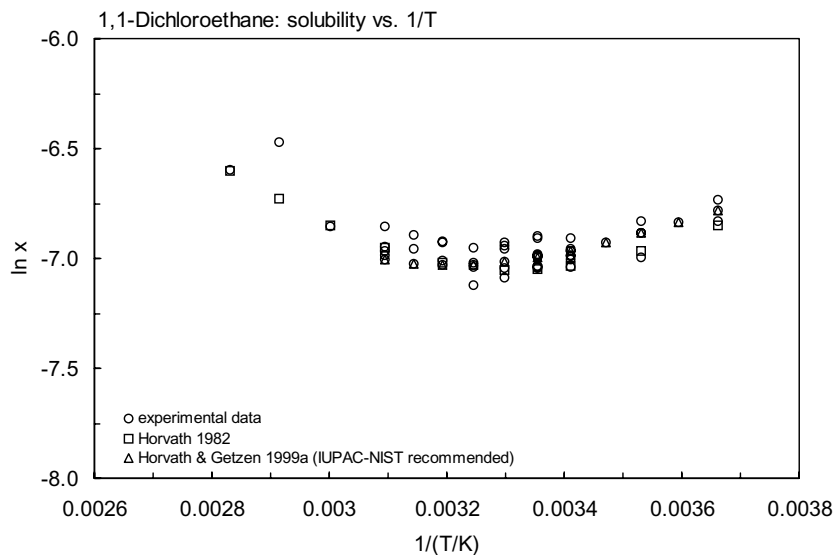


FIGURE 5.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.2

Reported vapor pressures of 1,1-dichloroethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)		
$\log P = A - B/(C + T/K)$	(3)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)				
Stull 1947	Li & Pitzer 1956				
summary of literature data	static-Hg manometer				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−60.7	133.3	−38.76	858.6	11.34	16536
−41.9	666.6	−29.61	1649	17.50	21876
−32.3	1333	−20.21	3020	17.62	22001
−21.9	2666	−19.18	3234		
−10.2	5333	−18.16	3301	mp/°C	−96.98
−2.90	7999	−17.69	3517		
7.20	13332	−16.82	3716	eq. 2	P/cmHg
22.4	26664	−12.61	4772	A	6.1560
39.8	53329	−12.20	4869	B	1258.1
57.4	101325	−2.23	8425	C	26.0
		1.18	10077	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 7.87$	
mp/°C	−96.7	11.10	16333	$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 31.02$	

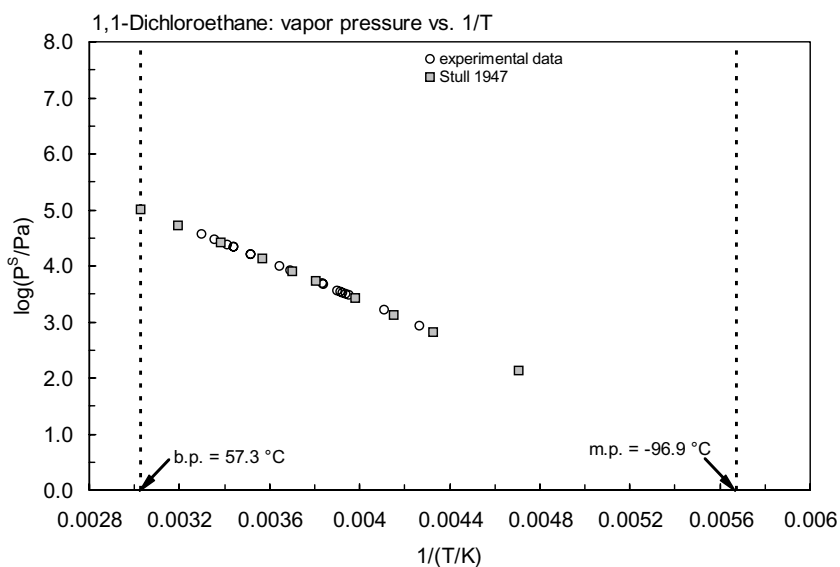


FIGURE 5.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.3

Reported Henry's law constants of 1,1-dichloroethane at various temperatures and temperature dependence equations

$$\begin{aligned} \ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln H &= A - B/(T/K) & (4) & \log H = A - B/(T/K) & (4a) \\ K_{AW} &= A - B \cdot (T/K) + C \cdot (T/K)^2 & (5) & & \end{aligned}$$

1.

Gossett 1987		Ashworth et al. 1988		Tse et al. 1992		Wright et al. 1992	
EPICS-GC		EPICS-GC		activity coefficient		activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
9.6	251.3	10	373	20	466	20	477
17.5	394.2	15	460	30	709	35	995
24.8	569.4	20	570	40	1034	45	1226
34.6	820.7	25	631				
		30	786				
eq. 4	H/(atm m ³ /mol)	eq. 4	H/(atm m ³ /mol)				
A	8.637	A	5.484				
B	4128	B	3137				

2.

Bhatia & Sandler 1995		Dewulf et al. 1995		Hovorka & Dohnal 1997		Görgényi et al. 2002	
activity coefficient		EPICS-GC		equilibrium air stripping-GC		EPICS-SPME method	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
25	588	2	152.1	10	273	2	174
35	1125	6	195.2	20	466	6	240.4
50	1844	10	194.7	30	692	10	283.9
		18.2	378.2	35	851	18	452.4
		25	510.6	40	1010	25	592.4
				45	1172	30	760.9
		eq. 1	K _{AW}	50	1338	40	1059
		A	11.727			50	1472
		B	3975			60	1907
						eq. 1	K _{AW}
						A	10.09
						B	3447.7

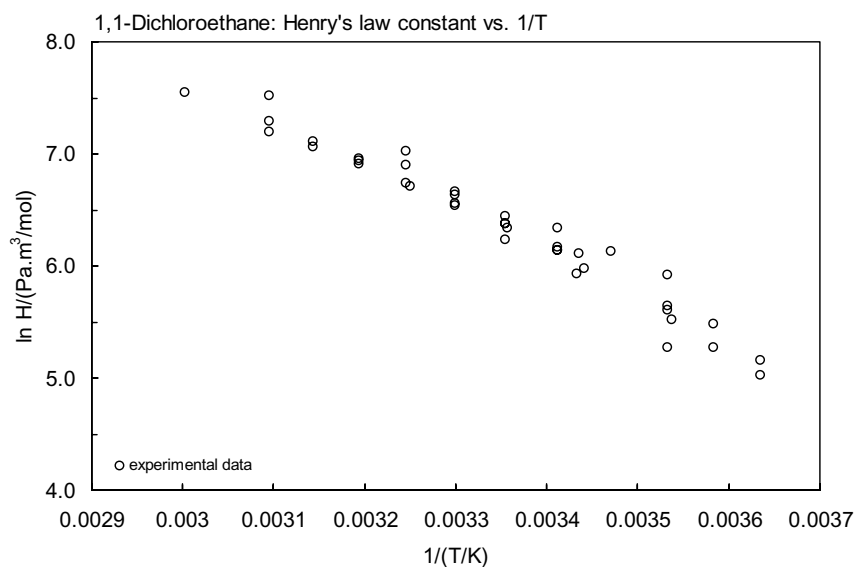


FIGURE 5.1.1.6.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1-dichloroethane.

TABLE 5.1.1.6.4

Reported octanol-water partition coefficients of 1,1-dichloroethane at various temperatures

Bhatia & Sandler 1995		DeWulf et al. 1999	
relative GC-RT technique		EPICS-GC	
$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$	$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$
25	1.82	2.2	1.70
35	1.66	4.0	1.69
50	1.68	10.0	1.74
		14.1	1.73
		18.7	1.78
		24.8	1.75
change in enthalpy:			
$\Delta H_{\text{OW}}/(\text{kJ mol}^{-1}) = 5.2$			
(0.0 to 10.4)			
enthalpy of transfer			
$\Delta H_{\text{OCT}}/(\text{kJ mol}^{-1}) = 2.5$			
(-2.7 to 7.7)			

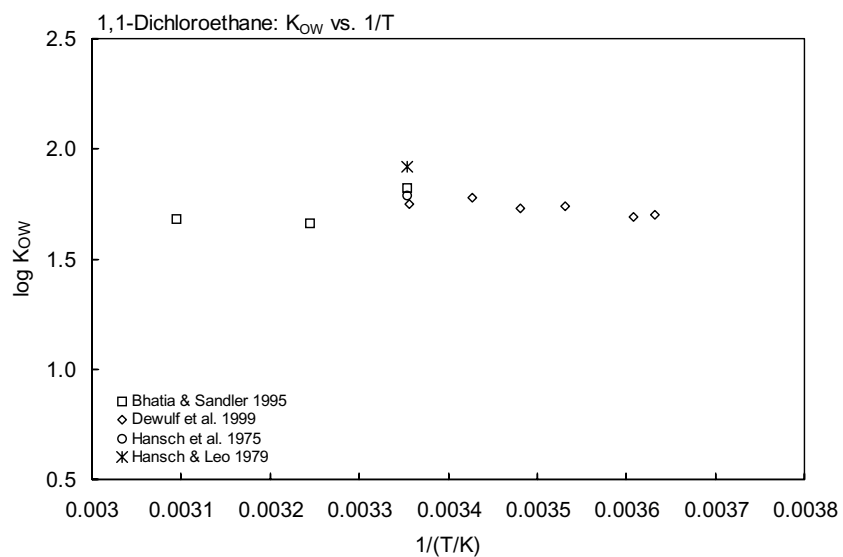
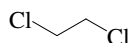


FIGURE 5.1.1.6.4 Logarithm of K_{OW} versus reciprocal temperature for 1,1-dichloroethane.

5.1.1.7 1,2-Dichloroethane



Common Name: 1,2-Dichloroethane

Synonym: ethylene chloride, ethylene dichloride, glycol dichloride, sym-dichloroethane, Dutch oil, EDC

Chemical Name: 1,2-dichloroethane

CAS Registry No: 107-06-2

Molecular Formula: $C_2H_4Cl_2$, CH_2ClCH_2Cl

Molecular Weight: 98.959

Melting Point ($^{\circ}C$):

−35.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

85.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2531, 1.2458 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Dean 1985)

1.25209, 1.24637 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

78.0 (calculated-density, Wang et al. 1992)

93.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.15, 32.02 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

1.982 (calculated, Dreisbach 1959)

2.112 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

8690* ($20^{\circ}C$, volumetric method, measured range $0-30^{\circ}C$, Rex 1906)

8650 (shake flask-interferometer, Gross 1929)

8720, 9000 ($15^{\circ}C$, $30^{\circ}C$, shake flask-interferometer, Gross & Saylor 1931)

8696 (volumetric method, Wright & Schaffer 1932)

8490* ($20^{\circ}C$, shake flask, measured range $0-56^{\circ}C$, Van Arkel & Vles 1936)

8620 (Seidell 1940)

8400 (data presented in graph, temp range $0-70^{\circ}C$, McGovern 1943; Horvath 1982)

8610* (shake flask-GC, temp range $0-80^{\circ}C$, Walraevens et al. 1974)

$\log [S/(mol/L)] = 2070/(T/K) - 15.369 + 0.0247 \cdot (T/K)$; temp range $0-80^{\circ}C$ (Walraevens et al. 1974)

8800 (shake flask-GC, McConnell et al. 1975)

8800 ($20^{\circ}C$, Pearson & McConnell 1975)

8570, 8390, 10250 (3, 20, $34^{\circ}C$, shake flask-GC/ECD, Chiou & Freed 1977)

8450 (shake flask-GC, Chiou et al. 1979)

8630 ($20^{\circ}C$, recommended, Sørensen & Arit 1979)

7987 (shake flask-LSC, Banerjee et al. 1980)

10600 (shake flask-titration, Coca & Diza 1980)

11000 (shake flask-titration/turbidity, Coca et al. 1980)

8000 (shake flask-LSC, Veith et al. 1980)

8608* (summary of literature data, temp range $0-80^{\circ}C$, Horvath 1982)

3506 ($30^{\circ}C$, shake flask-headspace-GC, McNally & Grob 1984)

8044 (calculated-UNIFAC activity coeff., Banerjee 1985)

8100 (Dean 1985, Riddick et al. 1986)

8782, 9102, 9960 (20, 35, $50^{\circ}C$, infinite dilution activity coeff. γ^{∞} -GC, Barr & Newsham 1987)

7200* ($19.7^{\circ}C$, shake flask-GC/TC, measured range $0-80^{\circ}C$, Stephenson 1992)

8500, 9013, 9163 (20, 30, $40^{\circ}C$, infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)

7809, 8727, 9209 (20, 30, 40°C, infinite dilution activity coeff. γ^∞ -UNIFAC, Tse et al. 1992)
 9400, 9209, 9835 (20, 35, 50°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 6537 (20°C, activity coeff. γ^∞ by inert air stripping-GC, Hovorka & Dohnal 1997)
 8600* (recommended, temp range 0–100°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
 $S/(\text{wt}\%) = 17.9147 - 0.11684 \cdot (T/K) + 2.0003 \times 10^{-4} \cdot (T/K)^2$, temp range 273–373 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)404

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

8130, 12980 (20°C, 30°C, Rex 1906)
 10519* (isotenoscope method, measured range –30.82 to 99.4°C, Pearce & Peters 1929)
 $\log (P/\text{mmHg}) = 128.756 - 4481.12/(T/K) - 52.3092 \cdot \log (T/K) + 0.07153 \cdot (T/K) - 4.1847 \times 10^{-5} \cdot (T/K)^2$; temp range 243–363 K (isotenoscope method, Pearce & Peters 1929)
 10660 (McGovern 1943)
 10740* (interpolated-Antoine eq., regression, temp range –30.8 to 99.4°C, Stull 1947)
 10700 (calculated-Antoine eq., Dreisbach 1959)
 $\log (P/\text{mmHg}) = 7.18431 - 1358.5/(252.0 + t/^\circ\text{C})$; temp range 6–161°C (Antoine eq. for liquid state, Dreisbach 1959)
 10150 (calculated-Antoine eq., Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 7950.7/(T/K)] + 7.708405$; temp range –44.5 to 285°C (Antoine eq., Weast 1972–73)
 10500 (calculated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.0253 - 1271.254/(222.927 + t/^\circ\text{C})$; temp range –30.82 to 99.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 8520 (McConnell et al. 1975)
 8400 (Pearson & McConnell 1975)
 13282*, 65145 (30, 70°C, vapor-liquid equilibrium VLE data, measured range 28.75–85.54°C, Gutsche & Knapp 1982)
 $\ln (P/\text{kPa}) = 14.142372 - 2896.480/[(T/K) - 52.506]$; temp range 301.9–357.69 K (vapor-liquid equilibrium VLE data, Gutsche & Knapp 1982)
 10500 (Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.16284 - 1278.323/(223.694 + t/^\circ\text{C})$; temp range –30.82 to 99.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.13975 - 1256.68/(220.504 + t/^\circ\text{C})$; temp range 28.75–84.54°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 7.0253 - 1271.3/(222.9 + t/^\circ\text{C})$; temp range –31 to 99°C (Antoine eq., Dean 1985, 1992)
 11110 (selected, Riddick et al. 1986)
 11100 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.07712 - 1247.8/(-50.15 + T/K)$; temp range 279–434 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.53278 - 1599.07/(-3.303 + T/K)$; temp range 356–558 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.07287 - 1245.488/(-50.392 + T/K)$; temp range 279–374 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.40918 - 1505.414/(-14.406 + T/K)$; temp range 368–524 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.5198 - 2129.577/(T/K)$; temp range 523–561 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 10462 (resistance measurements-Antoine eq., Foco et al. 1992)
 8270, 13320, 16720 (20, 30, 35°C, quoted from DIPPR, Tse et al. 1992)
 $\log (P/\text{mmHg}) = 48.4226 - 3.1803 \times 10^3/(T/K) - 15.37 \cdot \log (T/K) + 7.2935 \times 10^{-3} \cdot (T/K) + 2.6844 \times 10^{-14} \cdot (T/K)^2$; temp range 237–561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.1 (exptl., $1/K_{AW} (C_W/C_A)$, Hine & Mookerjee 1975)
 92.3 (calculated- C_W/C_A , McConnell et al. 1975; Pearson & McConnell 1975)

- 99.0, 123.9 (exptl., calculated-P/C, Dilling 1977)
 111.3 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
 174* (27.0°C, equilibrium cell-concn ratio-GC/FID, measured range 1.0–27.0°C, Leighton & Calo 1981)
 $\ln(k_H/\text{atm}) = 18.51 - 3482/(T/K)$; temp range: 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
 110 (recommended, Mackay & Shiu 1981)
 111.5 (gas stripping-GC, Warner et al. 1987)
 143* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln[H/(\text{atm}\cdot\text{m}^3/\text{mol})] = -1.371 - 1522/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 92.0 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 70.8 (computed value, Yaws et al. 1991)
 101, 152, 182 (20, 30, 40°C, infinite dilution activity coeff. γ° -GC, Tse et al. 1992)
 110, 185, 319 (20, 35, 50°C, activity coeff. γ° -differential pressure transducer, Wright et al. 1992)
 122.5 (γ° from gas stripping-GC, Li et al. 1993)
 5.30, 8.99 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 102.1* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)
 55.9, 123 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
 $\ln K_{AW} = -4329/(T/K) + 0.00473\cdot Z + 11.377$; with Z salinity 0–35.5‰, temp range: 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)
 110 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 95.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1998)
 185.2 (EPICS-GC, Ayuttaya et al. 2001)
 102 (20°C, selected from reported experimentally determined values, Staudinger & Roberts 2001)
 $\log K_{AW} = 4.434 - 1705/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 1.48 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979, 1987)
 1.45 (shake flask-LSC, Banerjee et al. 1980; Veith et al. 1980)
 1.58, 1.54 (calculated-octanol and water mutual solubility not considered, calculated-octanol and water mutual solubility considered, Arbuckle 1983)
 1.44 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
 1.48 (recommended, Sangster 1993)
 1.55 (calculated-from activity coefficients, Tse & Sandler 1994)
 1.51* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
 1.48 (recommended, Hansch et al. 1995)
 1.46* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 2.78 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 0.30 (bluegill sunfish, Barrows et al. 1980)
 0.301 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
 0.954 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982; quoted, Ma et al. 1990)
 0.30 (bluegill sunfish, Davies & Dobbs; quoted, Sabljic 1987; Ma et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 1.28 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
 1.51 (soil, quoted from Chiou et al. 1979, Karickhoff 1981)
 1.06, 1.19, 1.48 (estimated- K_{OW} , estimated-S and mp, estimated-S, Karickhoff 1981)
 2.18 (estimated- K_{OW} , Lyman et al. 1982;)
 1.15 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 1.09 (BUA 1987; quoted, Brüggemann et al. 1991)

1.34 (soil, selected, Jury et al. 1990)

1.64, 1.645, 1.64, 1.68, 1.70, 1.65, 1.68 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)

Sorption Partition Coefficient, $\log K_{OM}$:

1.28, 1.50 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental half-life of volatilization from aqueous solution of 1 mg/L to be (28 ± 1) min when stirred at 200 rpm in water at approx. 25°C in an open container (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation $t_{1/2}(\text{exptl}) = 28.0$ min, $t_{1/2}(\text{calc}) = 4.5$ min, 24.5 min from water (Dilling 1977)

rate of evaporation $k = 2.4 \text{ g m}^{-2} \text{ s}^{-1}$ (Environment Canada 1984);

$t_{1/2} = 90$ d, estimated volatilization loss from soil (Jury et al. 1990).

Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 1.1 ppm/min per gram of catalyst (Ollis 1985)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.2 \pm 0.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-laser magnetic resonance, Howard & Everson 1976b; quoted, Callahan et al. 1979)

$k_{OH} = 0.1 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 234$ h (Radding et al. 1977; quoted, Callahan et al. 1979)

$k_{OH} = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with residence time of 53 d, loss of 1.9% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{OH} = 1.3 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, estimated, at 300 K (Lyman 1982)

$k < 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k < 1 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radicals at 25°C (Mabey et al. 1982)

photooxidation $t_{1/2} = 292\text{--}2917$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k(\text{aq.}) \leq 0.05 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with a $t_{1/2} \geq 8$ d at pH 7 (Yao & Haag 1991).

Hydrolysis:

$k = 5 \times 10^{-13} \text{ s}^{-1}$ with a max. $t_{1/2} = 50,000$ yr at pH 7 and 25°C from experimental data at 100–150°C (Radding et al. 1977; quoted, Callahan et al. 1979);

$k = 1.80 \times 10^{-9} \text{ h}^{-1}$ for neutral process (Mabey et al. 1982; quoted, Ma et al. 1990)

$t_{1/2}(\text{abiotic})$ or $t_{1/2}(\text{dehydrohalogenation}) = 50$ months (Mabey et al. 1983; quoted, Olsen & Davis 1990)

$k(\text{neutral}) = .63 \text{ yr}^{-1}$ with first-order $t_{1/2} = 1.1$ yr (Kollig et al. 1987; quoted, Howard et al. 1991)

$k = 1.1 \times 10^{-6} \text{ h}^{-1}$ at pH 7 and 25°C with calculated $t_{1/2} = 72$ yr (Jeffers et al. 1989; quoted, Ellington 1989; Brüggemann et al. 1991)

$t_{1/2} = 400$ d at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: relatively undegradable (Lyman et al. 1982; quoted, Brüggemann et al. 1991)

$k < 1.4 \times 10^{-5} \text{ min}^{-1}$ disappearance rate in sediment-water sample, with $t_{1/2} > 35$ d (Jafvert & Wolfe 1987)

$t_{1/2}(\text{aq. aerobic}) = 2400\text{--}4320$ h, based on unacclimated grab sample of aerobic soil from ground water aquifers and acclimated river die-away rate data (Wilson et al. 1983; Mudder 1981; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 9600\text{--}17280$ h (Howard et al. 1991)

$t_{1/2} > 60$ d (Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 100$ d, $t_{1/2}(\text{anaerobic}) = 400$ d in natural waters (Capel & Larson 1995)

Biotransformation: estimated to be $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 17$ wk when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

lifetime of 1.7 months at 296 K based on reaction with OH radical (Callahan et al. 1979);

residence time of 53 d, loss of 1.9% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 292\text{--}2917$ h, based on photooxidation half-life in air from measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 0.09 yr (Nimitz & Skaggs 1992).

Surface water: $t_{1/2} = 2400\text{--}4320$ h, based on unacclimated grab sample of aerobic soil from ground water aquifers and acclimated river die-away rate data (Wilson et al. 1983; Mudder 1981; quoted, Howard et al. 1991);

$t_{1/2} > 35$ d in sediment-water sample (Jafvert & Wolfe 1987)

$t_{1/2}(\text{aerobic}) = 100$ d, $t_{1/2}(\text{anaerobic}) = 400$ d in natural waters (Capel & Larson 1995)

measured rate constant $k \leq 0.05 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with $t_{1/2} \geq 8$ d at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 2400\text{--}8640$ h, based on unacclimated grab sample of aerobic soil from ground water aquifers and estimated aqueous aerobic biodegradation half-life (Wilson et al. 1983; Howard et al. 1991).

Sediment: $t_{1/2} > 35$ d in Bar-H sediment-water sample (Jafvert & Wolfe 1987)

Soil: $t_{1/2} = 10\text{--}50$ d (Ryan et al. 1988);

$t_{1/2} = 90$ d, estimated volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 2400\text{--}4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $1 < t_{1/2} < 2$ d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{1/2} = 10\text{--}50$ d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.7.1

Reported aqueous solubilities of 1,2-dichloroethane at various temperatures

$$\log [S/(\text{mol/L})] = -A + 2070/(T/K) + B(T/K) \quad (1)$$

$$S/(\text{wt}\%) = 0.888 - 4.0468 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 9.37388 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 9.8465 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (2)$$

$$S/(\text{wt}\%) = 17.9147 - 0.11684 \cdot (T/K) + 2.0003 \times 10^{-4} \cdot (T/K)^2 \quad (3)$$

1.

Rex 1906		Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982	
volumetric method		shake flask		shake flask		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ^{-3*}	t/°C	S/g·m ⁻³
0	9220	0	8370	10	8520	0	8880
10	8650	20	8490	20	8490	10	8579
20	8690	36	8950	25	8610	20	8524
30	8904	56	10300	30	8800	25	8608
				40	9440	30	8775
				50	10460	40	9391
				60	11920	50	10430
				70	13950	60	11951
				80	16720	70	14014
						80	16678
Gross & Saylor 1931							
shake flask-IR							
t/°C	S/g·m ⁻³						
15	8720			eq. 1	S/(mol/L)		
30	9000			A	15.369	eq. 1	S/wt%
				B	0.0247		

*data calculated by Horvath 1982

(Continued)

TABLE 5.1.1.7.1 (Continued)

2.

Barr & Newsham 1987		Stephenson 1992		Tse et al. 1992		Wright et al. 1992	
infinite dilution activity coeff.		shake flask-GC		activity coefficient		activity coefficient	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	8782	0	8200	20	8500	20	9400
35	9102	9.3	7700	30	9013	35	9209
50	9960	19.7	7200	40	9163	50	9835
		29.7	8100				
		39.4	9800				
		50.3	10600				
		61.0	10800				
		70.6	11300				
		80.7	10600				

3.

Horvath & Getzen 1999a					
recommended, IUPAC-NIST					
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	9240	40	9410	80	15990
5	8910	45	9890	85	17270
10	8680	50	10460	90	18640
15	8550	55	11130	95	20110
20	8520	60	11900	100	21680
25	8600	65	12780		
30	8770	70	13750	eq. 2	S/wt%
35	9040	75	14820	temp range 273–373 K	

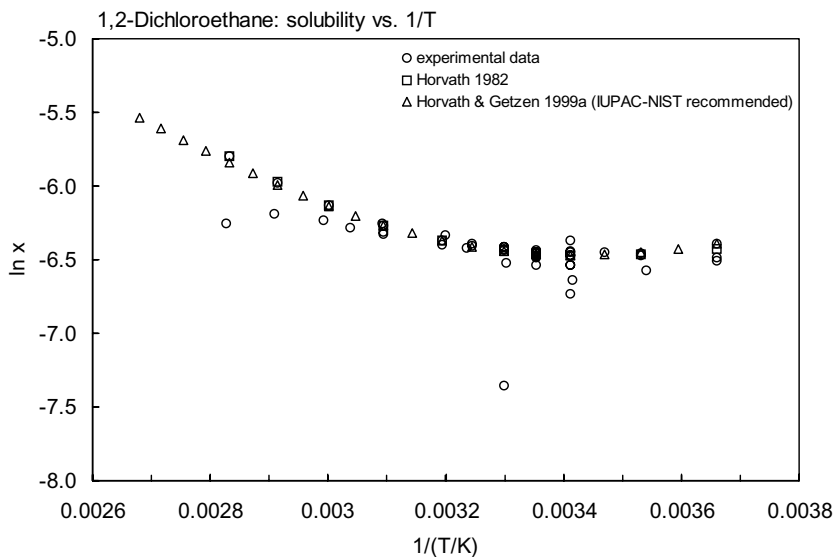


FIGURE 5.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,2-dichloroethane.

TABLE 5.1.1.7.2

Reported vapor pressures of 1,2-dichloroethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Pearce & Peters 1929		Stull 1947		Gutsche & Knapp 1982	
isoteniscope method		summary of literature data		Bourdon-tube manometer	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-30.82	427	-44.5	133.3	28.75	12530
-24.92	613	-24.0	666.6	38.65	19521
-19.32	860	-13.6	1333	46.39	27004
-15.02	1093	-2.40	2666	51.72	33373
-10.42	1547	10.0	5333	56.63	40285
-5.12	2120	18.1	7999	60.79	47009
0.070	2800	29.4	13332	64.19	53158
5.09	3760	45.7	26664	67.62	60006
10.07	4893	64.0	53329	70.24	65669
15.52	6546	82.4	101325	73.85	74207
20.21	8279			76.36	80633
25.25	10639	mp/ $^{\circ}\text{C}$	-35.3	78.67	86926
30.23	13452			80.80	93115
35.24	16839			82.74	98997
39.79	20425			84.54	104743
45.13	25544				
51.12	31304			eq. 3	P/kPa
55.22	37997			A	14.142372
60.28	45969			B	2896.480
65.27	55035			C	52.506
70.27	65448				
75.36	77220				
80.43	91046				
85.45	105938				
91.03	124603				
bp/ $^{\circ}\text{C}$	84.1				
$\Delta H_v/(\text{kJ mol}^{-1}) = 32.41$ at bp					
vapor pressure eq. see ref.					

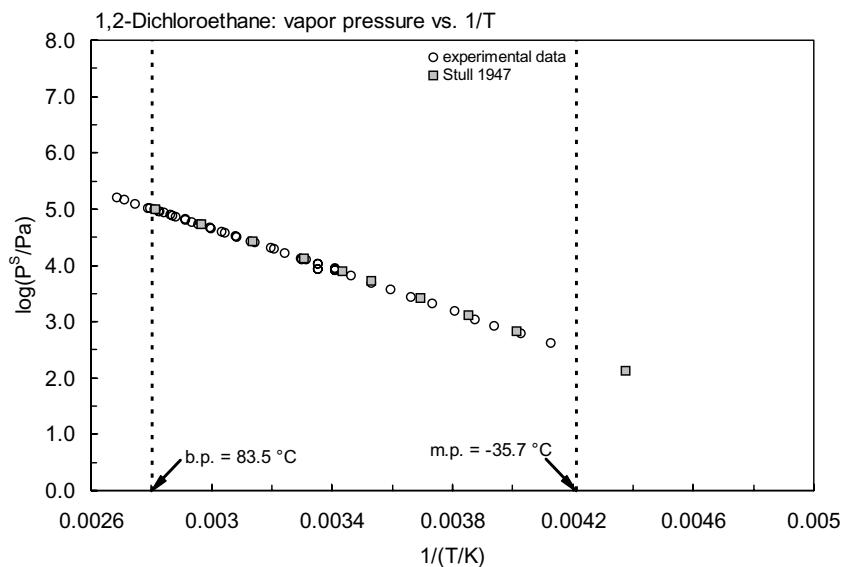


FIGURE 5.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichloroethane.

TABLE 5.1.1.7.3
Reported Henry’s law constants of 1,2-dichlorethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
Leighton & Calo 1981		Ashworth et al. 1988		Dewulf et al. 1995	
equilibrium cell-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
1.0	55.85	10	118.6	2.0	32.03
1.3	56.34	15	131.7	6.0	42.47
11.0	84.92	20	148.95	10.0	39.55
21.0	125.6	25	142.87	18.2	75.4
22.0	139.7	30	176.3	25.0	102.1
27.2	174.1				
25	119.3	eq. 4	H/(atm m ³ /mol)	eq. 1	K _{AW}
		A	−1.371	A	11.377
eq. 3	H/atm	B	1522	B	4329
A	16.05				
B	3539				

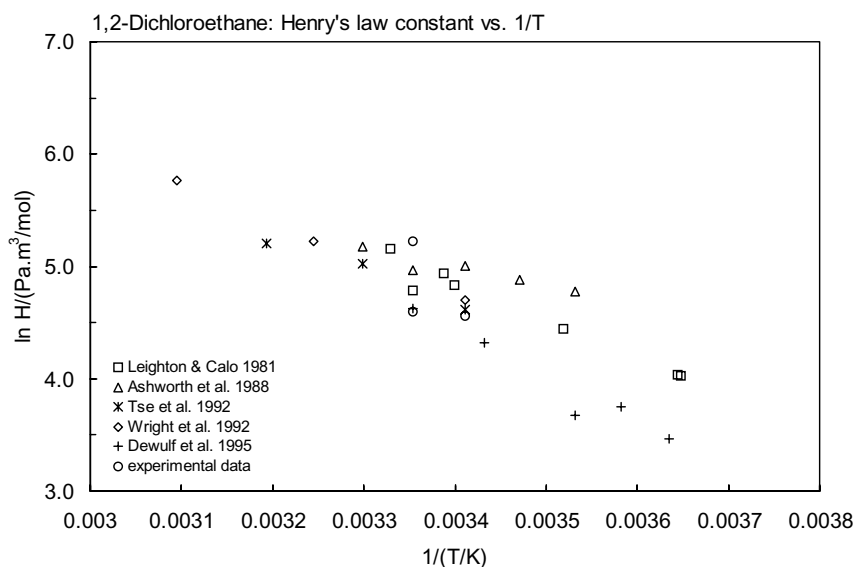


FIGURE 5.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dichloroethane.

TABLE 5.1.1.7.4
Reported octanol-water partition coefficients of 1,2-dichloroethane at various temperatures

Bhatia & Sandler 1995		DeWulf et al. 1999	
relative GC-RT technique		EPICS-GC	
$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$	$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$
25	1.51	2.2	1.43
35	1.51	4.0	1.46
50	1.53	10.0	1.47
		14.1	1.44
		18.7	1.50
		24.8	1.46

change in enthalpy:
 $\Delta H_{\text{OW}}/(\text{kJ mol}^{-1}) = 3.3$
 (−2.1 to 8.6)

enthalpy of transfer
 $\Delta H_{\text{oct}}/(\text{kJ mol}^{-1}) = 0.2$
 (−5.2 to 5.5)

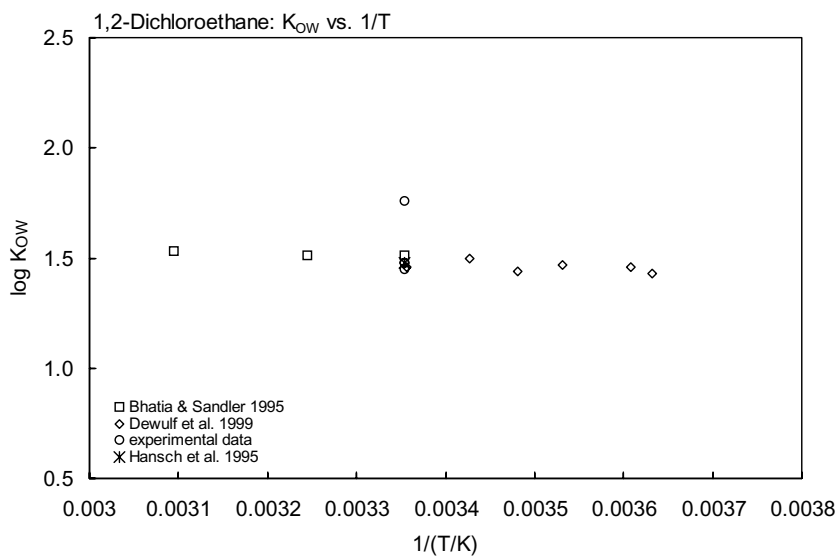


FIGURE 5.1.1.7.4 Logarithm of K_{OW} versus reciprocal temperature for 1,2-dichloroethane.

5.1.1.8 1,1,1-Trichloroethane



Common Name: 1,1,1-Trichloroethane

Synonym: methyl chloroform, chlorotene, Genklene, Baltana

Chemical Name: 1,1,1-trichloroethane

CAS Registry No: 71-55-6

Molecular Formula: CH_3CCl_3

Molecular Weight: 133.404

Melting Point ($^{\circ}\text{C}$):

−30.01 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

74.09 (Lide 2003)

Density (g/cm^3 at 20°C):

1.3390 (Dreisbach 1961; Horvath 1982; Weast 1982–83; McNally & Grob 1984)

1.3381, 1.3299 (20°C , 25°C , Riddick et al. 1986)

Molar Volume (cm^3/mol):

99.0, 52.0 (calculated-density, intrinsic volume-van der Waals method, Abernethy et al. 1988)

100.0 (calculated-density, Wang et al. 1992)

114.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.74, 29.74 (25°C , bp, Dreisbach 1961)

32.39, 29.708 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

2.35 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section):

1320* (20°C , shake flask, measured range 0 – 50°C , Van Arkel & Vles 1936)

1304 (Seidell 1940)

1490* (shake flask-GC, measured range 10 – 80°C , Walraevens et al. 1974)

$\log [S/(\text{mol}/\text{L})] = 2070/(T/\text{K}) - 14.860 + 0.020 \cdot (T/\text{K})$; temp range 2630353 K (shake flask, Walraevens et al. 1974)

480 (20°C , shake flask-GC, Pearson & McConnell 1975; McConnell et al. 1975)

880, 720 (1.5, 25°C , average literature values, Dilling 1977)

1360 (shake flask, Chiou et al. 1979)

1320 (20°C , recommended, Sørensen & Arit 1979)

100 (shake flask-titration, Coca & Diaz 1980)

1334 (shake flask-LSC, Banerjee et al. 1980)

1150, 1200 (23.5°C , elution chromatography, Schwarz 1980)

1850* (20°C , elution chromatography, measured range 10 – 30°C , Schwarz & Miller 1980)

1334; 278.7 (shake flask-LSC; calculated-f const., Veith et al. 1980)

1260 (calculated-group contribution as per Irmann 1965, Horvath 1982)

1485* (summary of literature data, temp range 0 – 80°C , Horvath 1982)

3200 (calculated-UNIFAC activity coeff., Arbuckle 1983)

479.8 (30°C , headspace-GC, McNally & Grob 1984)

1334 (calculated-UNIFAC activity coeff., Banerjee 1985)

1320 (20°C , selected, Riddick et al. 1986)

1310, 1194, 1267 (20 , 35 , 50°C , infinite dilution activity coeff. γ^{∞} -GC, Barr & Newsham 1987)

1252 (23 – 24°C , shake flask-GC, Broholm et al. 1992)

700* (20.2°C , shake flask-GC/TC, measured range 0 – 71.5°C , Stephenson 1992)

1260, 1353, 1370 (20, 30, 40°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 1413, 1392, 1454, 1489 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞ -GC, Tse et al. 1992)
 2935, 3228, 3536, 3749 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞ -UNIFAC, Tse et al. 1992)
 1758 (γ^∞ from gas stripping-GC, Li et al. 1993)
 1250 (shake flask-GC, Broholm & Feenstra 1995)
 1380 (20°C, activity coeff. γ^∞ by inert air stripping-GC, Hovorka & Dohnal 1997)
 1290* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
 $S/(\text{wt}\%) = 1.09092 - 6.52776 \times 10^{-3} \cdot (T/K) + 1.10747 \times 10^{-5} \cdot (T/K)^2$, temp range 273–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

12159* (17.68°C, static method-Hg manometer, measured range 268–290 K, Rubin et al. 1944)
 $\log(P/\text{cmHg}) = 6.92013 - 1729/(T/K)$; temp range 268–290 K (Hg manometer, Rubin et al. 1944)
 16190* (interpolated from Antoine eq. regression, temp range –52 to 74.1°C, Stull 1947)
 16100 (calculated-Antoine eq., Dreisbach 1961)
 $\log(P/\text{mmHg}) = 6.94983 - 1217.0/(225.0 + t/^\circ\text{C})$; temp range –3 to 111°C (Antoine eq. for liquid state, Dreisbach 1961)
 16170 (calculated-Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 8012.7/(T/K)] + 7.955902$; temp range –52 to 74.1°C (Antoine eq., Weast 1972–73)
 16490* (ebulliometry, measured range –77.15 to 25°C, Ambrose et al. 1975)
 16490 (ebulliometry, measured –77.15 to 25°C, Boublik et al. 1984)
 17800 (calculated-Antoine eq., Boublik et al. 1973, 1984)
 $\log(P/\text{mmHg}) = 8.64344 - 2136.621/(302.769 + t/^\circ\text{C})$; temp range –5.36 to 16.92°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 12800 (20°C, Pearson & McConnell 1975; McConnell et al. 1975)
 17800, 16490 (calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 7.78612 - 2147.034/(303.568 + t/^\circ\text{C})$; temp range –5.36 to 16.92°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.13297 - 1260.034/(231.327 + t/^\circ\text{C})$; temp range –77.2 to 25°C (Antoine eq. from reported exptl. data of Ambrose et al. 1973, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = 8.6434 - 2136.6/(302.8 + t/^\circ\text{C})$; temp range –6 to 17°C (Antoine eq., Dean 1985, 1992)
 16490 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.98755 - 1182.527/(222.594 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 16490 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.98755 - 1182.527/(-50.256 + T/K)$; temp range; 295–372 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.00452 - 1193.604/(-48.734 + T/K)$; temp range 349–408 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.36873 - 1474.394/(-8.08 + T/K)$; temp range 399–487 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 16530, 960 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
 13150, 20520, 25300, 30940 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
 $\log(P/\text{mmHg}) = 36.5468 - 2.821 \times 10^3/(T/K) - 10.205 \cdot \log(T/K) - 2.6369 \times 10^{-9} \cdot (T/K) + 3.7075 \times 10^{-6} \cdot (T/K)^2$; temp range 243–545 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1638 (calculated as $1/K_{\text{AW}}, C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
 3433 (20°C, McConnell et al. 1975)
 2800, 2875 (exptl., calculated-P/C, Dilling 1977)
 2025 (20°C, batch stripping-GC, Mackay et al. 1979)
 730 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
 $\log(k_{\text{H}}/\text{atm}) = 9.39 - 1992.95/(T/K)$, (least-square regression of data from lit., Kavanaugh & Trussell 1980)
 1996* (equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)

- $\ln (k_H/\text{atm}) = 21.68 - 4375/(T/K)$; temp range 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
 1520 (20°C, batch air stripping, Munz & Roberts 1982)
 836, 1317, 2155 (10, 20, 30°C, multiple equilibrium-GC, Munz 1985)
 606.9 (20°C, predicted-UNIFAC activity coeff., Arbuckle 1983)
 1319* (multiple equilibrium technique-GC, temp range 5–33°C, Hunter-Smith et al. 1983)
 $\ln K_{AW} = 9.15 - 2915/(T/K)$; measured range 5–33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)
 $\ln K_{AW} = 13.04 - 3905/(T/K)$; measured range 5–33°C (seawater, multiply equilibrium-GC, Hunter-Smith 1983)
 1743 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
 1337, 1358 (20°C, EPICS-GC/FID, batch air stripping-GC, Lincoff & Gossett 1984)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 10.21 - 4262/(T/K)$; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.975 - 4186/(T/K)$; temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)
 498.5 (adsorption isotherm, Urano & Murata 1985)
 1360 (20°C, multiple equilibration, Munz & Roberts 1986; quoted, Yurteri et al. 1987)
 $\log K_{AW} = 5.327 - 1636/(T/K)$; temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)
 498.5 (gas stripping-GC, Warner et al. 1987)
 1345, 1413* (20, 25°C, EPICS-GC/FID, measured range 9.6–24.6°C, Gossett 1987)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.777 - 4133/(T/K)$; temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)
 1572 (20°C, EPICS, Yurteri et al. 1987)
 1763* (EPICS-GC, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 7.351 - 3399/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 1317 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 1578* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 $\ln (1/K_{AW}) = -2.52 + 950/(T/K)$; temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
 1277, 2027, 2381, 2847 (20, 30, 35, 40°C, from measured activity coeff. γ^∞ -GC, Tse et al. 1992)
 1380, 1998, 2952 (20, 30, 40°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 1763* (26.3°C, EPICS-GC, measured range 26.3–44.8°C, Hansen et al. 1993)
 $\ln [H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -3120/(T/K) + 11.0$; temp range 26.3–45°C (EPICS-GC, Hansen et al. 1993)
 1783* (static headspace-GC, measured range 25–50°C, Robbins et al. 1993)
 1507* (EPICS-GC/FID, measured range 2.0–25°C, Dewulf et al. 1995)
 800, 2010 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
 $\ln K_{AW} = -3834/(T/K) + 0.00897 \cdot Z + 12.351$; with Z salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID measurements, Dewulf et al. 1995)
 1387 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 2072 (vapor-liquid equilibrium-GC, Turner et al. 1996)
 $K_{AW} = 0.204 + 0.0182 \cdot (T/K) + 0.000173 \cdot (T/K)^2$; temp range 0–35°C (vapor-liquid equilibrium-GC with additional lit. data, Turner et al. 1996)
 1280 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)
 1614, 1750, 1415; 1380 (direct calculated method, gas-phase EPICS method, liquid-phase EPICS method; quoted lit. Chiang et al. 1998)
 1370 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
 $\log K_{AW} = 5.163 - 1588/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 2.17 (Tute 1971)
 2.49 (shake flask, Hansch & Leo 1979; Hansch & Leo 1985)
 2.47 (shake flask-LSC, Banerjee et al. 1980)
 2.47 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982)
 2.35, 2.29 (calculated-UNIFAC with octanol and water mutual solubility not considered, calculated-UNIFAC with octanol and water mutual solubility considered, Arbuckle 1983)
 1.96 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
 2.49 (recommended, Sangster 1993)
 2.60 (calculated-activity coefficients, Tse & Sandler 1994)

- 2.47* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
 2.20* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 2.70 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 1.40 (calculated- K_{OW} , Veith et al. 1979; Veith et al. 1980)
 0.954 (bluegill sunfish, Veith et al. 1980)
 0.954 (bluegill sunfish, Barrows et al. 1980)
 1.908 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 0.950 (bluegill sunfish, Veith & Kosian 1982)
 1.70 (calculated-MCI χ , Koch 1983)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 2.02 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
 2.25 (quoted from Chiou et al. 1979, Karickhoff 1981, 1985)
 2.08, 2.04, 2.02 (estimated- K_{OW} , estimated-S and mp, estimated-S, Karickhoff 1981)
 2.182 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 2.20 (soil, best estimate, Karickhoff 1985)
 1.70 (calculated-MCI χ , Bahnick & Doucette 1988)
 2.26 (20°C, soil, Chiou et al. 1988)
 1.65 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
 2.22 (20°C, weathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
 3.02 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
 2.053 (soil, selected, Jury et al. 1990)
 1.95, 1.98, 1.99, 2.01, 1.98, 2.03 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)
 3.20 (soil, calculated-universal solvation model, Winget et al. 2000)
 2.16 (soil: organic carbon $OC \geq 0.1\%$, average, Delle Site 2001)

Sorption Partition Coefficient, $\log K_{OM}$:

- 2.02, 1.55 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization: evaporation $t_{1/2}(\text{exptl}) = 21$ min, $t_{1/2}(\text{calc}) = 0.34$ min from water (Dilling et al. 1975)
 $t_{1/2}(\text{exptl}) \sim (20 \pm 3)$ min at 25°C for an aqueous solution of 1 mg L⁻¹ when stirred at 200 rpm in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);
 Evaporation $t_{1/2}(\text{exptl}) = (17.3\text{--}24.9)$ min, $t_{1/2}(\text{calc}) = 0.19$ min, 23.7 min at 20–25°C, and $t_{1/2} = 30.2$ min at 15°C from water (Dilling 1977);
 estimated $t_{1/2} \sim 3.7$ h from water (Thomas 1982);
 $k = 0.029$ d⁻¹, $t_{1/2} = 24$ d in spring at 8–16°C, $k = 0.058$ d⁻¹, $t_{1/2} = 12$ d in summer at 20–22°C, $k = 0.063$ d⁻¹, $t_{1/2} = 11$ d in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.60$ d⁻¹, $t_{1/2} = 11.5$ d with HgCl₂, and $k = 0.072$ d⁻¹, $t_{1/2} = 9.6$ d without HgCl₂ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);
 estimated $t_{1/2} \sim 365$ d for volatilization loss from soil to be 365 d (Jury et al. 1990).

Photolysis: not expected to be important (Howard et al. 1991).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

- $k_{OH} = 3.36 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹ with a troposphere life time of 1.1 yr at 298 K (relative rate method, Cox et al. 1976; quoted, Callahan et al. 1979)
 $k_{OH} = (1.5 \pm 0.3) \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹ at 296 K (discharge flow-resonance fluorescence, Howard & Evenson 1976b)

$k_{\text{OH}}^* = (2.19 \pm 0.26) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 275–405 K, with calculated lifetime of 3.8–6.0 yr in troposphere (discharge flow system-resonance fluorescence, Chang & Kaufman 1977)

$k_{\text{OH}} = (1.59 \pm 0.16) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K with lifetime of 13 yr (flash photolysis-resonance fluorescence, Watson et al. 1977; quoted, Callahan et al. 1979; Altshuller 1980)

$k_{\text{OH}}^* = (1.06 \pm 0.09) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 293 K, measured range 278–461 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1979)

$k_{\text{OH}}^* = (1.08 \pm 0.20) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 222–363 K (flash photolysis resonance fluorescence, Kurylo et al. 1979)

$k_{\text{OH}} = 1.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, with an estimated toxic chemical residence time of 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k = 9.0 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, estimated at 300 K (Lyman 1982)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $1.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation $t_{1/2} = 5393\text{--}53929 \text{ h}$, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k_{\text{OH}}(\text{calc}) = 1.3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}}^* = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 1.19 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a troposphere lifetime of 1.7 yr for a global average concentration of OH radical (Prinn et al. 1987; quoted, Bunce et al. 1991)

$k_{\text{O}_3}(\text{aq.}) \leq 0.012 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 32 \text{ d}$ at pH 7 (Yao & Haag 1991).

Hydrolysis: $k = 0.12 \text{ month}^{-1}$ with $t_{1/2}(\text{exptl.}) = 6 \text{ months}$ at pH 7 and 25°C (Dilling et al. 1975; quoted, Callahan et al. 1979; Mabey et al. 1979; Neely 1985);

$k = 0.96 \text{ yr}^{-1}$ at pH 7 and 25°C with a first-order hydrolysis $t_{1/2} = 0.73 \text{ yr}$ (Kollig et al. 1987);

$k = (1.93 \pm 0.40) \times 10^{-8} \text{ s}^{-1}$ in distilled water contained 0.1% w/w CH_2O as sterilant with 39% conversion,

$k = (2.04 \pm 0.47) \times 10^{-8} \text{ s}^{-1}$ in autoclaved distilled water with 40% conversion and

$k = (1.80 \pm 0.90) \times 10^{-8} \text{ s}^{-1}$ in sediment contained 0.1% w/w CH_2O as sterilant with 25% conversion at 25°C, calculated $t_{1/2} = 350 \text{ d}$ at 25°C (Haag & Mill 1988)

$t_{1/2} = 6 \text{ months}$, abiotic hydrolysis or dehydrohalogenation half-life (Olsen & Davis 1990)

$t_{1/2} = 0.73 \text{ yr}$, based on reported rate constant at pH 7 at 25°C (Howard et al. 1991)

Biodegradation:

$k = 0.043 \text{ d}^{-1}$ in fresh water plus sediment incubated under anaerobic conditions (Wood et al. 1981; quoted, Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 3360\text{--}6552 \text{ h}$, based on unacclimated aerobic seawater grab sample data and sub-soil sample data from a ground water aquifer (Pearson & McConnell 1975; Wilson et al. 1983; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 13440\text{--}26208 \text{ h}$, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 26 \text{ wk}$, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

estimated troposphere residence time of 1.1 yr for reaction with OH radical (CEQ 1975);

estimated N. troposphere residence time of 7.2 yr by one compartment non-steady state model (Singh et al. 1978);

estimated troposphere residence time of 8–10 yr by two compartment non-steady state model (Singh 1977; Singh et al. 1979);

lifetime of 8 yr in troposphere (Altshuller 1980);

estimated toxic chemical residence time of 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

atmospheric lifetime $\tau = 6.3 \text{ yr}$ (Prinn et al. 1987);

troposphere lifetime of 1.7 yr for a global average concentration of OH radical (Bunce et al. 1991)

$t_{1/2} = 5393\text{--}53929$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

estimated tropospheric lifetime of 7.8 yr and 6.1 yr by rigorous calculations (Nimitz & Skaggs 1992).

Surface water: $t_{1/2} = 24$ d in the spring at $8\text{--}16^\circ\text{C}$, $t_{1/2} = 12$ d in the summer at $20\text{--}22^\circ\text{C}$, $t_{1/2} = 11$ d in the winter at $3\text{--}7^\circ\text{C}$ when volatilization dominates, and $t_{1/2} = 11.5$ d and 9.6 d for experiments with and without HgCl_2 as poison, respectively, in September 9–15 in marine mesocosm experiment (Wakeham et al. 1983);

calculated hydrolysis $t_{1/2} = 350$ d at 25°C (Haag & Mill 1988);

$t_{1/2} = 3360\text{--}6552$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$k(\text{exptl}) \leq 0.012 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C , with $t_{1/2} \geq 32$ d at pH 7 (Yao & Haag 1991).

Ground water: estimated $t_{1/2} \sim 1.0$ yr in the groundwater of the Netherlands (Zoeteman et al. 1981);

$t_{1/2} = 3360\text{--}13104$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and sub-soil grab sample data from a ground water aquifer (Howard et al. 1991; Wilson et al. 1983).

Sediment: measured $t_{1/2} = 450$ d at 25°C , based on neutral and base-catalyzed hydrolysis rates studied in pure water and in barely saturated subsurface sediment at $25\text{--}60^\circ\text{C}$ (Haag & Mill 1988).

Soil: $t_{1/2} = 365$ d, estimated volatilization loss (Jury et al. 1990);

$t_{1/2} = 3360\text{--}6552$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 5.1.1.8.1

Reported aqueous solubilities of 1,1,1-trichloroethane at various temperatures

$$S/(\text{wt}\%) = 0.1910 - 2.2811 \times 10^{-3} \cdot (t/^\circ\text{C}) + 2.5529 \times 10^{-5} \cdot (t/^\circ\text{C})^2 - 2.4775 \times 10^{-8} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 1.09092 - 6.52776 \times 10^{-3} \cdot (T/\text{K}) + 1.10747 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Schwarz & Miller 1980		Horvath 1982	
shake flask		shake flask-GC		elution chromatography		summary of literature data	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	1590	10	1730	10	1800	0	1910
20	1320	20	1550	20	1850	10	1707
35	1260	25	1490	30	1590	20	1554
50	1280	30	1440			25	1495
		40	1390			30	1449
		50	1380			40	1390
		60	1410			50	1377
		70	1480			60	1407
		80	1590			70	1479
						80	1592
						eq. 1	$S/\text{wt}\%$

TABLE 5.1.1.8.1 (Continued)

2.

Barr & Newsham 1987		Stephenson 1992		Tse et al 1992		Horvath & Getzen 1999a	
activity coefficient		shake flask-GC		activity coefficient		recommended, IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	1310	0	1470	20	1413	0	1340
35	1194	20.2	700	30	1392	5	1320
50	1267	31.6	760	35	1454	10	1300
		41.1	1010	40	1489	15	1290
		51.3	1060			20	1290
		61.5	1030			25	1290
		71.5	1140			30	1300
				Wright et al. 1992		35	1310
				activity coefficient		40	1330
				t/°C	S/g·m ⁻³	45	1350
				20	1260	50	1380
				30	1353		
				40	1370		
						eq. 2 S/wt% temp range 273–323 K	

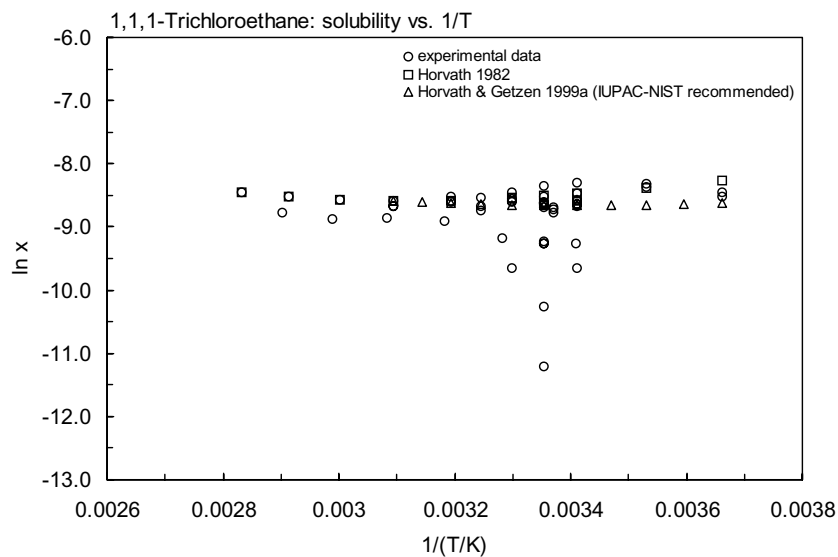


FIGURE 5.1.1.8.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.2

Reported vapor pressures of 1,1,1-trichloroethane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Rubin et al. 1944		Stull 1947		Ambrose et al. 1975	
static-mercury manometer		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-5.534	3840	-52.0	133.3	-77.15	20
-0.207	5160	-32.0	666.6	-55.15	100
5.12	6733	-21.9	1333	-25.85	1000
11.33	9239	-10.8	2666	14.15	10000
16.93	12159	1.6	5333	25.0	16490
		9.5	7999		
mp/K	240.2	20.0	13332		
		36.2	26664		
eq. 1	P/cmHg	54.6	53329		
A	6.92013	74.1	101325		
B	1729				
		mp/°C	-30.6		
$\Delta H_v/(\text{kJ mol}^{-1}) = 33.42$					
at 286.53 K					

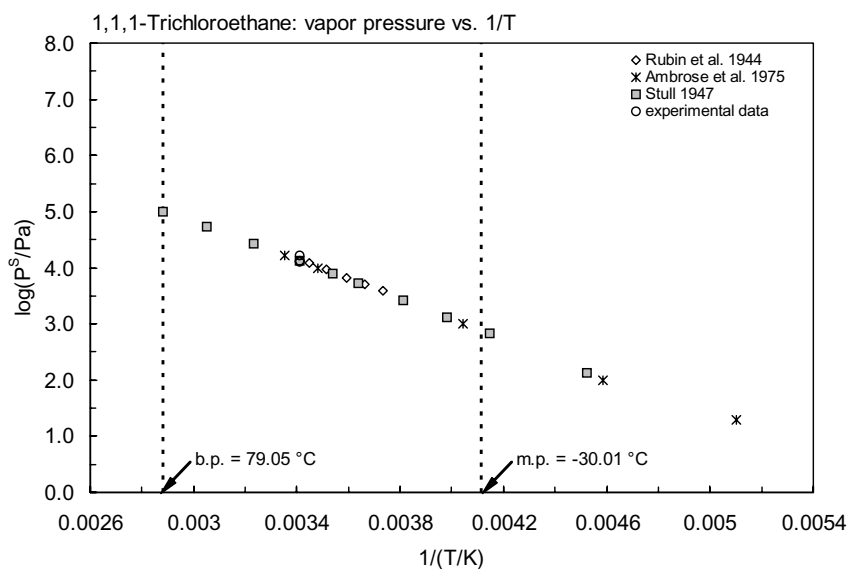


FIGURE 5.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.3

Reported Henry's law constants of 1,1,1-trichloroethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

1.

Leighton & Calo 1981		Hunter-Smith 1983		Gossett 1987		Ashworth et al. 1988	
equilibrium cell-GC		multiple equilibrium-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
1.0	541.7	5	612	9.6	771	10	978
1.0	543.3	10	749	17.5	1216	15	1165
1.2	555.9	15	912	24.8	1743	20	1479
2.5	597.9	20	1102	34.6	2523	25	1763
7.0	763.3	25	1324			30	2138
10.0	919.2	33	1738	eq. 4	H/(atm m ³ /mol)	eq. 4	H/(atm m ³ /mol)
12.0	1016			A	9.777	A	7.351
12.0	1039			B	4133	B	3399
12.9	1069						
14.0	1190						
18.0	1398						
18.0	1447						
18.0	1464						
19.0	1511						
19.2	1526						
19.5	1437						
24.3	1874						
25.2	1995						
25.3	2026						
26.0	1988						
26.0	2064						
26.1	1958						
$\ln (k_H/\text{atm}) = A - B/(T/K)$							
A	21.68						
B	4375						

2.

Kolb et al. 1992		Tse et al. 1992		Wright et al. 1992		Hansen et al. 1993	
equilibrium headspace-GC		activity coefficient		activity coefficient		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
40	1578	20	1277	20	1380	26.3	1763
60	1884	30	2027	30	1998	35.0	2412
70	2264	35	2381	40	2952	44.8	3232
80	2488	40	2847				
						eq. 4	H/(kPa m ³ /mol)
eq. 2	1/K _{AW}					A	11 ± 0.30
A	-2.52					B	3120 ± 93
B	-950						

(Continued)

TABLE 5.1.1.8.3 (Continued)

3.

Robbins et al. 1993		Dewulf et al. 1995	
static headspace-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
25	1783	2.0	152.1
30	2209	6.0	195.2
40	2675	10.0	194.7
45	3597	18.2	378.2
50	4164	25.0	510.6
		eq. 1	K _{AW}
		A	12.351
		B	3834

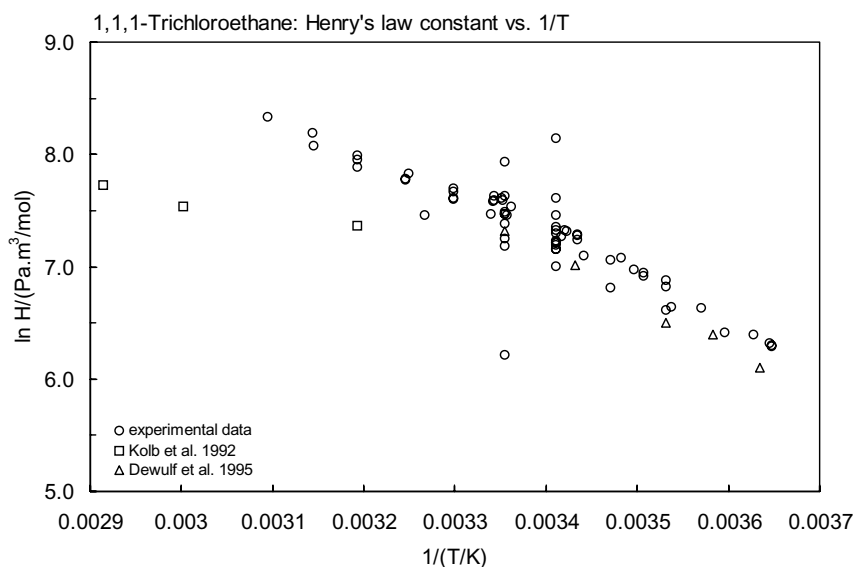


FIGURE 5.1.1.8.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,1-trichloroethane.

TABLE 5.1.1.8.4

Reported octanol-water partition coefficients of 1,1,1-trichloroethane at various temperatures

Bhatia & Sandler 1995		Dewulf et al. 1999	
relative GC-RT technique		shake flask-GC	
t/°C	log K _{OW}	t/°C	log K _{OW}
25	2.47	2.2	2.18
35	2.50	6.0	2.18
50	2.52	10.0	2.28
		14.1	2.24
		18.7	2.285
		24.8	2.20
enthalpy of transfer			
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$			
$\log K_{OW} = A - \Delta H/2.303RT$			
A	1.0195		
ΔH	-20.2		

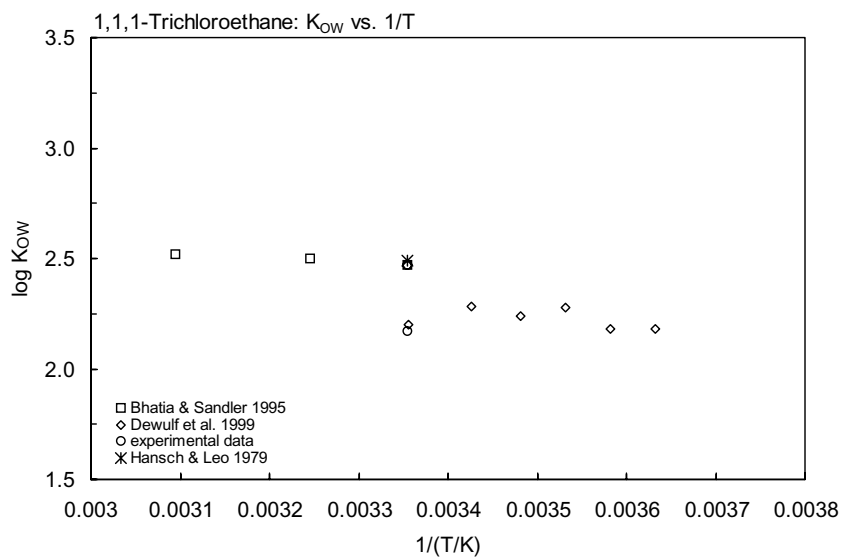
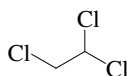


FIGURE 5.1.1.8.4 Logarithm of K_{OW} versus reciprocal temperature for 1,1,1-trichloroethane.

5.1.1.9 1,1,2-Trichloroethane



Common Name: 1,1,2-Trichloroethane

Synonym: vinyl trichloride

Chemical Name: 1,1,2-trichloroethane

CAS Registry No: 79-00-5

Molecular Formula: $\text{CH}_2\text{ClCHCl}_2$

Molecular Weight: 133.404

Melting Point ($^{\circ}\text{C}$):

-36.3 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

113.8 (Lide 2003)

Density (g/cm^3 at 20°C):

1.440 (Dreisbach 1959; Weast 1982–83; Verschueren 1983;)

1.43931, 1.43213(20°C , 25°C , Riddick et al. 1986)Molar Volume (cm^3/mol):

93.0 (calculated-density, Wang et al. 1992)

114.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):46.77, 37.07 (25°C , bp, Dreisbach 1961)40.28, 34.23 (25°C , bp, Riddick et al. 1986)Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.543 (Dreisbach 1959; quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3704 (volumetric method, Wright & Schaffer 1932)

4580* (shake flask, measured range 0 – 55°C , Van Arkel & Vles 1936)

4418 (Seidell 1940)

4400 (data presented in graph, temp range 0 – 70°C , McGovern 1943)

4400 (shake flask-refractive index and density, Treybal et al. 1946)

4380* (shake flask-GC, measured range 0 – 80°C , Walraevens et al. 1974) $\log [S/(\text{mol}/\text{L})] = 2070/(T/K) - 15.285 + 0.0230 \cdot (T/K)$; temp range 0 – 80°C (Walraevens et al. 1974)

4420 (literature average, Dilling 1977)

4500 (20°C , Verschueren 1977, 1983)4370 (20°C , recommended, Sørensen & Arit 1979)

5100 (shake flask-titration/turbidity, Coca & Diaz 1980, Coca et al. 1980)

1490 (shake flask-LSC, Veith et al. 1980)

4394* (summary of literature data, temp range 0 – 80°C , Horvath 1982)4365 (30°C , headspace-GC, McNally & Grob 1984)

4800 (Dean 1985)

4941, 4876, 5183 (20 , 35 , 50°C , infinite dilution activity coeff. γ^{∞} -GC, Barr & Newsham 1987)2858, 1469 (predicted-MCI χ and polarizability, Nirmalakhandan & Speece 1988)4580* (31.3°C , shake flask-GC/TC, measured range 0 – 90.8°C , Stephenson 1992)4813, 5035, 5205 (20 , 30 , 40°C , infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)2574, 2960, 3378 (20 , 30 , 40°C , infinite dilution activity coeff. γ^{∞} -UNIFAC, Tse et al. 1992)4877, 5257, 6075 (20 , 35 , 50°C , activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)4460 (20°C , activity coeff. γ^{∞} by inert air stripping-GC, Hovorka & Dohnal 1997)

4590* (tentative values, temp range 0–55°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(\text{wt}\%) = 2.89796 - 1.8585 \times 10^{-2} \cdot (T/K) + 3.48961 \times 10^{-5} \cdot (T/K)^2$, temp range 273–328 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):

26664* (73.5°C, ebulliometry, measured range 73.5–113.5°C, Treybal et al. 1946)

3090* (Antoine eq. regression, temp range –24 to 113.9°C, Stull 1947)

19114* (49.97°C, ebulliometry, measured range 49.97–113.67°C, Dreisbach & Shrader 1949)

2998 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/\text{mmHg}) = 6.84165 - 1262.6/(205.0 + t/^\circ\text{C})$; temp range 30–186°C (Antoine eq. for liquid state, Dreisbach 1959)

3217 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/\text{mmHg}) = 6.96527 - 1351.0/(217.0 + t/^\circ\text{C})$; temp range 29–155°C (Antoine eq. for liquid state, Dreisbach 1961)

3088 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 9163.2/(T/K)] + 8.079996$; temp range –24 to 113.9°C, (Antoine eq., Weast 1972–73)

2910 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)

$\log(P/\text{mmHg}) = 6.95185 - 1314.41/(209.197 + t/^\circ\text{C})$; temp range 49.97–113.7°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)

3066 (literature average, Dilling 1977)

2533, 4266 (20, 30°C, Verschuereen 1983)

$\log(P/\text{kPa}) = 6.13975 - 1313.598/(209.106 + t/^\circ\text{C})$; temp range 49.97–113.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

$\log(P/\text{mmHg}) = 6.95185 - 1314.41/(209.20 + t/^\circ\text{C})$; temp range 50–114°C (Antoine eq., Dean 1985, 1992)

2998 (selected lit., Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.10301 - 1332.6/(211.38 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

3218 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.09017 - 1351.0/(-56.15 + T/K)$; temp range 302–428 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.13875 - 1351.685/(-59.953 + T/K)$; temp range 316–384 K (Antoine eq., Stephenson & Malanowski 1987)

2369, 4012, 6590 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)

$\log(P/\text{mmHg}) = 25.0845 - 2.7368 \times 10^3/(T/K) - 5.9182 \cdot \log(T/K) + 2.5155 \times 10^{-10} \cdot (T/K) + 1.1831 \times 10^{-6} \cdot (T/K)^2$; temp range 237–602 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

92.1 (calculated as $1/K_{\text{AW}} \cdot C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

94.2 (calculated-P/C, Dilling 1977)

78.4 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)

122, 120 (calculated-P/C, recommended, Mackay & Shiu 1981, 1990)

81.4* (24.3°C, equilibrium cell-concn ratio-GC/FID, measured range 2.5–26.1°C, Leighton & Calo 1981)

$\ln(k_{\text{H}}/\text{atm}) = 16.20 - 3690/(T/K)$; temp range 2.5–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

92.2* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

$\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 9.320 - 4943/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

74.97 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

97.34 (computed value, Yaws et al. 1991)

70.9, 115.5, 172.3 (20, 30, 40°C, infinite dilution activity coeff. γ^∞ -GC, Tse et al. 1992)

67.1, 136, 234 (20, 35, 50°C, activity coeff γ^∞ -differential pressure transducer, Wright et al. 1992)

82* (26.2°C, EPICS-GC, measured range 26.2–44.8°C, Hansen et al. 1993)

$\ln[H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -5091/(T/K) + 17.0$; temp range 26.2–45°C (EPICS-GC measurements, Hansen et al. 1993)

- 1.30, 2.48 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 122 (quoted from Howard 1989–1991, Capel & Larson 1995)
 66.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1998)
 65.7 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 66.78 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 5.219 - 1989/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperature designated * are compiled at the end of this section:

- 2.17 (calculated as per Tute 1971, Callahan et al. 1979; Ryan et al. 1988)
 2.38 (Hansch & Leo 1979)
 1.89 (shake flask, Log P Database, Hansch & Leo 1987)
 1.89 (recommended, Sangster 1993)
 2.07 (calculated-activity coefficients, Tse & Sandler 1994)
 1.98* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)
 1.89 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 3.40 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- < 1.0 (Kawasaki 1980; quoted, Howard 1990)
 1.519 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 1.23 (quoted, Isnard & Lambert 1988)
 1.049 (calculated- K_{OW} , McCarty et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.845 (sandy soil column, Wilson et al. 1981)
 1.748 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 3.20; 1.90 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
 1.88 (soil: organic carbon OC $\geq 0.1\%$, average, Delle Site 2001)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 21$ min, estimated from lab. experiment of initial 1 mg/L in water stirred at 200 rpm at 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982; Howard 1990)

Evaporation $t_{1/2}(\text{exptl}) = 35.1$ min, $t_{1/2}(\text{calc}) = 6.1$ min, 30.1 min from water (Dilling 1977)

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
 $k_{OH}^* = (3.18 \pm 0.06) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 278–461 K (discharge flow-resonance fluorescence, Jeong & Kaufman 1979)

$k_{OH} = 3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, with estimated residence time of 35 d, loss of 2.8% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 3.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)
 photooxidation $t_{1/2} \sim 196$ –1956 h, based on measured rate constants for reaction with hydroxyl radical in air (estimated, Atkinson 1985; quoted, Howard et al. 1991)

$k_{OH}^* = (3.18 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 277–461 K (discharge flow-resonance fluorescence, Jeong et al. 1984)

$k_{O_3}(\text{aq.}) \leq 0.08 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 5$ d at pH 7 (Yao & Haag 1991).

$k_{OH}(\text{aq.}) = 1.1 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

Hydrolysis:

$k = 1.2 \times 10^{-7} \text{ h}^{-1}$ at 25°C and pH 7 (estimated, Mabey et al. 1982)

$k = 5.9 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 3263 \text{ h}$, based on alkaline catalyzed hydrolysis reaction at pH 9 and 25°C;
 $t_{1/2} = 37 \text{ yr}$, based on hydrolysis rate constant measured at pH 7 and 25°C (Mabey et al. 1983; quoted, Howard 1990; Howard et al. 1991)

$t_{1/2}(\text{abiotic})$ or $t_{1/2}(\text{dehydrohalogenation}) = 170 \text{ months}$ (Olsen & Davis 1990)

$t_{1/2} = 14000 \text{ d}$ at pH 7, $t_{1/2} = 0.14 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 4320\text{--}8760 \text{ h}$, based on the extremely low or no biodegradation which was observed in screening tests and a river die-away test (Tabak et al. 1981; Kawasaki 1980; Mudder & Musterman 1982; quoted, Howard 1990; Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 17280\text{--}35040 \text{ h}$, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991)

$k = 0.04 \text{ yr}^{-1}$ with $t_{1/2} = 24 \text{ d}$ (Wood et al. 1985; quoted, Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 180 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 720 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant $k = 3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 0.763 \text{ h}^{-1}$ (flagfish, calculated-BCF $\times k_2$, McCarty et al. 1992)

$k_2 = 0.0676 \text{ h}^{-1}$ (flagfish, estimated from one compartment first-order kinetic, McCarty et al. 1992)

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the reaction with OH radical in air (Darnall et al. 1976);

photodecomposition $t_{1/2} = 15.9 \text{ h}$ with NO under simulated atmospheric conditions (Dilling et al. 1976);

estimated residence time of 35 d, loss of 2.8% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 196\text{--}1956 \text{ h}$, based on measured rate constants for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: estimated $t_{1/2} = 1.9 \text{ d}$ in surface waters in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2} = 3263\text{--}8760 \text{ h}$, based on estimated hydrolysis half-life at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and estimated unacclimated aerobic aqueous degradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 100 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 400 \text{ d}$ and hydrolysis $t_{1/2} = 14000 \text{ d}$ at pH 7, $t_{1/2} = 0.14 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

$k(\text{exptl}) \leq 0.08 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 5 \text{ d}$ at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 3263\text{--}117520 \text{ h}$, based on estimated hydrolysis half-life pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and data from estimated unacclimated aerobic aqueous biodegradation half-life as well as a ground water die-away study in which no biodegradation was observed (Wilson et al. 1984; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 3263\text{--}8760 \text{ h}$, based on estimated hydrolysis half-life at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991) and estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991) and a soil column test in which no biodegradation was observed (Wilson et al. 1981; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.1.9.1

Reported aqueous solubilities of 1,1,2-trichloroethane at various temperatures

$$S/(\text{wt}\%) = 0.48137 - 2.9594 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 4.3162 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 3.2190 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 2.89796 - 1.8585 \times 10^{-2} \cdot (T/\text{K}) + 3.48961 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982		Barr & Newsham 1987	
shake flask				summary of literature data		activity coefficient	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	4660	10	4600	0	4814	20	4941
20	4360	20	4410	10	4546	35	4876
25	4580	25	4380	20	4420	50	5183
55	5320	30	4390	25	4394		
		40	4530	30	4401		
		50	4830	40	4527		
		60	5290	50	4815		
		70	5950	60	5287		
		80	6860	70	6961		
				80	6857		
				eq. 1	S/wt%		

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999a	
shake flask-GC		activity coefficient		activity coefficient		tentative, IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	4640	20	4813	20	4877	0	4250
9.2	4390	30	5035	35	5257	5	4280
31.3	4580	40	5205	50	6075	10	4330
41	4830					15	4400
50.6	5180					20	4490
60.5	4970					25	4590
710	5550					30	4710
81.7	6380					35	4850
90.8	7030					40	5000
						45	5170
						50	5360
						55	5570
						eq. 2	S/wt%
						temp range 263–328 K	

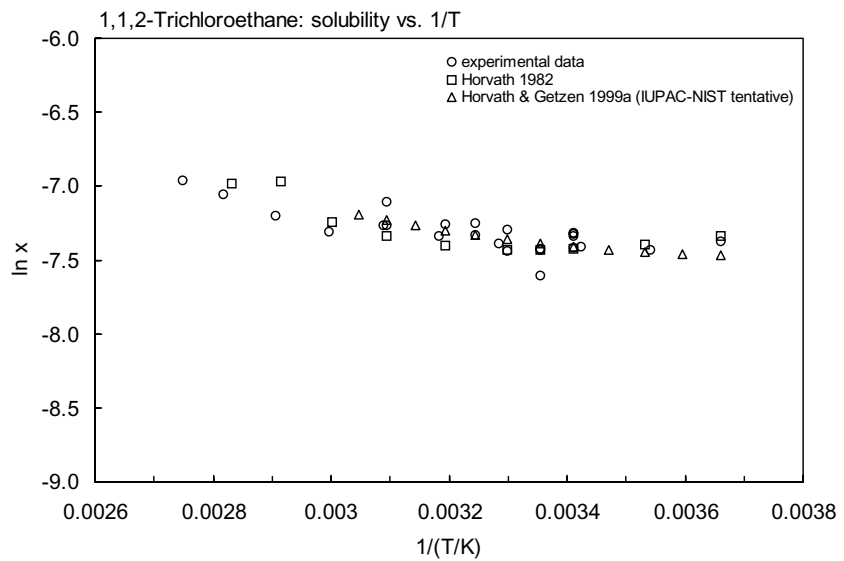
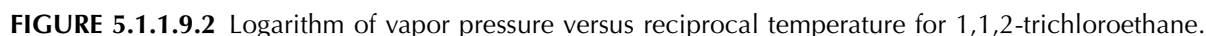


FIGURE 5.1.1.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.9.2
Reported vapor pressures of 1,1,2-trichloroethane at various temperatures

Treybal et al. 1946		Stull 1947		Dreisbach & Shrader 1949	
ebulliometry		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
73.5	26664	−24.0	133.3	49.97	19114
80.3	34397	−2.0	666.6	61.29	16500
82.4	37064	8.3	1333	85.99	42066
83.8	38530	21.6	2666	100.34	67661
85.6	41597	35.2	5333	113.67	101325
96.2	59328	44.0	7999		
104.6	77594	55.7	13332		
108.7	87326	73.3	26664		
109.8	90393	93.0	53329		
111.3	94392	113.9	101325		
113.5	101325				


$$\begin{array}{ll}
\ln K_{AW} = A - B/(T/K) & (1) \\
\ln (1/K_{AW}) = A - B/(T/K) & (2) \\
\ln (k_H/\text{atm}) = A - B/(T/K) & (3) \\
\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) & (4) \\
K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 & (5)
\end{array}
\qquad
\begin{array}{ll}
\log K_{AW} = A - B/(T/K) & (1a) \\
\log (1/K_{AW}) = A - B/(T/K) & (2a) \\
\log [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) & (4a)
\end{array}$$

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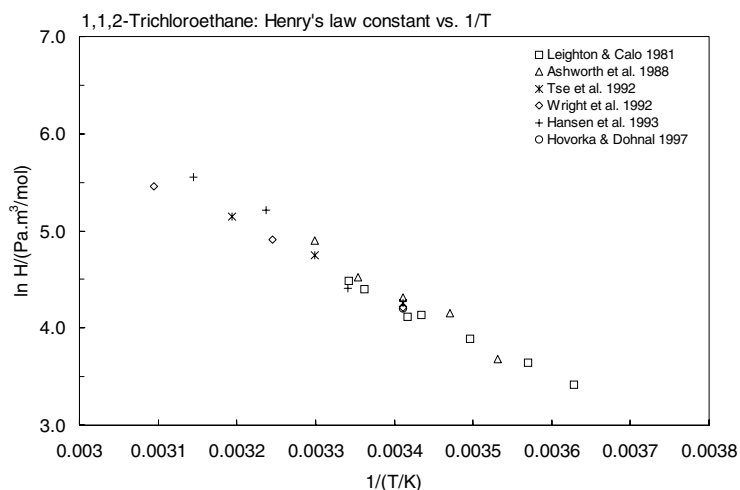


FIGURE 5.1.1.9.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.9.4

Reported octanol-water partition coefficients of 1,1,2-trichloroethane at various temperatures

Bhatia & Sandler 1995	
relative GC-RT technique	
$t/^{\circ}\text{C}$	$\log K_{\text{OW}}$
25	1.98
35	1.93
50	1.94
enthalpy of transfer	
$\Delta H/(\text{kJ mol}^{-1}) = -20.2.$	
$\log K_{\text{OW}} = A - \Delta H/2.303RT$	
A	1.0195
ΔH	-20.2

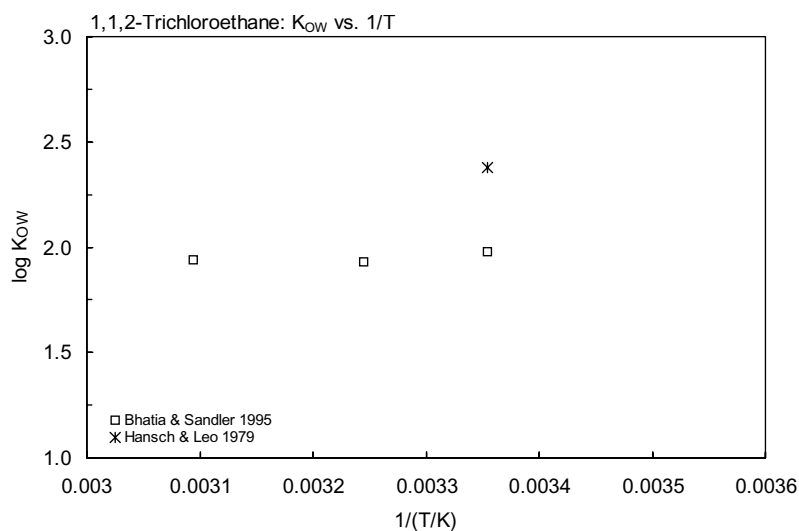
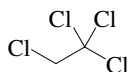


FIGURE 5.1.1.9.4 Logarithm of K_{OW} versus reciprocal temperature for 1,1,2-trichloroethane.

5.1.1.10 1,1,1,2-Tetrachloroethane



Common Name: 1,1,1,2-Tetrachloroethane

Synonym:

Chemical Name: 1,1,1,2-tetrachloroethane

CAS Registry No: 630-20-6

Molecular Formula: $\text{CH}_2\text{ClCCl}_3$

Molecular Weight: 167.849

Melting Point ($^{\circ}\text{C}$):

-70.2 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

130.2 (Lide 2003)

Density (g/cm^3 at 20°C):

1.5406 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

1.5328 (25°C , Dreisbach 1961)

1.4819 (Dean 1985)

Molar Volume (cm^3/mol):

109.0 (20°C , calculated-density)

135.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

34.78, 42.18 (normal boiling point, 25°C , Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

1090* (20°C , shake flask, measured range 0 – 50°C , Van Arkel & Vles 1936)

1110 (Seidell 1940)

1100* (shake flask, temp range 10 – 80°C , Walraevens et al. 1974)

$\log [S/(\text{mol}/\text{L})] = 2070/(T/\text{K}) - 16.165 + 0.0236 \cdot (T/\text{K})$, temp range 283 – 353 K (Walraevens et al. 1974)

1100 (interpolation of literature values, Dilling 1977)

215, 200, 202 (3, 20, 34°C , shake flask-GC, Chiou & Freed 1977)

1110* (summary of literature data, temp range 0 – 80°C , Horvath 1982)

1206, 1280, 1292, 1321 (20, 30, 35, 40°C , infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)

1178, 1382, 1492, 1607 (20, 30, 40°C , infinite dilution activity coeff. γ^{∞} -UNIFAC, Tse et al. 1992)

1005, 1093, 1056 (20, 30, 40°C , activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)

1070* (recommended, temp range 0 – 50°C , IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(\text{wt}\%) = 2.17896 - 1.3966 \times 10^{-3} \cdot (T/\text{K}) + 2.93282 \times 10^{-5} \cdot (T/\text{K})^2$, temp range 273 – 323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1767* (Antoine eq. regression, temp range 58 – 200°C , Stull 1947)

8851* (59.31°C , ebulliometry, measured range 59.31 – 130.2°C , Dreisbach & Shrader 1949)

1578 (calculated-Antoine eq., Dreisbach 1961)

$\log (P/\text{mmHg}) = 6.97560 - 1410.7/(214.0 + t/^{\circ}\text{C})$; temp range 43 – 174°C (Antoine eq. for liquid state, Dreisbach 1961)

1778 (calculated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 9296.5/(T/\text{K})] + 7.938042$; temp range -16.3 to 130.5°C (Antoine eq., Weast 1972–73)

1604 (calculated-Antoine eq., Boublik et al. 1973, 1984)

$\log(P/\text{mmHg}) = 6.89875 - 1365.876/(209.744 + t/^{\circ}\text{C})$; temp range 59–130°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)

1853 (20°C, interpolation of literature values, Dilling 1977)

$\log(P/\text{kPa}) = 6.02534 - 1366.919/(209.861 + t/^{\circ}\text{C})$; temp range 59.31–130.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

$\log(P/\text{mmHg}) = 6.89875 - 1365.88/(209.74 + t/^{\circ}\text{C})$; temp range 59–130°C (Antoine eq., Dean 1985, 1992)

1578 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.1005 - 1410.7/(-59.15 + T/\text{K})$; temp range 316–417 K (Antoine eq., Stephenson & Malanowski 1987)

1201, 2120, 2765, 3575 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)

$\log(P/\text{mmHg}) = -1.0712 - 2.5074 \times 10^3/(T/\text{K}) + 6.1536 \cdot \log(T/\text{K}) - 1.8763 \times 10^{-2} \cdot (T/\text{K}) + 1.0462 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 203–624 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

272.7 (calculated-P/C, Dilling 1977)

283, 280 (calculated-P/C, recommended, Mackay & Shiu 1981)

172, 2, 284, 365, 486 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)

196, 320, 560 (20, 30, 40°C, activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)

0.496, 0.80 (30, 40°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.03 (calculated, Müller & Klein 1992)

2.62, 2.62 (30, 40°C, infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 43$ min for the evaporation from dilute aqueous solution (Dilling et al. 1975)

Evaporation $t_{1/2}(\text{exptl}) = 42.3$ min, $t_{1/2}(\text{calc}) = 2.01$ min, 48.8 min from water (Dilling 1977)

Photolysis:

Oxidation:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} < 1.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time > 1160 d, loss $< 0.1\%$ in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

photooxidation $t_{1/2} = 2236\text{--}22361$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $k = 1.2 \text{ M}^{-1} \text{ s}^{-1}$ for reaction at pH 7 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991);

$k = 4320 \text{ M}^{-1} \text{ h}^{-1}$ for base reaction at pH 9 and 25°C (Mabey et al. 1983; quoted, Howard et al. 1991);

abiotic hydrolysis or dehydrohalogenation $t_{1/2} = 384$ months (Mabey et al. 1983; quoted, Olsen & Davis 1990).

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on acclimated river die-away rate data for 1,1,2,2-tetrachloroethane (Mudder 1981; quoted, Howard et al. 1991), unacclimated sea water (Pearson & McConnell 1975; quoted, Howard et al. 1991) and sub-soil grab sample data for a ground water aquifer for 1,1,1-trichloroethane (Wilson et al. 1983; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}17280$ h, based on aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976)
residence time > 1160 d, loss $< 0.1\%$ in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical with OH radical (Singh et al. 1981)

$t_{1/2} = 2236\text{--}22361$ h, based on an estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated tropospheric lifetime of 1.9 yr (Nimitz & Skaggs 1992).

Surface water: $t_{1/2} = 16\text{--}1604$ h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 16\text{--}1604$ h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 16\text{--}1604$ h, based on hydrolysis half-lives at pH 7 and 9 (Mabey et al. 1983; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.1.10.1

Reported aqueous solubilities of 1,1,1,2-tetrachloroethane at various temperatures

$$S/(\text{wt}\%) = 0.11968 - 7.87116 \times 10^{-4} \cdot (t/^{\circ}\text{C}) + 1.42253 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 7.24354 \times 10^{-8} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 2.17896 - 1.3966 \times 10^{-3} \cdot (T/\text{K}) + 2.93282 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Van Arkel & Vles 1936		Walraevens et al. 1974		Horvath 1982		Tse et al. 1992	
shake flask		shake flask-GC		summary of literature data		activity coefficient	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	1200	10	1130	0	1197	20	1206
20	1090	20	1100	10	1133	30	1280
35	1150	25	1100	20	1102	35	1292
50	1250	30	1110	25	1100	40	1321
		40	1160	30	1108		
		50	1250	40	1156		
		60	1390	50	1249		
		70	1590	60	1393		
		80	1850	70	1591		
				80	1848		
				eq. 1	$S/\text{wt}\%$		

2.

Wright et al. 1992		Horvath & Getzen 1999a	
activity coefficient		recommended, IUPAC-NIST	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
20	1005	0	1200
30	1093	5	1150
40	1056	10	1110
		15	1080
		20	1070
		25	1070
		30	1080
		35	1100
		40	1130
		45	1170
		50	1230
		eq. 2	$S/\text{wt}\%$
		temp range 273–323 K	

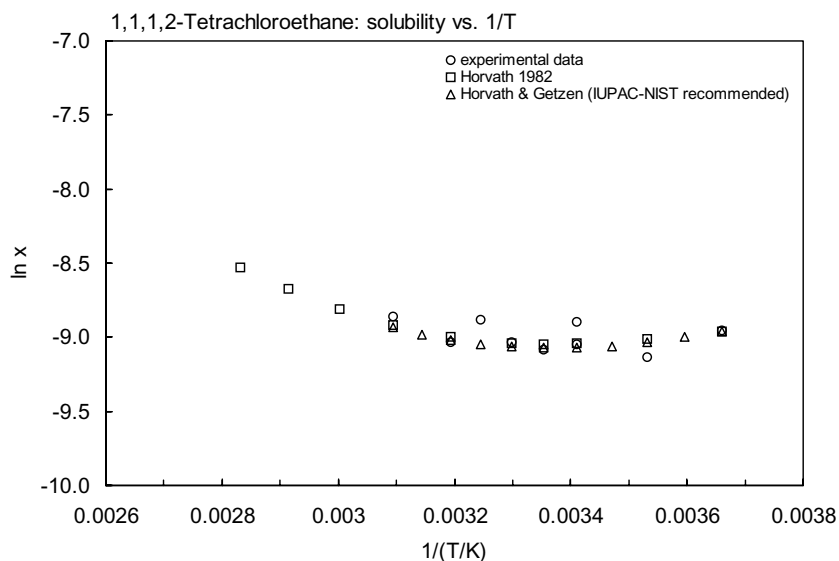


FIGURE 5.1.1.10.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

TABLE 5.1.1.10.2

Reported vapor pressures and octanol-water partition coefficients of 1,1,1,2-tetrachloroethane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Vapor pressure				log K_{OW}	
Stull 1947		Dreisbach & Shrader 1949		Bhatia & Sandler 1995	
summary of literature data		ebulliometry		relative GC-RT technique	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	log K_{OW}
-16.3	133.3	59.31	8851	30	2.62
7.40	666.6	62.39	10114	40	2.62
19.3	1333	74.47	16500		
32.1	2666	199.69	42066		enthalpy of transfer
46.7	5333	115.99	67881		$\Delta H/(\text{kJ mol}^{-1}) = -20.2.$
56.0	7999	130.2	101325		
68.0	13332				$\log K_{OW} = A - \Delta H/2.303RT$
87.2	26664				A 1.0195.
108.2	53329				ΔH -20.2
130.5	101325				
mp/ $^{\circ}\text{C}$	-68.7				

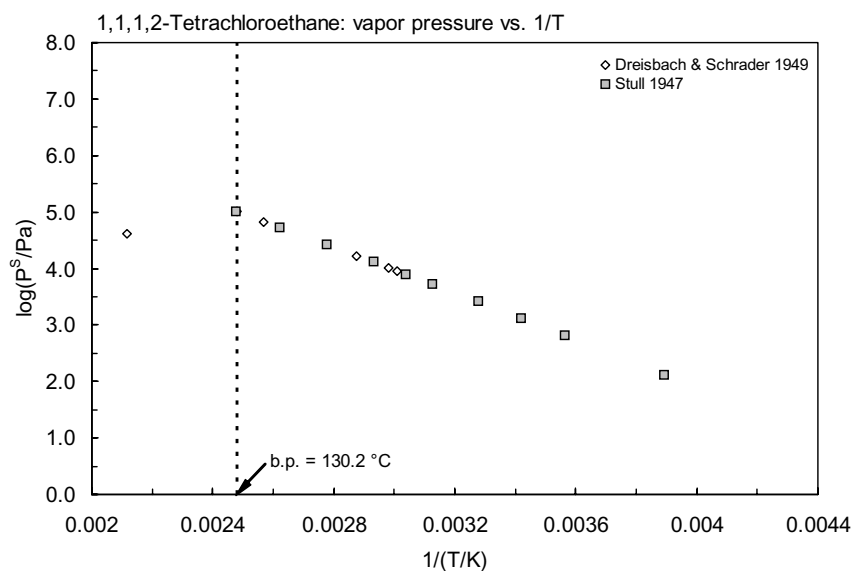


FIGURE 5.1.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

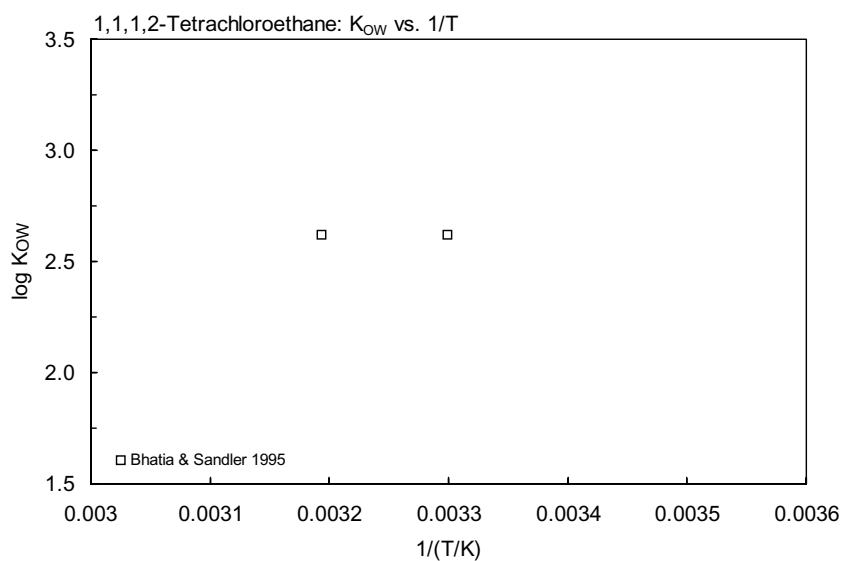
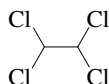


FIGURE 5.1.1.10.3 Logarithm of K_{OW} versus reciprocal temperature for 1,1,1,2-tetrachloroethane.

5.1.1.11 1,1,2,2-Tetrachloroethane



Common Name: 1,1,2,2-Tetrachloroethane

Synonym: sym-tetrachloroethane, acetylene tetrachloride

Chemical Name: 1,1,2,2-tetrachloroethane

CAS Registry No: 79-34-5

Molecular Formula: $C_2H_2Cl_4$, $CHCl_2CHCl_2$

Molecular Weight: 167.849

Melting Point ($^{\circ}C$):

−42.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

145.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5953 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

1.59449, 1.58666 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

105.0 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

135.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

44.89, 36.18 ($25^{\circ}C$, at normal boiling point, Dreisbach 1961)

45.78, 38.65 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2857 (volumetric method, Wright & Schaffer 1932)

2880, 3360 (20 , $55.6^{\circ}C$, Van Arkel & Vles 1936)

2850 (Seidell 1940)

2900 (data presented in graph, temp range 0 – $70^{\circ}C$, McGovern 1943)

2960* (shake flask-GC, measured range 10 – $80^{\circ}C$, Walraevens et al. 1974)

$\log [S/(mol/L)] = 2070/(T/K) - 16.316 + 0.0222 \cdot (T/K)$, temp range 283 – $353 K$ (Walraevens et al. 1974)

3790, 3220, 3210 (3 , 20 , $34^{\circ}C$, shake flask-GC, Chiou & Freed 1977)

3000 (literature average, Dilling 1977)

3230 (shake flask-GC, Chiou et al. 1979)

3041 ($37^{\circ}C$, shake flask-GC, Sato & Nakijima 1979)

2880 ($20^{\circ}C$, recommended, Sørensen & Arit 1979)

2970 (shake flask-LSC, Banerjee et al. 1980)

2960 ($23.5^{\circ}C$, elution chromatography, Schwartz 1980)

3850* ($20^{\circ}C$, elution chromatography, measured range 10 – $30^{\circ}C$, Schwarz & Miller 1980)

2985 (shake flask-LSC, Veith et al. 1980)

2962* (summary of literature data, temp range 0 – $80^{\circ}C$, Horvath 1982)

866.4 (calculated-UNIFAC activity coeff., Arbuckle 1983)

2915 ($30^{\circ}C$, headspace-GC, McNally & Grob 1984)

2985 (calculated-UNIFAC activity coeff., Banerjee 1985)

2870 ($20^{\circ}C$, selected, Riddick et al. 1986)

2355, 2695, 3008 (20 , 35 , $50^{\circ}C$, infinite dilution activity coeff. γ^{∞} -GC, Barr & Newsham 1987)

2910* ($20^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.8^{\circ}C$, Stephenson 1992)

2481, 2503, 2917, 3008 (20 , 30 , 35 , $40^{\circ}C$, infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)

778, 918, 994, 1074 (20 , 30 , 35 , $40^{\circ}C$, infinite dilution activity coeff. γ^{∞} -UNIFAC, Tse et al. 1992)

2422, 3140, 2612 (20, 30, 40°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 2570 (20°C, activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 2830* (recommended, temp range 0–50°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)
 $S/(\text{wt}\%) = 4.87975 - 3.0937 \times 10^{-3} \cdot (T/K) + 5.20513 \times 10^{-5} \cdot (T/K)^2$, temp range 276–323 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

827* (static method, extrapolated, measured range 31.1–146.7°C, Nelson 1930)
 $\log(P/\text{mmHg}) = 8.06938 - 2167.83/(T/K)$; temp range 31.1–146.7°C (static method, Nelson 1930)
 850* (Antoine eq. regression, temp range 65–243.5°C, Stull 1947)
 560* (Ramsay-Young method, measured range 25–130°C, Matthews et al. 1950)
 793 (calculated-Antoine eq., Dreisbach 1961)
 $\log(P/\text{mmHg}) = 6.98240 - 1465.1/(211.0 + t/^\circ\text{C})$; temp range 55–191°C (Antoine eq. for liquid state, Dreisbach 1961)
 851 (interpolated-Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 9917.1/(T/K)] + 8.072583$; temp range –3.8 to 146°C (Antoine eq., Weast 1972–73)
 582 (calculated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{kPa}) = 6.63168 - 1228.062/(179.972 + t/^\circ\text{C})$; temp range 25–120°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 867 (literature average, Dilling 1977)
 585 (calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.77919 - 1240.857/(181.401 + t/^\circ\text{C})$; temp range 25–130°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 2133 (McNally & Grob 1984)
 $\log(P/\text{mmHg}) = 6.6317 - 1228.1/(279.9 + t/^\circ\text{C})$; temp range 25–130°C (Antoine eq., Dean 1985, 1992)
 793 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.1295 - 1444.3/(205.1 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 793 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.1073 - 1465.1/(-62.15 + T/K)$; temp range 328–464 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 5.98931 - 1365.692/(-76.476 + T/K)$; temp range 377–419 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 440, 848, 1154, 2550 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
 $\log(P/\text{mmHg}) = 56.2356 - 4.4615 \times 10^3/(T/K) - 1.6556 \cdot \log(T/K) - 3.5724 \times 10^{-10} \cdot (T/K) + 4.0425 \times 10^{-6} \cdot (T/K)^2$; temp range 229–645 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

46.2 (exptl. $1/K_{AW} (C_W/C_A)$, Hine & Mookerjee 1975)
 47.1 (calculated-P/C, Dilling 1977)
 35.38* (22.0°C, equilibrium cell-GC, measured range 11.0–27.2°C, Leighton & Calo 1981)
 48.5, 48.0 (calculated-P/C, recommended, Mackay & Shiu 1981)
 25.3* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 1.726 - 2810/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 38.5 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 33.45 (computed value, Yaws et al. 1991)
 30.4, 50.7, 60.8, 91.2 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞ -GC, Tse et al. 1992)
 40.3, 57.06, 120 (20, 30, 40°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 34.4 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 34.12 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 2.493 - 1255/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.56 (calculated as per Tute 1971, Callahan et al. 1979)
 2.39 (shake flask-LSC, Banerjee et al. 1980)

- 2.39 (shake flask-LSC, Veith et al. 1980)
 2.79, 2.84 (calculated-UNIFAC with octanol and water mutual solubility considered, calculated-UNIFAC with octanol and water mutual solubility not considered; Arbuckle 1983)
 2.39 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
 2.93 (recommended, Sangster 1993)
 2.39 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 0.9–1.0 (bluegill sunfish, Barrows et al. 1980; Kawasaki 1980)
 0.90 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
 1.96 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 0.91 (fathead minnow, Veith & Kosian 1982)
 2.03 (calculated- K_{OW} , McCarty et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

- 1.66 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
 1.90 (silt loam, quoted from Chiou et al. 1979; Karickhoff 1981; Howard 1990)
 2.00, 1.80, 1.87 (estimated- K_{OW} , estimated-S and mp, estimated-S, Karickhoff 1981)
 2.07 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 3.60 (soil, calculated-universal solvation model; Winget et al. 2000)

Sorption Partition Coefficient, log K_{OM} :

- 1.66, 1.90 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental $t_{1/2} = 56$ min for initial concentration of 1 mg/L when stirred at 200 rpm in water at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

Evaporation $t_{1/2}(\text{exptl}) = 55.2$ min, $t_{1/2}(\text{calc}) = 12.0$ min, 40.5 min from water (Dilling 1977);

estimated $t_{1/2} \sim 6.3$ h for a model river of 1 m deep flowing at 1 m/s with a wind speed of 3 m/s, based on calculated Henry's law constant (Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2} \sim 3.5$ d for a model pond was based on the effect of adsorption (USEPA 1987; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 2.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k_{OH} < 1.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, estimated as toxic chemical residence time > 1160 d, loss < 0.1% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 213\text{--}2131$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: $k = 1.2 \times 10^{-7} \text{ h}^{-1}$ at 25°C and pH 7 (estimated, Mabey et al. 1982);

$t_{1/2}(\text{abiotic})$ or $t_{1/2}(\text{dehydrohalogenation}) = 10$ months (Mabey et al. 1983; quoted, Olsen & Davis 1990)

$t_{1/2}(\text{abiotic}) = 3.3$ months (Cooper et al. 1987; quoted, Olsen & Davis 1990);

$k = 2.3 \times 10^7 \text{ M}^{-1} \text{ yr}^{-1}$ at pH 9 and 25°C with $t_{1/2} = 1.1$ d in alkaline soil, and $k = 111$ d at pH 7 (Kollig et al. 1987; quoted, Howard 1990)

$k = 1.8 \text{ M}^{-1} \text{ s}^{-1}$ for base-catalyzed reaction at 25°C and pH 7 with $t_{1/2} = 45$ d; $k = 6480 \text{ M}^{-1} \text{ h}^{-1}$ for base reaction at pH 9 and 25°C; $k = (27.6 \pm 4.0) \times 10^{-8} \text{ s}^{-1}$ in sediment with 61% conversion (Haag & Mill 1988)

Biodegradation: $k = (7.3 \pm 0.1) \times 10^{-5} \text{ min}^{-1}$ with $t_{1/2} = 6.6$ d in sediment-water sample (Jafvert & Wolfe 1987)

$t_{1/2}(\text{abiotic}) > 800$ d for the reaction with photochemically produced hydroxyl radical (Singh et al. 1981; quoted, Howard 1990)

$t_{1/2}(\text{aq. aerobic}) = 672\text{--}4320$ h, based on acclimated river die-away rate data (Mudder 1981; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 168\text{--}672$ h, based on anaerobic sediment grab sample data (Jafvert & Wolfe 1987) and anaerobic screening test data (Hallen et al. 1986; quoted, Howard et al. 1991).

Biotransformation: estimated rate constant of 3×10^{-12} mL cell⁻¹ h⁻¹ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 13.2$ h⁻¹ (flagfish, calculated-BCF $\times k_2$, McCarty et al. 1992)

$k_2 = 0.123$ h⁻¹ (flagfish, estimated-one compartment first-order kinetic, McCarty et al. 1992)

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976); estimated as toxic chemical residence time > 1160 d, loss $< 0.1\%$ in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 213\text{--}2131$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

estimated tropospheric lifetime of 0.09 yr (Nimitz & Skaggs 1992).

Surface water: $t_{1/2} = 6.6$ d in sediment-water sample (Jafvert & Wolfe 1987);

$t_{1/2} = 45$ d at pH 7 and 25°C, based on base-catalyzed hydrolysis rate constant (Haag & Mill 1988);

$t_{1/2} = 10.7\text{--}1056$ h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Ground water: $t_{1/2} = 10.7\text{--}1056$ h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Sediment: $t_{1/2} = 6.6$ d in Bar-H sediment-water sample (Jafvert & Wolfe 1987);

measured $t_{1/2} = 29$ d at 25°C, based on neutral and base-catalyzed hydrolysis rates studies in pure water and in barely saturated subsurface sediment at 25–60°C (Haag & Mill 1988).

Soil: $t_{1/2} < 10$ d (Ryan et al. 1988);

$t_{1/2} = 10.7\text{--}1056$ h, based on hydrolysis half-lives at pH 7 and 9 (Howard et al. 1991).

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{1/2} < 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.11.1

Reported aqueous solubilities of 1,1,2,2-tetrachloroethane at various temperatures

$$\log S/(\text{mol/L}) = -15.316 + 2070/(T/K) + B(T/K) \quad (1)$$

$$S/(\text{wt}\%) = 0.32934 - 2.10434 \times 10^{-3} \cdot (t/^\circ\text{C}) + 2.54796 \times 10^{-5} \cdot (t/^\circ\text{C})^2 + 1.86126 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (2)$$

$$S/(\text{wt}\%) = 4.87975 - 3.0937 \times 10^{-3} \cdot (T/K) + 5.20513 \times 10^{-5} \cdot (T/K)^2 \quad (3)$$

1.

Walraevens et al. 1974		Schwarz & Miller 1980		Horvath 1982		Barr & Newsham 1987	
shake flask-GC		elution chromatography		summary of literature data		activity coefficient	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	3200	10	3720	0	3299	20	2235
20	3010	20	3850	10	3116	35	2595
25	2960	30	3670	20	2995	50	3008
30	2940			25	2962		
40	2980			30	2948		
50	3120			40	2984		
60	3360			50	3118		
70	3710			60	3356		
80	4200			70	3713		
				80	4199		
eq. 1	S/(mol/L)						
A	15.316						
B	0.0222			eq. 2	S/wt%		

TABLE 5.1.1.11.1 (Continued)

2.

Stephenson 1992		Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999a	
shake flask-GC		activity coefficient		activity coefficient		recommended, IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	3170	20	2481	20	2422	5	3020
9.5	2900	30	2503	30	3140	10	2830
20	2910	35	2917	40	2612	15	2870
29.7	2920	40	3008			25	2840
39.6	3010					30	2830
50.1	3160					35	2850
61	3570					40	2890
70.5	3850					45	3060
80.6	4250					50	3160
90.8	4740						

eq. 3 S/wt%
temp range 276–323 K

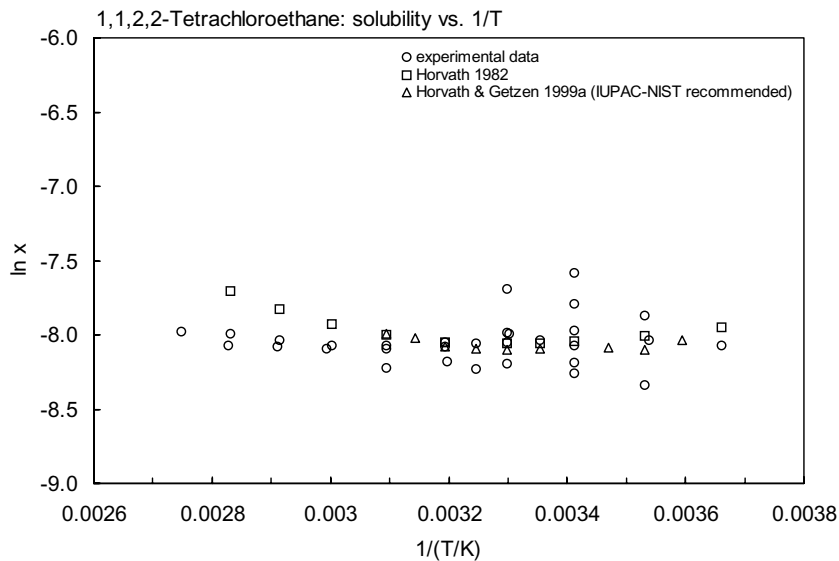


FIGURE 5.1.1.11.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

TABLE 5.1.1.11.2

Reported vapor pressures of 1,1,2,2-tetrachloroethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Nelson 1930		Stull 1947		Matthews et al. 1950	
static method		summary of literature data		Ramsay-Young method	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
31.1	1000	-3.80	133.3	25.0	560
34.6	1067	20.7	666.6	30.0	667
39.3	1533	33.0	1333	35.0	1080
44.3	2200	46.2	2666	40.0	1493
50.4	3120	60.8	5333	45.0	2000
57.8	4253	70.0	7999	50.0	2680
64.6	5893	83.2	13332	55.0	3480
72.3	8293	102.2	26664	60.0	4440
79.0	10879	124.0	53329	65.0	5626
85.0	13865	145.9	101325	70.0	6933
89.9	16785			75.0	8533
94.9	20438	mp/ $^{\circ}\text{C}$	-36	80.0	10666
99.9	24611			85.0	13066
105	29851			90.0	16079
109.1	34770			95.0	19532
114.9	41730			100	23665
119.9	47703			105	28331
120.1	48569			110	33130
124.5	54865			115	38930
130.4	66328			120	45663
135.2	92139			135	53329
141.5	102285			130	62795
146.7	106938				
20	626.6*			bp/K	420.4
25	826.6*			$\Delta H_v = 38.42 \text{ kJ/mol at bp}$	
				Kirchhoff, Rankine, Dupre eq.	
eq. 1	P/mmHg			eq. 4	P/mmHg
A	8.08938			A	35.117
B	2167.83			B	3646
				C	8.981

*extrapolated

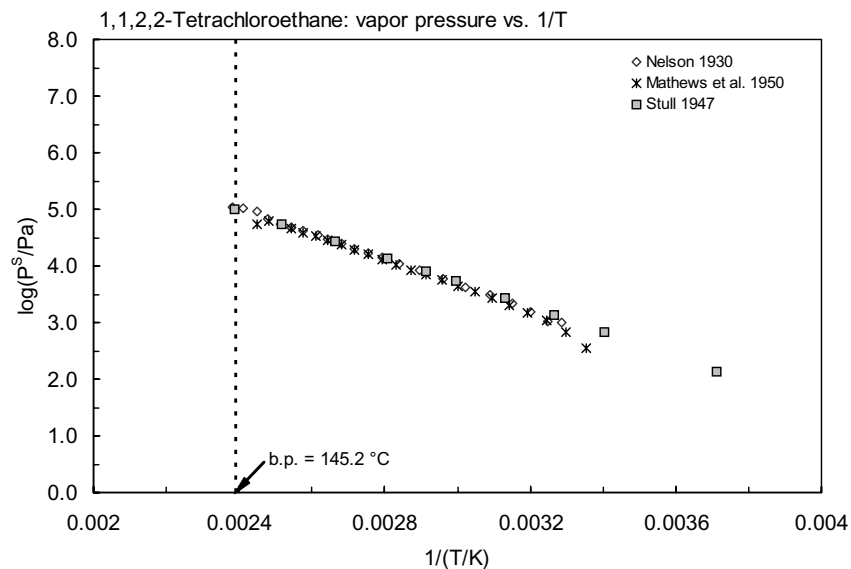


FIGURE 5.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

TABLE 5.1.11.3
Reported Henry’s law constants of 1,1,2,2-tetrachloroethane at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$
$$\ln (1/K_{AW}) = A - B/(T/K)$$
$$\ln (k_H/\text{atm}) = A - B/(T/K)$$
$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

(1)

(2)

(3)

(4)

(5)

$$\log K_{AW} = A - B/(T/K)$$
$$\log (1/K_{AW}) = A - B/(T/K)$$

(1a)

(2a)

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

(4a)

Leighton & Calo 1981		Ashworth et al. 1988		Tse et al. 1992		Wright et al. 1992	
equilibrium cell-GC		EPICS-GC		activity coefficient		activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
11.0	19.95	10	33.44	20	30.4	20	40.3
13.0	22.83	15	20.27	30	50.7	30	57.06
21.0	31.06	20	73.97	35	60.8	40	120
22.0	35.38	25	25.33	40	91.2		
27.2	38.19	30	70.93				
eq. 3	H/atm	eq. 4a	H/(atm m ³ /mol)				
A	14.91	A	1.726				
B	3547	B	2810				

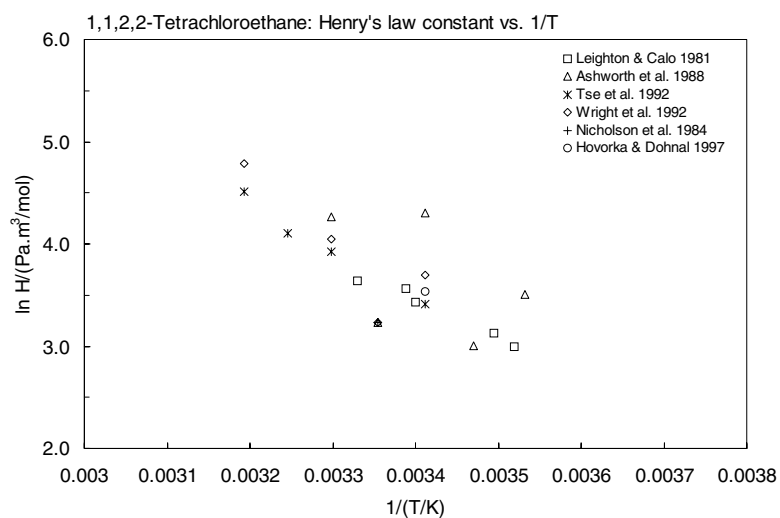
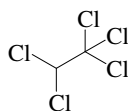


FIGURE 5.1.1.11.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2,2-tetrachloroethane.

5.1.1.12 Pentachloroethane



Common Name: Pentachloroethane

Synonym: 1,1,1,2,2-pentachloroethane, pentalin

Chemical Name: pentachloroethane

CAS Registry No: 76-01-7

Molecular Formula: C_2HCl_5 , $CHCl_2CCl_3$

Molecular Weight: 202.294

Melting Point ($^{\circ}C$):

-28.78 (Lide 2003)

Boiling Point ($^{\circ}C$):

162.0 (Horvath 1982; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.6796 (Horvath 1982; Weast 1982–83)

1.6808, 1.6732 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

120 (calculated-density, Abernethy et al. 1988)

156.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.79, 36.941 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.34 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

345 (volumetric method, Wright & Schaffer 1932)

470 ($20^{\circ}C$, shake flask, Van Arkel & Vles 1936)

463 (Seidell 1940)

500 (data presented in graph, temp range 0 – $70^{\circ}C$, McGovern 1943)

500* (shake flask-GC, temp range 10 – $80^{\circ}C$, Walraevens et al. 1974)

$\log [S/(mol\ dm^{-3})] = 2070/(T/K) - 16.412 + 0.0230 \cdot (T/K)$; temp range 283 – $353\ K$ (Walraevens et al. 1974)

480 (literature average, Dilling et al. 1975; Dilling 1977)

776 (shake flask-LSC, Veith et al. 1980)

500* (summary of literature data, temp range 0 – $80^{\circ}C$, Horvath 1982)

500 (Dean 1985; Riddick et al. 1986)

470, 490 ($20^{\circ}C$, $25^{\circ}C$, recommended, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):

467* ($25.1^{\circ}C$, static method, measured range 25.1 – $162.2^{\circ}C$, Nelson 1930)

$\log (P/mmHg) = 7.80304 - 2129.6/(T/K)$; temp range 25.1 – $162.2^{\circ}C$ (static method, Nelson 1930)

596* (Antoine eq. regression, temp range 1.0 – $160.5^{\circ}C$, Stull 1947)

596 (calculated-Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 9800.1/(T/K)] + 7.832202$; temp range 1.0 – $160.6^{\circ}C$ (Antoine eq., Weast 1972–73)

465 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 6.74011 - 1378.096/(197.367 + t/^{\circ}C)$; temp range 25.1 – $162^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

600 (literature average, Dilling 1977)

453, 800 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

- 467 (calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.92765 - 1419.719/(202.285 + t/^{\circ}\text{C})$; temp range 25.1–162°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = 6.740 - 1378/(197 + t/^{\circ}\text{C})$, temp range: 25–162°C (Antoine eq., Dean 1985, 1992)
 590 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 5.7199 - 1295.67/(188.96 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 625 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.69025 - 1982.65/(-10.577 + T/\text{K})$; temp range 274–434 K (Antoine eq., Stephenson & Malanowski 1987)
 467, 453 (quoted, calculated-UNIFAC, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 72.1134 - 4.6522 \times 10^3/(T/\text{K}) - 23.777 \cdot \log(T/\text{K}) + 9.6908 \times 10^{-3} \cdot (T/\text{K}) - 3.3886 \times 10^{-13} \cdot (T/\text{K})^2$;
 temp range 244–665 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 247.9 (exptl $-1/K_{\text{AW}} = C_{\text{W}}/C_{\text{A}}$, Hine & Mookerjee 1975)
 247.9 (calculated-P/C, Dilling 1977)
 96.44 (calculated-QSAR, Nirmalakhandan & Speece 1988)
 196.5 (calculated-P/C, Howard 1990)
 188.9, 53.73 (quoted, calculated-bond contribution method, Meylan & Howard 1991)
 183.9 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.89 (shake flask-LSC, Veith et al. 1980)
 3.05 (HPLC-RT correlation, McDuffie 1981; quoted, Sangster 1993)
 3.22 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.826 (bluegill sunfish, Barrows et al. 1980)
 1.83 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
 1.78 (fathead minnow, Veith & Kosian 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constant, k and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental $t_{1/2} = 48$ min for 1 mg/L aqueous solution when stirred at 200 rpm at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975)

Evaporation $t_{1/2}(\text{exptl}) = 46.5$ min, $t_{1/2}(\text{calc}) = 2.3$ min, 32 min from water (Dilling 1977)

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = 1.93 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{exptl}) = 2.33 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4$ –24 h from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

estimated tropospheric lifetime of 0.58 h (Nimitz & Skaggs 1992).

Surface water:

Ground water:

Sediment:

Soil:

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 5.1.1.12.1

Reported aqueous solubilities and vapor pressures of pentachloroethane at various temperatures

$$S/(\text{wt}\%) = 5.41068 \times 10^{-2} - 2.81268 \times 10^{-4} \cdot (t/^{\circ}\text{C}) + 3.41333 \times 10^{-6} \cdot (t/^{\circ}\text{C})^2 + 4.76167 \times 10^{-8} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$\log S = A/(T/K) - B + C \cdot (T/K) \quad (2)$$

Aqueous solubility				Vapor pressure			
Walraevens et al. 1974		Horvath 1982		Nelson 1930		Stull 1947	
shake flask-GC		summary of literature data		static method		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
10	520	0	541.1	25.1	467	1.0	133.3
20	500	10	516.8	41.1	1733	27.2	666.6
25	500	20	502.3	50.0	2133	39.8	1333
30	500	25	499.5	55.0	2666	53.9	2666
40	510	30	500.3	65.0	4453	69.9	5333
50	550	40	513.6	69.0	4986	80.0	7999
60	600	50	545.3	75.0	6573	93.5	13332
70	670	60	598.0	80.0	7973	114.0	26664
80	780	70	674.8	88.2	10959	137.2	53329
		80	778.3	95.7	14212	160.5	101325
eq. 2	S/(mol/L)			100.2	16732		
A	2070	eq.1	S/wt%	105.0	19852	mp/°C	57
B	16.412			110.0	23771		
C	0.0230			115.6	28491		
				119.9	33064		
				124.9	39170		
				125.6	39957		
				128.7	43876		
				132.4	49049		
				134.6	50249		
				139.4	59555		
				145.3	70741		
				151.3	80660		
				157.3	94859		
				162.2	108137		

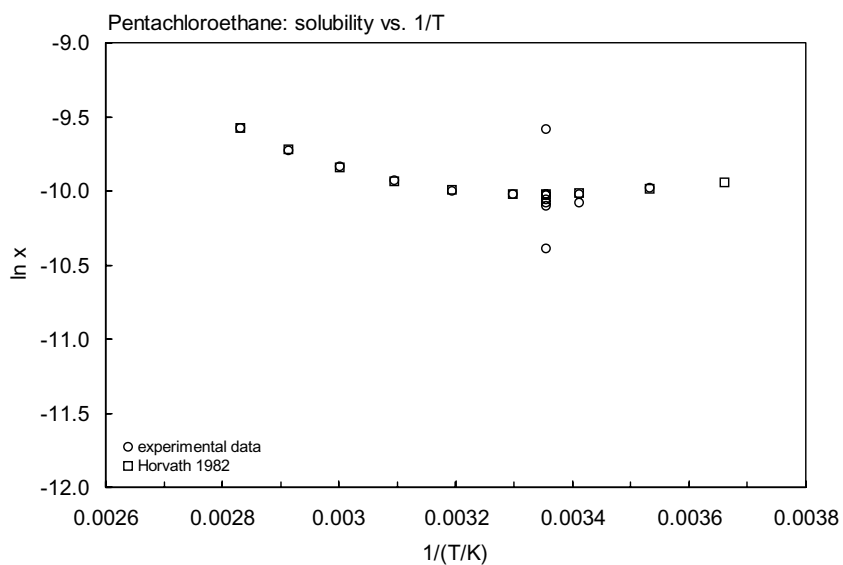


FIGURE 5.1.1.12.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for pentachloroethane.

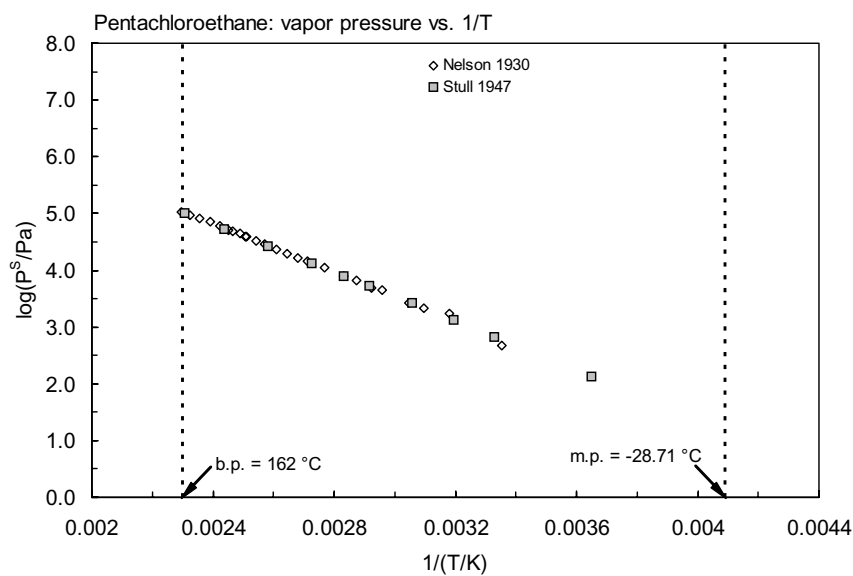
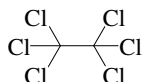


FIGURE 5.1.1.12.2 Logarithm of vapor pressure versus reciprocal temperature for pentachloroethane.

5.1.1.13 Hexachloroethane



Common Name: Hexachloroethane

Synonym: carbon hexachloride, perchloroethane, phenohep, HCE

Chemical Name: hexachloroethane

CAS Registry No: 67-72-1

Molecular Formula: C_2Cl_6 , CCl_3CCl_3

Molecular Weight: 236.739

Melting Point ($^{\circ}C$):

186.8 (triple point) (Lide 2003)

Boiling Point ($^{\circ}C$):

184.7 (sublimation point) (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

2.091 (McGovern 1943; Horvath 1982; Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

113 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

177.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

50 ($22.3^{\circ}C$, shake flask, Van Arkel & Vles 1936)

50 ($22.3^{\circ}C$, McGovern 1943)

27.2 (shake flask-LSC, Veith et al. 1980)

50 ($22.3^{\circ}C$, recommended, Horvath 1982)

77.1 ($20^{\circ}C$, EPICS-LSC, Munz & Roberts 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

42.7* (gas saturation method, extrapolated, measured range 31 – $55^{\circ}C$, Nelson 1930)

75.4* (extrapolated-Antoine eq. regression, temp range 32.7 – $186.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11711.3/(T/K)] + 8.440623$; temp range 32.7 – $185.6^{\circ}C$ (Antoine eq., Weast 1972–73)

49.5 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 7.9015 - 3077/(T/K)$; temp range 317 – $345\ K$ (Antoine eq.-I, solid, rhombic, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 7.856 - 2677/(T/K)$; temp range 345 – $460\ K$ (Antoine eq.-II, solid, cubic, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.6075 - 2103.6/(T/K)$; temp range 460 – $513\ K$ (Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -366.2243 + 6.67893 \times 10^3/(T/K) + 155.63 \cdot \log(T/K) - 0.15563 \cdot (T/K) + 5.56 \times 10^{-5} \cdot (T/K)^2$; temp range 306 – $698\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

231.3 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

123.9 (calculated-P/C, Dilling 1977)

285* ($20^{\circ}C$, EPICS-LSC, measured range 10 – $30^{\circ}C$, Munz 1985)

$\log K_{AW} = 6.982 - 2320/(T/K)$, temp range 10 – $30^{\circ}C$ (EPICS-LSC measurements, Munz & Roberts 1987)

- 846* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 3.744 - 2550/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 253.3 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 226.7 (computed value, Yaws et al. 1991)
 285 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 6.982 - 2320/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.14 (20°C, shake flask-GC, both phases, Chiou et al. 1977)
 3.82 (HPLC- k' correlation, Könemann et al. 1979)
 3.93 (shake flask-LSC, Veith et al. 1980)
 4.05 (RP-HPLC-RT correlation, Veith et al. 1980)
 4.04 (HPLC-RT correlation, McDuffie 1981)
 4.14 (recommended, Sangster 1993)
 4.14 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 4.47 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 0.92–3.23 (calculated- K_{OW} , Veith et al. 1979, 1980)
 2.143 (bluegill sunfish, Barrows et al. 1980)
 2.14 (bluegill sunfish, Veith et al. 1980)
 3.83 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 2.14 (bluegill sunfish, Veith & Kosian 1982)
 2.85 (fathead minnow, Veith & Kosian 1982)
 4.57 (calculated- K_{OW} , Thomann 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.3 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental $t_{1/2} = 40$ –45 min from dilute aqueous solution in open container of depth 65mm and stirring at 200 rpm (Dilling et al. 1975)

Evaporation $t_{1/2}(\text{exptl}) = 28.0$ min, $t_{1/2}(\text{calc}) = 4.5$ min, 24.5 min from water (Dilling 1977)

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} < 1.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, estimated residence time > 11600 d, loss $\approx 0.0\%$ in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} > 7.3$ –73 yr, based on estimated maximum rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991)

Hydrolysis: not significant, based on hydrolysis studies after 13 d at 85°C and pH 3, 7, and 11 (Ellington et al. 1987; quoted, Howard et al. 1991)

Biodegradation:

$k = (5.0 \pm 0.34) \times 10^{-2} \text{ min}^{-1}$ in Bar-H sediment-water slurry, $k = (2.0 \pm 0.17) \times 10^{-2} \text{ min}^{-1}$ in Beaver Dam sediment-water slurry, $k = (2.6 \pm 0.2) \times 10^{-2} \text{ min}^{-1}$ in Hickory Hill sediment-water slurry, $k = (1.9 \pm 0.16) \times 10^{-2} \text{ min}^{-1}$ in Memorial Park sediment-water slurry and $k = (1.9 \pm 0.1) \times 10^{-2} \text{ min}^{-1}$ with $t_{1/2} = 36$ min in anoxic Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

$t_{1/2}(\text{aq. aerobic}) = 672$ h–4320 h, based on aqueous screening studies (Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 2688$ –17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 28$ d, $t_{1/2}(\text{anaerobic}) = 110$ d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of $1 \times 10^{-10} \text{ ml cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

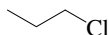
Half-Lives in the Environment:

- Air: disappearance $t_{1/2} > 10$ d for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);
 $t_{1/2} > 7.3$ –73 yr, based on estimated maximum rate constant for reaction with hydroxyl radical (Singh et al. 1980; quoted, Howard et al. 1991);
 residence time > 11600 d, loss ≈ 0.0 in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical K for the reaction with OH radical (Singh et al. 1981)
- Surface water: $t_{1/2} = 36$ min in anoxic sediment-water suspension (Jafvert & Wolfe 1987);
 $t_{1/2} = 672$ –4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
 $t_{1/2}(\text{aerobic}) = 28$ d, $t_{1/2}(\text{anaerobic}) = 110$ d in natural waters (Capel & Larson 1995).
- Ground water: $t_{1/2} = 1344$ –8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Sediment: disappearance $k = (5.0 \pm 0.34) \times 10^{-2} \text{ min}^{-1}$ in Bar-H sediment-water slurry, $k = (2.0 \pm 0.17) \times 10^{-2} \text{ min}^{-1}$ in Beaver Dam sediment-water slurry, $k = (2.6 \pm 0.2) \times 10^{-2} \text{ min}^{-1}$ in Hickory Hill sediment-water slurry, $k = (1.9 \pm 0.16) \times 10^{-2} \text{ min}^{-1}$ in Memorial Park sediment-water slurry and $k = (1.9 \pm 0.1) \times 10^{-2} \text{ min}^{-1}$ with $t_{1/2} = 36$ min in Bar-H sediment-water suspension (Jafvert & Wolfe 1987)
- Soil: $t_{1/2} = 672$ –4320 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980)

TABLE 5.1.1.13.1

Reported vapor pressures and Henry's law constant of hexachloroethane at various temperatures

Vapor pressure				Henry's law constant			
Nelson 1930		Stull 1947		Ashworth et al. 1988		Munz 1985	
gas saturation		summary of literature data		EPICS-GC		EPICS-LSC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
31	73.3	32.7	133.3	10	601	10	74.2
35	93.3	49.8	666.6	15	566.4	20	285
40	133.3	73.5	1333	20	598.8	30	537
45	198.7	87.6	2666	25	846.1		
50	282.6	102.3	5333	30	1044		
55	390.6	112.0	7999				
		124.2	13332	$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$			
		143.1	26664	A	3.744		
		163.8	53332	B	2550		
		185.6	101325				

5.1.1.14 1-Chloropropane (*n*-Propyl chloride)

Common Name: 1-Chloropropane

Synonym: *n*-Propyl chloride, propyl chloride

Chemical Name: 1-chloropropane, *n*-Propyl chloride, propyl chloride

CAS Registry No: 540-54-5

Molecular Formula: $\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$

Molecular Weight: 78.541

Melting Point ($^{\circ}\text{C}$):

−122.9 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

46.5 (Lide 2003)

Density (g/cm^3 at 20°C):

0.8909 (Dreisbach 1961; Horvath 1982)

0.8899, 0.8830 (20°C , 25°C , Riddick et al. 1986)

Molar Volume (cm^3/mol):

88.3 (20°C , calculated-density)

94.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

28.48, 27.25 (25°C , normal bp, Dreisbach 1961)

28.50, 27.24 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.544 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2720* (20°C , measured range 0 – 30°C , volumetric method, Rex 1906)

2500 (Wright & Schaffer 1932)

2772 (30°C , shake flask, Van Arkel & Vles 1936)

2334 (Seidell 1941)

2333 (20°C , Saracco & Spaccamela Marchetti 1958)

2700 (20°C , Verschueren 1983)

2651* (summary of literature data, Horvath 1982)

2710 (20°C , quoted, Riddick et al. 1986)

2500* (reported value of IUPAC-NIST Solubility Data Series, temp range 0 – 37°C , Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

37360, 55240 (20°C , 30°C , Rex 1906)

46500* (interpolated-Antoine eq. regression, temp range -68.3 to 36.5°C , Stull 1947)

46000 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/\text{mmHg}) = 6.93111 - 1121.123/(230.2 + t/^{\circ}\text{C})$; temp range -25 to 88°C (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/\text{mmHg}) = 6.93111 - 1121.123/(230.20 + t/^{\circ}\text{C})$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

40517* (21.8°C , differential thermal analysis, measured range -25.1 to 47.1°C , Kemme & Kreps 1969)

$\log(P/\text{mmHg}) = [-0.2185 \times 7485.7/(T/\text{K})] + 8.028733$; temp range -63.8 to 46.4°C (Antoine eq., Weast 1972–73)

$\log(P/\text{kPa}) = 6.07206 - 1120.381/(229.061 + t/^{\circ}\text{C})$; temp range -25.1 to 47.1°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log(P/\text{mmHg}) = 6.92648 - 1110.19/(227.94 + t/^{\circ}\text{C})$; temp range -25 to 47°C (Antoine eq., Dean 1985, 1992)

45920 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.07655 - 1125.09/(229.86 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

46060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.09145 - 1126.383/(-43.78 + T/\text{K})$; temp range 248–320 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 32.3325 - 2.485 \times 10^3/(T/\text{K}) - 8.8052 \cdot \log (T/\text{K}) + 8.9119 \times 10^{-11} \cdot (T/\text{K}) + 3.6803 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 150–503 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1341 (calculated-P/C, using Hine & Mookerjee 1975 data)

1600 (calculated-QSAR, Nirmalakhandan & Speece 1988)

1091 (computed value, Yaws et al. 1991)

1450 (γ^{∞} from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.04 (shake flask, Log P Database, Hansch & Leo 1987)

2.04 (recommended, Sangster 1989)

2.04 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.24 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 5.1.1.14.1

Reported aqueous solubilities of 1-chloropropane at various temperatures

$$S/(\text{wt}\%) = 0.3746 - 0.007725 \cdot (t/^{\circ}\text{C}) + 1.05001 \times 10^{-6} \cdot (t/^{\circ}\text{C})^2 + 1.14998 \times 10^{-6} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		reported, IUPAC-NIST	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	3760	0	3746	0	3750
10	3230	10	3090	10	3220
20	2720	20	2713	12.5	2320
30	2770	25	2651	20	2710
		30	2684	25	2500
				30	2760
		eq. 1	$S/\text{wt}\%$	30	2770
				37	2440

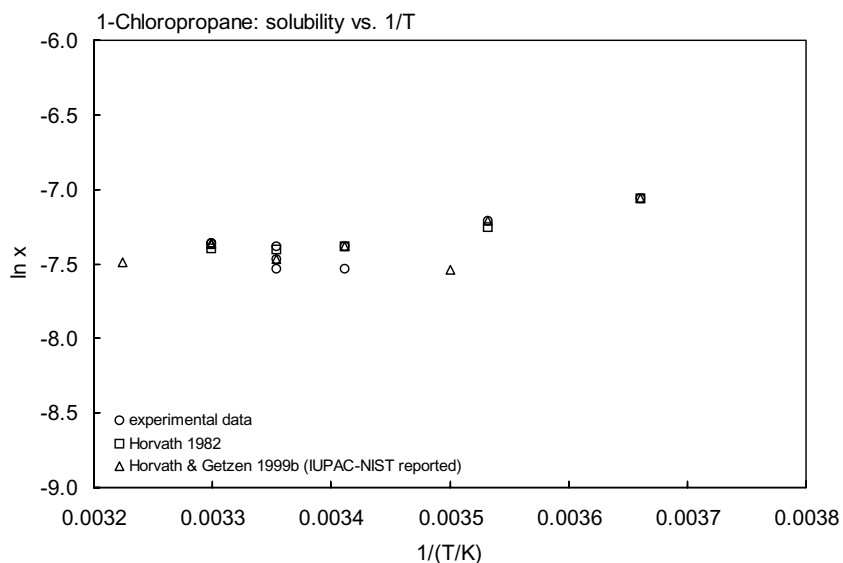


FIGURE 5.1.1.14.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-chloropropane.

TABLE 5.1.1.14.2

Reported vapor pressures of 1-chloropropane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & \end{aligned}$$

Stull 1947		Kempe & Kreps 1969	
summary of literature data		differential thermal analysis	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-63.8	133.3	-25.1	3840
-50.0	666.6	-19.6	5320
-41.0	1333	-13.7	7386
-31.0	2666	-6.90	10599
-19.5	5333	1.20	16065
-12.1	7999	12.1	26691
-2.50	13332	21.8	40517
12.1	26664	34.9	67194
29.4	53329	47.1	103458
46.4	101325		
mp/ $^{\circ}\text{C}$	-117	eq. 2	P/mmHg
		A	8.18894
		B	1690.864
		C	221.346

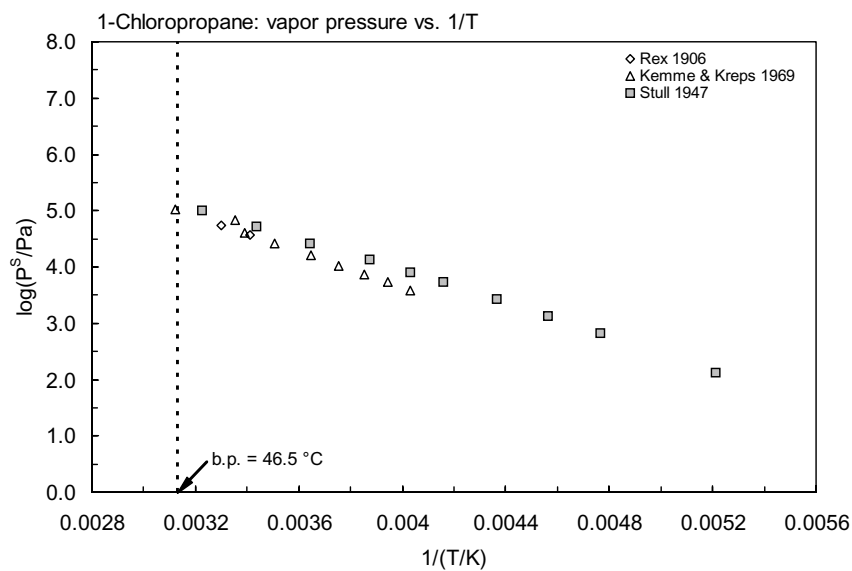


FIGURE 5.1.14.2 Logarithm of vapor pressure versus reciprocal temperature for 1-chloropropane.

5.1.1.15 2-Chloropropane



Common Name: 2-Chloropropane

Synonym: isopropyl chloride

Chemical Name: 2-chloropropane, isopropyl chloride

CAS Registry No: 75-29-6

Molecular Formula: C_3H_7Cl , $CH_3CHClCH_3$

Molecular Weight: 78.541

Melting Point ($^{\circ}C$):

-117.18 (Lide 2003)

Boiling Point ($^{\circ}C$):

35.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8626, 0.8560 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

0.8617, 0.8563 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961; Riddick et al. 1986)

Molar Volume (cm^3/mol):

91.2 ($20^{\circ}C$, calculated from density)

94.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

26.86, 26.26 ($25^{\circ}C$, normal bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.39 (calculated, Dreisbach 1959)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

3050* ($20^{\circ}C$, measured range $0-30^{\circ}C$, volumetric method, Rex 1906)

3444 (shake flask, Fühner 1924)

3056 (Seidell 1940)

3000 (Seidell 1941)

2950 (selected exptl., Horvath 1982)

3400 (Dean 1985)

3040* ($20^{\circ}C$, tentative values, temp range $0-30^{\circ}C$, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

58050, 83940 ($20^{\circ}C$, $30^{\circ}C$, Rex 1906)

53329* ($18.1^{\circ}C$, summary of literature data, temp range -78.8 to $36.5^{\circ}C$, Stull 1947)

70580 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.96540 - 1081.6/(230 + t/^{\circ}C)$; temp range -32 to $90^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

68700 (interpolated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 6.91997 - 1081.4/(232 + t/^{\circ}C)$; temp range -33 to $68^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 6855.2/(T/K)] + 7.75768$; temp range -78.8 to $36.5^{\circ}C$ (Antoine eq., Weast 1972-73)

70000 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.91429 - 1593.593/(289.355 + t/^{\circ}C)$; temp range $0-30^{\circ}C$ (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)

69440 (interpolated-Antoine eq., temp range $0-30^{\circ}C$, Dean 1985, 1992)

$\log(P/mmHg) = 7.771 - 1582.0/(288.0 + t/^{\circ}C)$; temp range $0-30^{\circ}C$ (Antoine eq., Dean 1985, 1992)

68700 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 5.3643 - 779.7/(196.5 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

68800 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.54823 - 860.49/(-66.25 + T/\text{K})$; temp range 239–310 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 115.1259 - 4.6278 \times 10^3/(T/\text{K}) - 42.197 \cdot \log(T/\text{K}) + 2.526 \times 10^{-2} \cdot (T/\text{K}) - 9.8906 \times 10^{-14} \cdot (T/\text{K})^2$; temp range 156–589 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1652 (calculated-P/C, using Hine & Mookerjee 1975 data)

1248 (calculated-QSAR, Nirmalakhandan & Speece 1988)

1468 (computed value, Yaws et al. 1991)

1836 (γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.69 (calculated- π const., Hansch et al. 1968)

1.90 (shake flask, Log P Database, Hansch & Leo 1987)

1.90 (recommended, Sangster 1989)

1.90 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Hydrolysis: rate constant $k = 2.12 \times 10^7 \text{ s}^{-1}$ with $t_{1/2} = 38 \text{ d}$ at 25°C and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

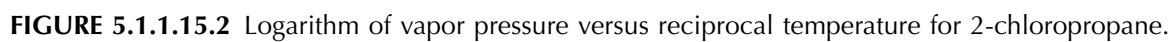
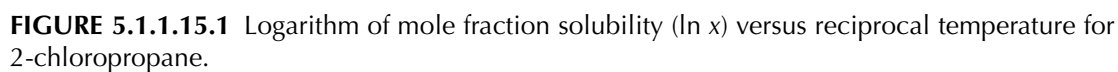
Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (Darnall et al. 1976).

Surface water: $t_{1/2} = 38 \text{ d}$ at 25°C and pH 7 based on hydrolysis rate constant (Mabey & Mill 1978)

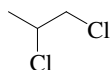
TABLE 5.1.1.15.1

Reported aqueous solubilities and vapor pressures of 2-chloropropane at various temperatures

Aqueous solubility				Vapor pressure			
Rex 1906		Horvath 1982		Rex 1906		Stull 1947	
volumetric method		summary of literature data				summary of literature data	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
0	440	0	4381	0	25558	−78.8	133.3
10	362	10	3607	10	38863	−61.1	666.6
20	305	20	3141	20	58062	−52.0	1333
30	304	25	2945	30	83953	−42.0	2666
		30	3031			−31.0	5333
						−23.5	7999
						−13.7	13332
						1.30	26664
						18.1	53329
						36.5	101325
						$\text{mp}/^\circ\text{C}$	−117



5.1.1.16 1,2-Dichloropropane



Common Name: 1,2-Dichloropropane

Synonym: propylene chloride, propylene dichloride, α,β -propylene dichloride

Chemical Name: 1,2-dichloropropane

CAS Registry No: 78-87-5

Molecular Formula: 1,2-C₃H₆Cl₂, CH₃CHClCH₂Cl

Molecular Weight: 112.986

Melting Point (°C):

−100.53 (Lide 2003)

Boiling Point (°C):

96.40 (McGovern 1943; Timmermans 1950; Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm³ at 20°C):

1.1560 (Dreisbach 1959, 1961; Horvath 1982; Weast 1982–83; Riddick et al. 1986)

1.1494 (25°C, Dreisbach 1959, 1961)

Molar Volume (cm³/mol):

98 (calculated-density, Abernethy et al. 1988; Wang et al. 1992)

115.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

36.33, 30.5 (25°C, normal bp, Dreisbach 1961)

36.40, 32.004 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.40 (calculated, Dreisbach 1959; quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2800 (shake flask-interferometer, Gross 1929; Stephen & Stephen 1963)

2773 (Seidell 1940)

2700 (20°C, McGovern 1943)

2750 (measured by Dow Chemical, Dreisbach 1955–1961)

2096 (shake flask-GC, Jones et al. 1977/1978)

3520 (shake flask-GC, Chiou et al. 1979)

2800* (summary of literature data, Horvath 1982)

2420 (headspace-GC, McNally & Grob 1983)

2070 (30°C, headspace-GC, McNally & Grob 1984)

2600 (Dean 1985)

2740 (selected, Riddick et al. 1986; Howard 1990)

3000*, 2900 (20°C, 29.7°C, shake flask-GC/TC, measured range 0–90.4°C, Stephenson 1992)

3005, 3129, 3261 (20, 30, 40°C, infinite dilution activity coeff. γ^∞ -GC, Tse et al. 1992)

3287, 3706, 4152 (20, 30, 40°C, infinite dilution activity coeff. γ^∞ -UNIFAC, Tse et al. 1992)

2683, 2717, 3003 (20, 30, 40°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)

2650 (20°C, limiting activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

2740* (recommended, temp range 278.15–313.15 K, IUPAC-NIST Series, Horvath & Getzen 1999)

$S/(wt\%) = 3.3285 - 0.021464 \cdot (T/K) + 3.7632 \times 10^{-5} \cdot (T/K)^2$, temp range 275–313 K (Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7200* (isoteniscope method, measured range 15–99.7°C, Nelson & Young 1933)

$\log (P/\text{mmHg}) = 7.7085 - 1782.8/(T/K)$; temp range 15–100°C (isoteniscope, Nelson & Young 1933)

6930 (McGovern 1943)

- 6780* (Antoine eq. regression, temp range -7 to 141.6°C, Stull 1947)
 16500* (44.78°C, ebulliometry, measured range 44.78–96.2°C, Dreisbach & Shrader 1949)
 6620 (calculated-Antoine eq., Dreisbach 1959, 1961)
 $\log(P/\text{mmHg}) = 6.96395 - 1295.9/(221.0 + t/^\circ\text{C})$; temp range 15–160°C (Antoine eq. for liquid state, Dreisbach 1959)
 $\log(P/\text{mmHg}) = 6.96546 - 1296.4/(221.0 + t/^\circ\text{C})$; temp range 15–135°C (Antoine eq. for liquid state, Dreisbach 1961)
 $\log(P/\text{mmHg}) = [-0.2185 \times 8428.5/(T/K)] + 7.882416$; temp range -38.5 to 96.8°C (Antoine eq., Weast 1972–73)
 6720 (calculated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 6.98047 - 1308.138/(222.845 + t/^\circ\text{C})$; temp range 44.8–96.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
 6720, 7120 (calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.10153 - 1305.689/(222.567 + t/^\circ\text{C})$, temp range 55.78–96.2°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.73547 - 1717.264/(266.9 + t/^\circ\text{C})$, temp range 15–99.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = 6.9807 - 1308.1/(222.8 + t/^\circ\text{C})$; temp range 45–96°C (Antoine eq., Dean 1985, 1992)
 6622 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.08885 - 1295.9/(221.0 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 6620 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_1/\text{kPa}) = 6.08324 - 1292.64/(-52.52 + T/K)$; temp range 239–373 K (Antoine eq., Stephenson & Malanowski 1987)
 5410, 8790, 13790 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
 $\log(P/\text{mmHg}) = 5.4819 - 2.1918 \times 10^3/(T/K) + 2.6014 \cdot \log(T/K) - 1.1751 \times 10^{-2} \cdot (T/K) + 7.3435 \times 10^{-6} \cdot (T/K)^2$; temp range 173–572 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 298 (calculated- $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
 31.21, 2261 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
 280* (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)
 $\ln(k_{\text{H}}/\text{atm}) = 19.60 - 4333/(T/K)$; temp range: 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
 210 (calculated-P/C, Mackay & Yuen 1983)
 286 (gas stripping-GC, Warner et al. 1987)
 362* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 9.843 - 4708/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 233 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 150 (computed value, Yaws et al. 1991)
 213, 324, 486 (20, 30, 40°C, infinite dilution activity coeff. γ^∞ -GC, Tse et al. 1992)
 216, 347, 497 (20, 35, 50°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 3.37, 5.93 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 222 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 226.8 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 232 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 4.878 - 1730/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)
 227.6* (EPICS-SPME, measured range 2–70°C, Görgényi et al. 2002)
 $\ln K_{\text{AW}} = 9.49 - 3494.7/(T/K)$; temp range 2–70°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 2.00 (Hansch & Leo 1979)
 1.98 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)
 1.99* (infinite dilution activity coefficient determined by relative GC technique, measured range 25–50°C, Bhatia & Sandler 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.96 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

< 1.0 (fish, Kawasaki 1980; quoted, Howard 1990)

1.29 (calculated- K_{OW} , Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.43 (soil, equilibrium sorption isotherm, Chiou et al. 1979)

1.67 (silt loam soil, quoted from Chiou et al. 1979; Howard 1990)

1.70 (calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} < 50$ min in water from stirring in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975; quoted, Mills et al. 1982);

$t_{1/2} = 8$ min from a stirred solution 1.6 cm deep (Chiou et al. 1980; quoted, Howard 1990);

$t_{1/2} = 1.7$ – 10 d, estimated from an EXAMS model of the fate of 1,2-dichloropropane in a pond, river, and two lakes (Burns 1981; quoted, Howard 1990);

$t_{1/2} = 8.3$ h at 1 m depth of stirred aqueous solution (Lyman et al. 1982; quoted, Howard 1990);

$t_{1/2} \sim 5.5$ h for the removal from a stream of 1 m depth with 1 m/s current, based on laboratory-determined relative transfer coefficients (Cadena et al. 1984; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 65$ – 646 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{O_3}(aq.) \leq 0.004 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C , with a half-life of 100 d at pH 7 (Yao & Haag 1991).

Hydrolysis: $k = 5.0 \times 10^{-6} \text{ h}^{-1}$ at pH 7 to 9 and 25°C with a calculated $t_{1/2} = 15.8$ yr (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biodegradation: aerobic $t_{1/2}(aq.) = 4008$ – 30936 h, based on acclimated aerobic soil grab sample data (Roberts & Stoydin 1976; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2}(aq.) = 16032$ – 123744 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4$ – 24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 65$ – 646 h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

$t_{1/2} > 23$ d, reaction with photochemically produced OH radical (Howard 1990).

Surface water: $t_{1/2} = 4008$ – 30936 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); measured rate constant $k \leq 0.004 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C , with $t_{1/2} \geq 100$ d at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 8016$ – 61872 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 4008$ – 30936 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.1.16.1

Reported aqueous solubilities of 1,2-dichloropropane at various temperatures

$$S/(\text{wt}\%) = 0.1300 + 1.43332 \times 10^{-2} \cdot (t/^{\circ}\text{C}) - 4.99992 \times 10^{-4} \cdot (t/^{\circ}\text{C})^2 + 6.66654 \times 10^{-6} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 3.3285 - 0.021464 \cdot (T/\text{K}) + 3.7632 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

Horvath 1982		Stephenson 1992		Tse et al. 1992		Horvath & Getzen 1999	
summary of literature data		shake flask-GC		activity coefficient		recommended IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	2300	0	2900	20	3005	5	2799
20	2700	9.5	2800	30	3129	10	2680
25	2800	20	3000	40	3261	15	268-
30	2900	29.7	2900			20	2700
		40.3	3000			25	2740
eq.1	S/wt%	49.8	3200	Wright et al. 1992 activity coefficient		30	2800
		60	3500			35	2880
		70.5	3900	t/°C	S/g·m ⁻³	40	2970
		80.2	4700				
		90.4		20	2583	eq. 2	S/wt%
				30	2717	temp range 275–313 K	
				40	3003		

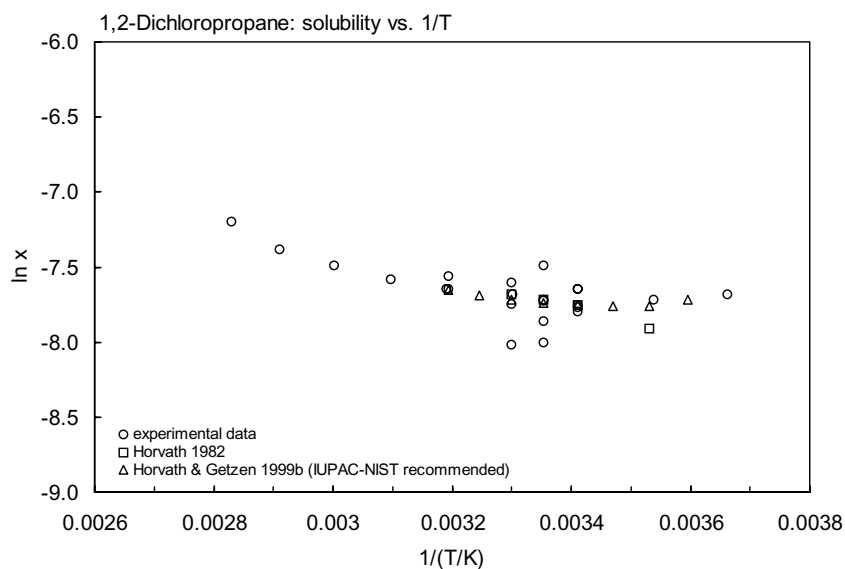


FIGURE 5.1.1.16.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,1,2-trichloroethane.

TABLE 5.1.1.16.2

Reported vapor pressures of 1,2-dichloropropane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & \end{aligned}$$

Nelson & Young 1933		Stull 1947		Dreisbach & Shrader 1949	
static method		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
15.0	4400	-7.0	133.3	44.78	16500
20.0	5600	17.3	666.6	69.0	42066
25.0	7199	29.4	1333	83.18	67661
30.0	8999	42.3	2666	96.2	101325
35.0	11199	57.2	5333		
40.0	13799	66.4	7999		
45.0	16839	75.7	13332		
50.0	20625	97.8	26664		
55.0	24065	118.5	53329		
60.0	30317	141.6	101325		
65.0	36397				
70.0	43570	mp/°C	-34.4		
75.0	51729				
80.0	61235				
85.0	71874				
90.0	84059				
95.0	97792				
96.0	100525				
96.4	101325				
99.7	112937				

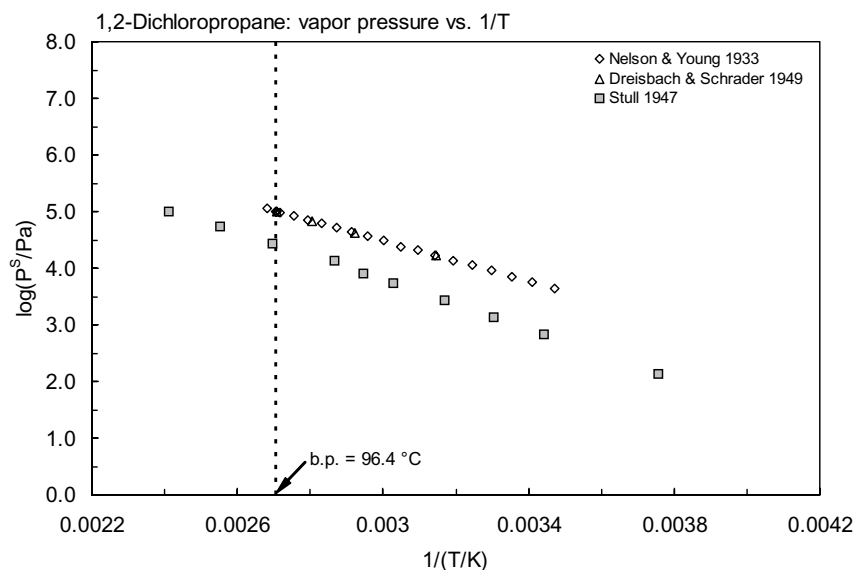


FIGURE 5.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichloropropane.

TABLE 5.1.1.16.3

Reported Henry's law constants of 1,2-dichloropropane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)				
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)				
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)						
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)				
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)						
Leighton & Calo 1981	Ashworth et al. 1988	Tse et al. 1992	Görgényi et al. 2002				
equilibrium cell-GC	EPICS-GC	activity coefficient	EPICS-SPME method				
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
1.90	83.5	10	123.6	20	213	2	82.35
13.5	164.5	15	127.7	30	324	6	109
15.7	185.3	20	192.5	40	486	10	134.2
17.1	239.7	25	361.7			18	203.3
22.0	239.7	30	289.8			25	227.6
24.9	280.0					30	341.8
				Wright et al. 1992			
				activity coefficient		40	524.9
eq. 3	k _H /atm	eq. 4	H/(atm m ³ /mol)	t/°C	H/(Pa m³/mol)	50	759.8
A	19.6	A	9.843			60	1014
B	4333	B	4708			70	1226
				20	216		
				35	347		
				50	497	eq. 1	K _{AW}
						A	9.49
						B	3494.7

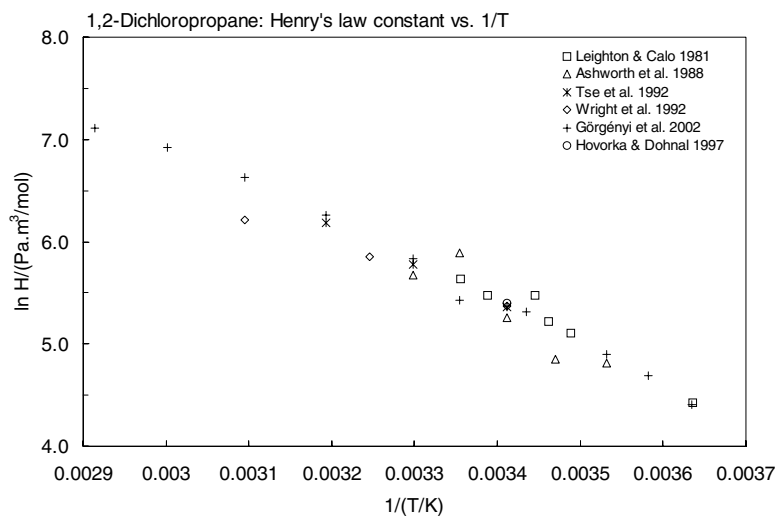


FIGURE 5.1.1.16.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dichloropropane.

TABLE 5.1.1.16.4
Reported octanol-water partition coefficient of
1,2-dichloropropane at various temperatures

Bhatia & Sandler 1995	
relative GC-RT technique	
t/°C	log K _{OW}
25	1.99
35	1.99
50	1.99
enthalpy of transfer	
$\Delta H/(\text{kJ mol}^{-1}) = -20.2$	
$\log K_{OW} = A - \Delta H/2.303RT$	
A	1.0195
ΔH	-20.2

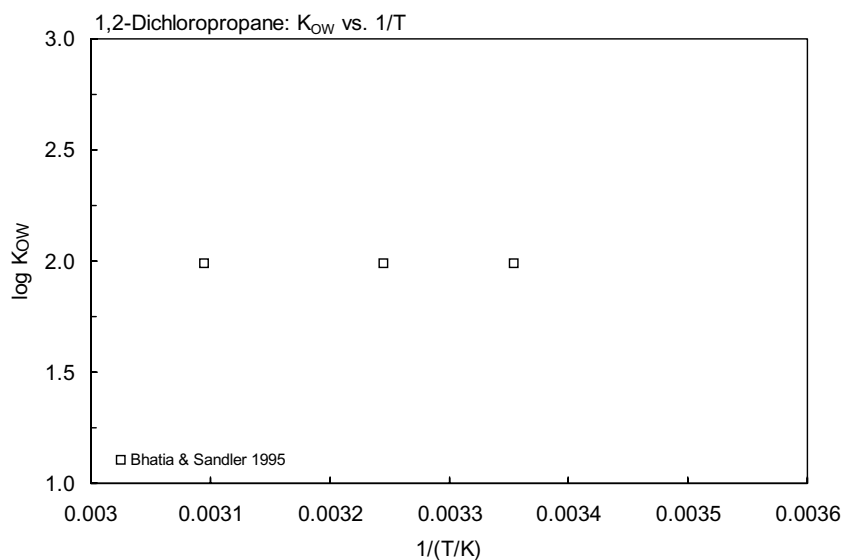
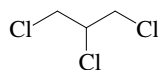


FIGURE 5.1.1.16.4 Logarithm of K_{OW} versus reciprocal temperature for 1,2-dichloropropane.

5.1.1.17 1,2,3-Trichloropropane



Common Name: 1,2,3-Trichloropropane

Synonym:

Chemical Name: 1,2,3-trichloropropane

CAS Registry No: 96-18-4

Molecular Formula: 1,2,3-C₃H₃Cl₃, CH₂ClCHClCH₂Cl

Molecular Weight: 147.431

Melting Point (°C):

-14.7 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

157 (Lide 2003)

Density (g/cm³ at 20°C):

1.3888 (Dreisbach 1961; Horvath 1982; Weast 1982–83)

1.3832 (25°C, Dreisbach 1961; Riddick et al. 1986)

Molar Volume (cm³/mol):

136.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

46.93, 37.12 (25°C, normal bp, Dreisbach 1961; Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

1900 (20°C, literature average, Dilling 1977)

1896 (recommended, Horvath 1982)

1900 (selected, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

492 (extrapolated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.98716 – 1502.3/(209.0 + t/°C); temp range 64–204°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = [–0.2185 × 10714.3/(T/K)] + 8.326893; temp range 9.0–158°C (Antoine eq., Weast 1972–73)

266.6, 533.2 (20°C, 30°C, Verschuereen 1983)

492.0 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.11206 – 1502.3/(–64.15 + T/K); temp range 337–477 K (Antoine eq., Stephenson & Malanowski 1987)

413, 960 (quoted, calculated-solvatochromic parameters. and UNIFAC, Banerjee et al. 1990)

log (P/mmHg) = –3.9501 – 2.4501 × 10³/(T/K) + 6.6887 · log (T/K) – 1.4991 × 10^{–2} · (T/K) + 7.3403 × 10^{–6} · (T/K)²; temp range 258–652 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

32.22 (calculated-C_A/C_w, Dilling 1977)

36.1* (24.9°C, equilibrium cell-concn ratio-GC/FID, measured range 1.9–24.9°C, Leighton & Calo 1981)

ln (k_H/atm) = 14.61 – 3477/(T/K); temp range: 1.9–24.9°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

24.91* (25.6°C, EPICS-GC, tap water, measured range 25.6–45°C, Tancrede & Yanagisawa 1990)

log K_{AW} = 3.351 – 1606/(T/K); temp range 26.5–45°C (EPICS measurements, Tancrede & Yanagisawa 1990)

34.4 (computed value, Yaws et al. 1991)

22.31 (interpolated from Tancrede & Yanagisawa 1990, Tancrede et al. 1992)

23.71 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 22.74 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
 $\log K_{AW} = 3.073 - 1496/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.63 (estimated, Abernethy et al. 1988)
 1.98 (quoted, Van Leeuwen et al. 1992; Verhaar et al. 1992)
 2.25, 2.36 (quoted, calculated-molar volume, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.98; 1.89; 1.92 (Captina silt loam, OC 1.49%, pH 4.97; McLaurin sandy loam, OC 0.66%, pH 4.43, batch equilibrium-sorption isotherm, Walton et al. 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2} = 51$ min from dilute aqueous solution (Dilling 1975)

Evaporation $t_{1/2}(\text{exptl}) = 56.1$ min, $t_{1/2}(\text{calc}) = 18$ min, 44.7 min from water (Dilling 1977)

Photolysis:

Oxidation: photooxidation $t_{1/2} = 61\text{--}613$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $k = 1.8 \times 10^{-6} \text{ h}^{-1}$ at pH 7 to 9 at 25°C with a calculated $t_{1/2} = 44$ yr (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biodegradation: aerobic $t_{1/2}(\text{aq.}) = 4320\text{--}8640$ h, based on acclimated aerobic grab sample test data for 1,3-dichloropropane (Roberts & Stoydin 1976; quoted, Howard et al. 1991); anaerobic $t_{1/2}(\text{aq.}) = 17280\text{--}34560$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 61\text{--}613$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 4320\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 8640\text{--}17280$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: disappearance $t_{1/2} = 2.7$ d was calculated from first-order kinetic for volatilization loss of mixtures in soils (Anderson et al. 1991);

$t_{1/2} = 4320\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.1.17.1
Reported Henry's law constants of 1,2,3-trichloropropane at various temperatures

Leighton & Calo 1981	
equilibrium cell-GC	
t/°C	H/(Pa m ³ /mol)
1.90	21.27
13.5	20.90
15.7	24.71
17.1	25.86
22.0	27.58
24.9	36.13
$\ln (k_H/\text{atm}) = A - B/(T/K)$	
A	14.61
B	3477

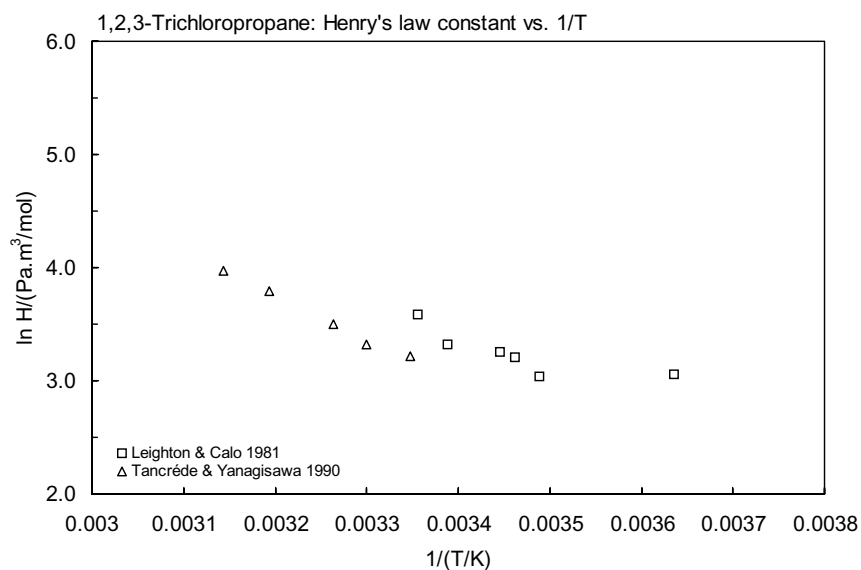
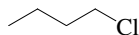


FIGURE 5.1.1.17.1 Logarithm of Henry's law constant versus reciprocal temperature for 1,2,3-trichloropropane.

5.1.1.18 1-Chlorobutane (*n*-Butyl chloride)

Common Name: 1-Chlorobutane

Synonym: *n*-butyl chloride, butyl chlorideChemical Name: 1-chlorobutane, *n*-butyl chloride

CAS Registry No: 109-69-3

Molecular Formula: C_4H_9Cl , $CH_3CH_2CH_2CH_2Cl$

Molecular Weight: 92.567

Melting Point ($^{\circ}C$):

-123.1 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

78.44 (Dreisbach 1959, 1961; Horvath 1982; Dean 1985)

78.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.8862, 0.8808 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959, 1961; Horvath 1982)0.8857, 0.8810 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)Molar Volume (cm^3/mol):

117.1 (calculated-Le Bas method at normal boiling point)

104.5 ($20^{\circ}C$, calculated-density)Enthalpy of Vaporization, ΔH_v (kJ/mol):30.02, 33.32 (normal bp, $25^{\circ}C$, Dreisbach 1961)Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

666 ($12.5^{\circ}C$, shake flask, Fühner 1924)

640 (Seidell 1940)

741 (Kakovsky 1957)

667 ($17.5^{\circ}C$, Saracco & Spaccamela Marchetti 1958)671 ($20^{\circ}C$, exptl., Korenman et al. 1971; Horvath 1982)

614.7* (summary of literature data, Horvath 1982)

872 (generator column-HPLC, Tewari et al. 1982)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4173* ($20^{\circ}C$, static method-manometer, measured range 20 – $70^{\circ}C$, Smyth & Engel 1929)14170* (interpolated compiled data, temp range -49 to $77.8^{\circ}C$, Stull 1947)

13650 (calculated-Antoine eq., Dreisbach 1959)

 $\log(P/\text{mmHg}) = 6.93790 - 1227.43/(224.1 + t/^{\circ}C)$; temp range 0 – $123^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

 $\log(P/\text{mmHg}) = 6.93790 - 1227.433/(224.1 + t/^{\circ}C)$; temp range 1 – $116^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

 $\log(P/\text{mmHg}) = 6.93790 - 1227.433/(224.10 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)
10639* ($19.7^{\circ}C$, differential thermal analysis, measured range -16.7 to $78.5^{\circ}C$, Kemme & Kreps 1969)
 $\log(P/\text{mmHg}) = [-0.2185 \times 8144.8/(T/K)] + 7.979366$; temp range -49 to $77.8^{\circ}C$ (Antoine eq., Weast 1972–73)
14719* ($26.85^{\circ}C$, differential thermal analysis, measured range 26.85 – $80.0^{\circ}C$, Gutsche & Knapp 1982)
 $\log(P/\text{mmHg}) = 6.83694 - 1173.79/(218.13 + t/^{\circ}C)$, temp range: -17 to $78.6^{\circ}C$ (Antoine eq., Dean 1985, 1992)
13300 ($24.47^{\circ}C$, selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.0514 - 1216.82/(222.33 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

13660 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.0628 - 1227.433/(-49.05 + T/\text{K})$; temp range 257–389 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 35.7808 - 2.8632 \times 10^3/(T/\text{K}) - 8.8957 \cdot \log (T/\text{K}) + 5.1598 \times 10^{-11} \cdot (T/\text{K}) + 3.5488 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 150–537 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1970 (exptl- $1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975)

1800, 8600 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1530* (23°C, equilibrium cell-concn ratio-GC/FID, measured range 1–23°C, Leighton & Calo 1981)

$\ln (k_H/\text{atm}) = 18.51 - 3482/(T/\text{K})$; temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

1708 (computed value, Yaws et al. 1991)

1878 (γ^∞ from gas stripping-GC, Li et al. 1993)

1485 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

1384 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.488 - 1388/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.39 (shake flask-GC, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)

2.64 (shake flask, Hansch & Leo 1979; 1987)

2.55 (generator column-GC, DeVoe et al. 1981)

2.55 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)

2.64 (recommended, Sangster 1989, 1993)

2.64 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.72 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 5.1.18.1

Reported aqueous solubilities and Henry's law constants of 1-chlorobutane at various temperatures

$$S/(\text{wt}\%) = 0.07703 - 6.75497 \times 10^{-4} \cdot (t/^\circ\text{C}) - 1.00170 \times 10^{-10} \cdot (t/^\circ\text{C})^2 + 8.50030 \times 10^{-8} \cdot (t/^\circ\text{C})^3 \quad (1)$$

Aqueous solubility		Henry's law constant	
Horvath 1982		Leighton & Calo 1981	
summary of literature data		equilibrium cell-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
0	770.3	1.0	593.7
10	703.6	3.0	684.5
20	642.0	12.4	979.2
25	614.7	12.5	1038
30	590.6	17.9	1265

TABLE 5.1.1.18.1 (Continued)

Aqueous solubility		Henry's law constant	
Horvath 1982		Leighton & Calo 1981	
summary of literature data		equilibrium cell-GC	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)
eq. 1	S/wt%	22.7	1251
		23.0	1530
		ln (k _H /atm) = A – B/(T/K)	
		A	18.51
		B	3482

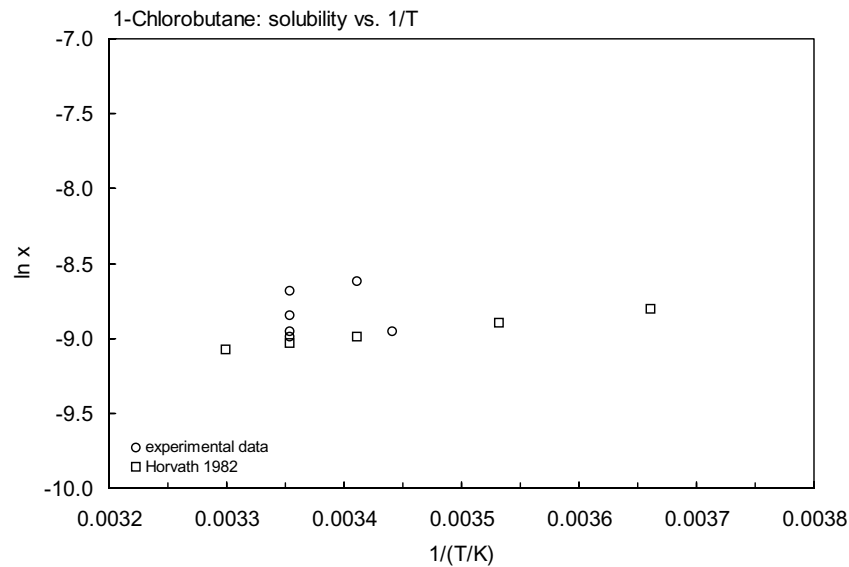


FIGURE 5.1.1.18.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-chlorobutane.

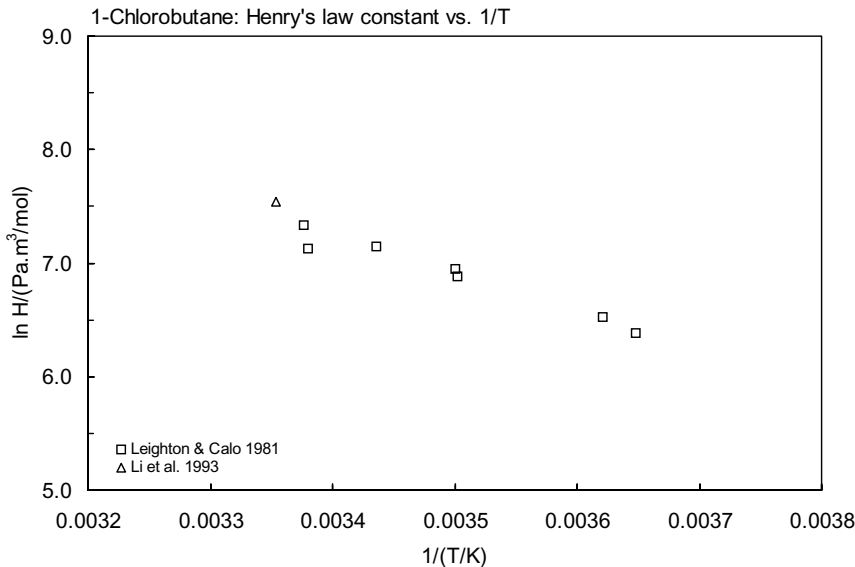


FIGURE 5.1.1.18.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chlorobutane.

TABLE 5.1.1.18.2

Reported vapor pressures of 1-chlorobutane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & \end{aligned}$$

Smyth & Engel 1929		Stull 1947		Kempe & Kreps 1969		Gutsche & Knapp 1982	
static-manometry		summary of literature data		static method-DTA*		Vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20.0	4173	-49.0	133.3	-16.7	1347	26.85	14719
30.0	6799	-28.9	666.6	-10.5	2026	30.0	17001
40.0	10959	-18.6	1333	-6.20	2640	50.0	38434
50.0	16892	-7.40	2666	0.80	3946	51.85	41397
60.0	25278	5.0	5333	6.20	5360	78.85	96925
70.0	36170	13.0	7999	12.0	7306	80.0	106255
		24.0	13332	19.7	10639		
		40.0	26664	28.8	16212		
		55.8	53329	41.1	27078		
		77.8	101325	51.3	40263		
				65.5	66541		
		mp/°C	-123.1	78.5	101165		
				eq. 2	P/mmHg		
				A	6.87098		
				B	1182.903		
				C	218.285		

*DTA—differential thermal analyzer

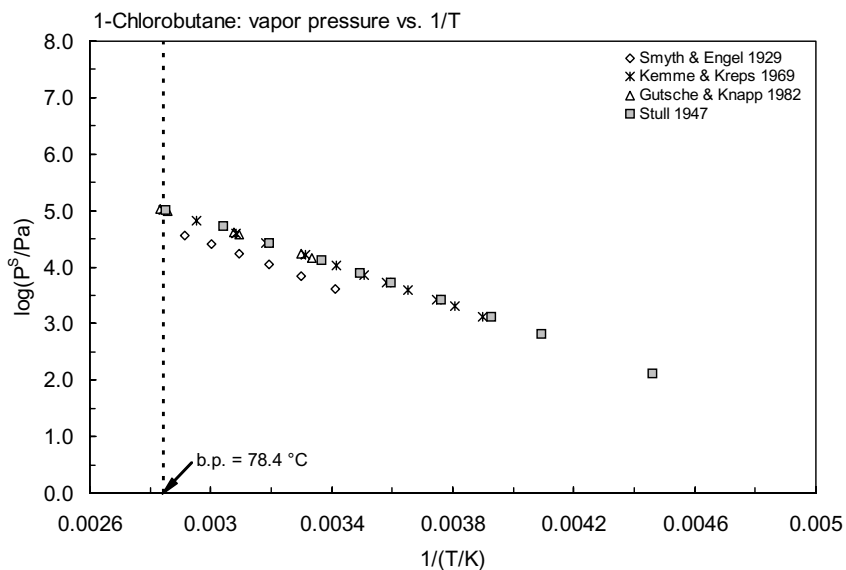


FIGURE 5.1.1.18.3 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorobutane.

5.1.1.19 2-Chlorobutane



Common Name: 2-Chlorobutane

Synonym: methylethylchloromethane, *sec*-butyl chloride

Chemical Name: 2-chlorobutane, methylethylchloromethane, *sec*-butyl chloride

CAS Registry No: 78-86-4

Molecular Formula: C_4H_9Cl , $CH_3CH_2CHClCH_3$

Molecular Weight: 92.567

Melting Point ($^{\circ}C$):

−131.3 (Dreisbach 1961; Horvath 1982; Lide 2003)

−113.3, −140.5 (racemic, active, Riddick et al. 1986)

Boiling Point ($^{\circ}C$):

68.25 (Dreisbach 1961; Horvath 1982; Riddick et al. 1986)

68.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8732, 0.8677 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961; Horvath 1982; Dean 1985)

0.8732 (racemic, Riddick et al. 1986)

Molar Volume (cm^3/mol):

117.1 (calculated-Le Bas method at normal boiling point)

106.0 ($20^{\circ}C$, calculated-density)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.81, 29.20 ($25^{\circ}C$, bp, Dreisbach 1961)

31.56, 29.20 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1000 (volumetric method, Wright & Schaffer 1932)

1000 (Dean 1985; Riddick et al. 1986)

1070, 930, 850, 820, 840, 920 (0, 5, 10, 15, 20, $35^{\circ}C$, tentative values, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

$S/(wt\%) = 8.9653 - 0.061598 \cdot (T/K) + 1.0678 \times 10^{-4} \cdot (T/K)^2$, temp range 273–298 K (equation derived from reported solubility data, Horvath & Getzen 1999)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

20210 (interpolated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 6.94469 - 1195.8/(226.0 + t/^{\circ}C)$; temp range -7 to $104^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 7407.9/(T/K)] + 7.625620$; temp range -60.2 to $68^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = 6.79923 - 1149.12/(224.68 + t/^{\circ}C)$; temp range 0 – $40^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/kPa) = 6.1222 - 1145.2/(234.4 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

20200 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.06958 - 1195.8/(-47.15 + T/K)$; temp range 266–377 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 28.2992 - 2.4355 \times 10^3/(T/K) - 7.359 \cdot \log(T/K) - 1.3048 \times 10^{-11} \cdot (T/K) + 3.0834 \times 10^{-6} \cdot (T/K)^2$; temp range 142–521 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2268* ($24.9^{\circ}C$, equilibrium cell-concn ratio-GC/FID, measured range 1.9 – $24.9^{\circ}C$, Leighton & Calo 1981)

$\ln(k_H/atm) = 22.29 - 4499/(T/K)$; temp range 1.9 – $24.9^{\circ}C$ (equilibrium cell-concn ratio, Leighton & Calo 1981)

1869 (computed value, Yaws et al. 1991)

1886 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.129 - 1829/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.51 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

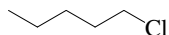
Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radicals (Darnall et al. 1976).

TABLE 5.1.1.19.1
Reported Henry's law constants of 2-chlorobutane at various temperatures

Leighton & Calo 1981

equilibrium cell-GC	
$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
1.90	653.3
13.5	1411
15.7	1545
17.1	1625
22.0	2023
24.9	2268
$\ln (k_H/\text{atm}) = A - B/(T/K)$	
A	22.29
B	4499

5.1.1.20 1-Chloropentane (*n*-Amyl chloride)

Common Name: 1-Chloropentane

Synonym: *n*-amyl chloride, monochloropentane, pentyl chloride

Chemical Name: *n*-amyl chloride, 1-chloropentane, pentyl chloride

CAS Registry No: 543-59-9

Molecular Formula: $C_5H_{11}Cl$, $CH_3CH_2CH_2CH_2CH_2Cl$

Molecular Weight: 106.594

Melting Point ($^{\circ}C$):

−99.0 (Dreisbach 1961; Horvath 1982; Riddick et al. 1982; Dean 1985; Lide 2003)

Boiling Point ($^{\circ}C$):

108.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8818 ($20^{\circ}C$, Weast 198–83; Horvath 1982)

0.8820, 0.8770 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

120.9 ($20^{\circ}C$, calculated-density)

139.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

38.24, 32.77 ($25^{\circ}C$, bp, Dreisbach 1961; Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

200 (volumetric method, Wright & Schaffer 1932)

789 (shake flask-residue volume method, Booth & Everson 1948)

190.6* ($24.3^{\circ}C$, converted-distribution coeff., temp range 2.5 – $26.1^{\circ}C$, Leighton & Calo 1981)

198.2* (summary of literature data, Horvath 1982)

200 (Dean 1985; Riddick et al. 1986)

201* (tentative values, measured range 5 – $35^{\circ}C$, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

$S/(wt\%) = 0.55726 - 3.7269 \times 10^{-3} \cdot (T/K) + 6.457 \times 10^{-6} \cdot (T/K)^2$, temp range 276 – $310\ K$ (equation derived from reported solubility data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4142 (calculated-Antoine eq, Dreisbach 1961)

$\log (P/mmHg) = 6.96617 - 1332.890/(218.5 + t/^{\circ}C)$; temp range 24 – $148^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.96617 - 1332.890/(218.50 + t/^{\circ}C)$; pressure range 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

4142 (selected, Riddick et al. 1986)

$\log (P/kPa) = 5.93641 - 1271.15/(215.0 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

4148 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.09107 - 1332.89/(T/K - 54.65)$; temp range 289 – $409\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = -4.4886 - 2.2604 \times 10^3/(T/K) + 7.8088 \cdot \log (T/K) - 2.3675 \times 10^{-2} \cdot (T/K) + 1.4884 \times 10^{-5} \cdot (T/K)^2$; temp range 174 – $568\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2209 (exptl.- $1/K_{\text{AW}} = C_{\text{W}}/C_{\text{A}}$, Hine & Mookerjee 1975)

2480, 13010 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2376* (24.3°C , equilibrium cell-concn ratio-GC/FID, measured range 2.5 – 26.1°C , Leighton & Calo 1981)

$\ln(k_{\text{H}}/\text{atm}) = 23.04 - 4727/(T/\text{K})$; temp range 2.5 – 26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

4942 (computed value, Yaws et al. 1991)

2407 (activity coefficient γ^∞ from gas stripping-GC, Li et al. 1993)

1835 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 6.455 - 1928/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.41 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4$ – 24 h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 5.1.1.20.1

Reported aqueous solubilities and Henry's law constant of 1-chloropentane at various temperatures

$$S/(\text{wt}\%) = 0.02426 - 1.79166 \times 10^{-4} \cdot (t/^\circ\text{C}) + 1.49999 \times 10^{-7} \cdot (t/^\circ\text{C})^2 - 3.33355 \times 10^{-9} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 0.55726 - 3.7269 \times 10^{-3} \cdot (T/\text{K}) + 6.457 \times 10^{-6} \cdot (T/\text{K})^2 \quad (2)$$

Aqueous solubility						Henry's law constant	
Leighton & Calo 1981		Horvath 1982		Horvath & Getzen 1999b		Leighton & Calo 1981	
converted-distribution coeff.		summary of literature data		summary of literature data		equilibrium cell-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
2.5	200.6	0	242.6	5	202	2.5	661
7.0	205.2	10	224.8	10	197	7.0	846.6
12.9	196.8	20	207.1	15	195	12.9	1246
18.0	195.0	25	198.2	20	196	18.0	1654
19.5	200.5	30	189.3	25	210	19.5	1742
24.3	190.6			30	209	24.3	2376
26.1	203.2	eq. 1	$S/\text{wt}\%$	35	220	26.1	2404
				eq. 2	$S/\text{wt}\%$	$\ln k_{\text{H}}/\text{atm} = A - B/(T/\text{K})$	
				temp range 276–310 K		A	23.04
						B	4727

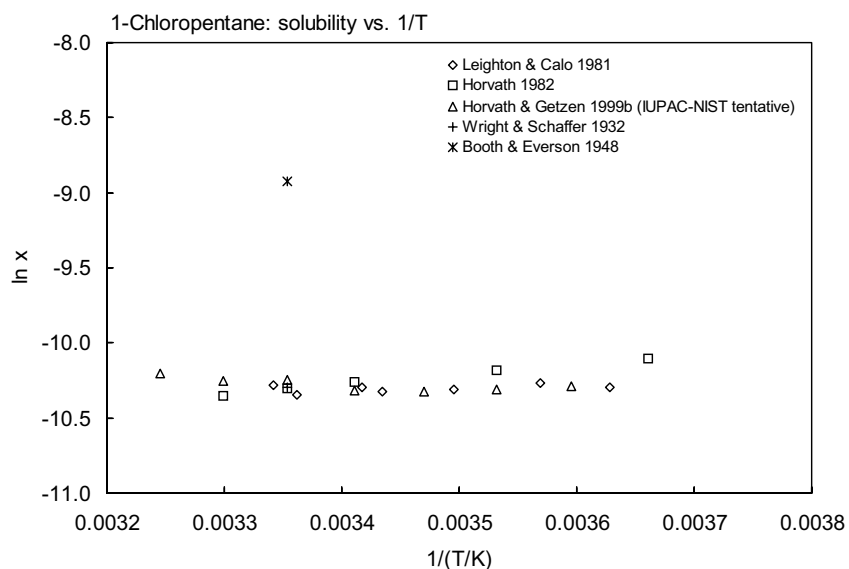


FIGURE 5.1.1.20.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-chloropentane.

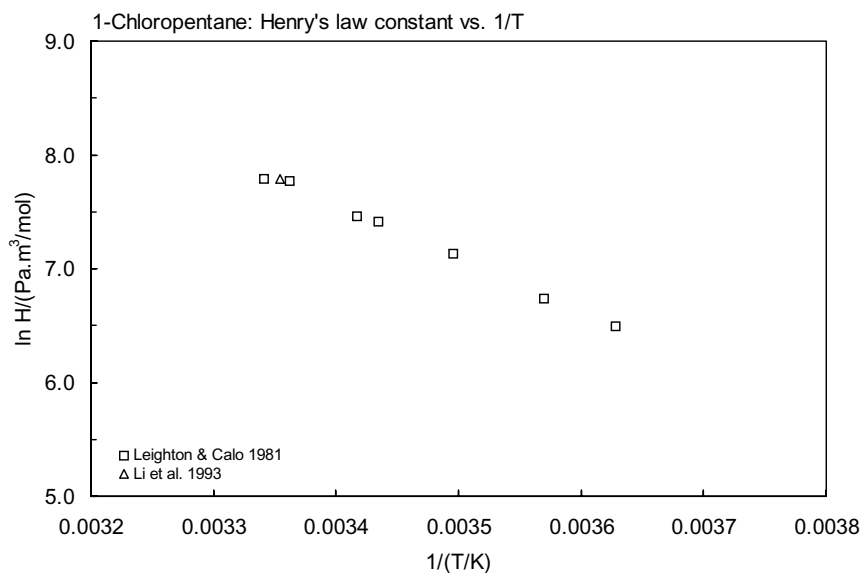
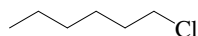


FIGURE 5.1.1.20.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chloropentane.

5.1.1.21 1-Chlorohexane



Common Name: 1-Chlorohexane

Synonym: *n*-hexyl chloride

Chemical Name: 1-chlorohexane

CAS Registry No: 544-10-5

Molecular Formula: C₆H₁₃Cl

Molecular Weight: 120.620

Melting Point (°C):

−94 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

135.1 (Lide 2003)

Density (g/cm³):

0.8785; 0.8739 (20°C, 25°C, Dreisbach 1961)

0.8785 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):

137.7 (20°C, calculated-density, Stephenson & Malanowski 1987)

161.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

43.22, 35.39 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

83.6 (volumetric method, Wright & Schaffer 1932)

57.93* (23.0°C, converted-distribution coeff., temp range 1.0–23.0°C, Leighton & Calo 1981)

91.01* (summary of literature data, Horvath 1982)

54.3* (tentative values, measured range 5–25°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

$S/(\text{wt}\%) = -0.019959 + 8.852 \times 10^{-5} \cdot (T/K)$, temp range 274–296 K (equation derived from reported solubility data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1284 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.0115 - 1437.05/(213.4 + t/^\circ\text{C})$; temp range 46–178°C (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.0115 - 1437.05/(213.4 + t/^\circ\text{C})$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

1387* (26.7°C, differential thermal analysis, measured range 15–135.6°C, Kemme & Kreps 1969)

$\log(P/\text{mmHg}) = 6.76886 - 1304.968/(t/^\circ\text{C} + 200.058)$; temp range 15–135.6°C (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

1230 (interpolated-Antoine eq., Boublik et al. 1973)

$\log(P/\text{mmHg}) = 7.05136 - 1461.72/(t/^\circ\text{C} + 136.92)$; temp range 15–136°C (Antoine eq. based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1973)

1246 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/\text{kPa}) = 5.89376 - 1304.968/(T/K - 73.092)$; temp range: 288–409 K (Antoine eq., Stephenson & Malanowski 1987)

1260 (interpolated-Antoine eq., Dean 1992)

$\log(P/\text{mmHg}) = 7.05136 - 1461.72/(t/^\circ\text{C} + 215.57)$; temp range 15–136°C (Antoine eq., Dean 1992)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2312* (23°C , equilibrium cell-concn ratio-GC/FID, measured range $1\text{--}23^\circ\text{C}$, Leighton & Calo 1981)
 $\ln(k_{\text{H}}/\text{atm}) = 22.16 - 4469/(T/\text{K})$; temp range $1.0\text{--}23.0^\circ\text{C}$ (equilibrium cell-concn ratio, Leighton & Calo 1981)
 1899 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 6.073 - 1812/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.68 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 5.1.1.21.1

Reported aqueous solubilities and Henry's law constant of 1-chlorohexane at various temperatures

$$S/(\text{wt}\%) = 0.01172 - 0.000313(t/^\circ\text{C}) - 1.078 \times 10^{-5} \cdot (t/^\circ\text{C})^2 - 4.58 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = -0.019959 + 8.852 \times 10^{-5} \cdot (T/\text{K}) \quad (2)$$

Aqueous solubility						Henry's law constant	
Leighton & Calo 1981		Horvath 1982		Horvath & Getzen 1999b		Leighton & Calo 1981	
converted-distribution coeff.		summary of literature data		summary of literature data		equilibrium cell-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
1.0	36.87	0	117.2	5	46.7	1.0	728.6
3.0	49.46	10	101.1	10	51.1	3.0	666.6
12.4	56.45	20	97.08	15	55.5	12.4	1219
12.5	52.48	25	91.01	20	59.9	12.5	1328
17.9	61.87	30	77.66	25	64.3	17.9	1593
19.1	59.29			30	209	22.7	2118
22.7	62.37	eq. 1	$S/\text{wt}\%$	35	220	23.0	2312
23.0	57.93			eq. 2	$S/\text{wt}\%$	$\ln k_{\text{H}}/\text{atm} = A - B/(T/\text{K})$	
				temp range 274–296 K		A	22.16
						B	4459

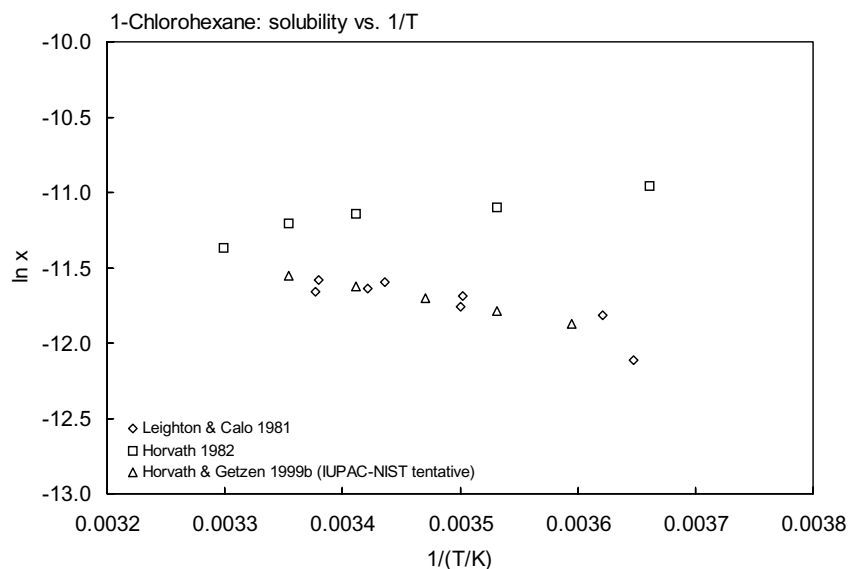


FIGURE 5.1.1.21.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-chlorohexane.

TABLE 5.1.1.21.2

Reported vapor pressures of 1-chlorohexane at various temperatures

Kemme & Kreps 1969

Static method-DTA*

t/°C	P/Pa	t/°C	P/Pa
15.0	667	104.6	40757
26.7	1387	120.3	66781
33.1	2000	135.6	103191
38.6	2680		
46.7	4013	$\log P = A - B/(C + t/^{\circ}\text{C})$ P/mmHg	
52.6	5320		
59.7	7333		
68.4	10639		
79.5	16745		
92.6	27091		

*DTA—differential thermal analyzer

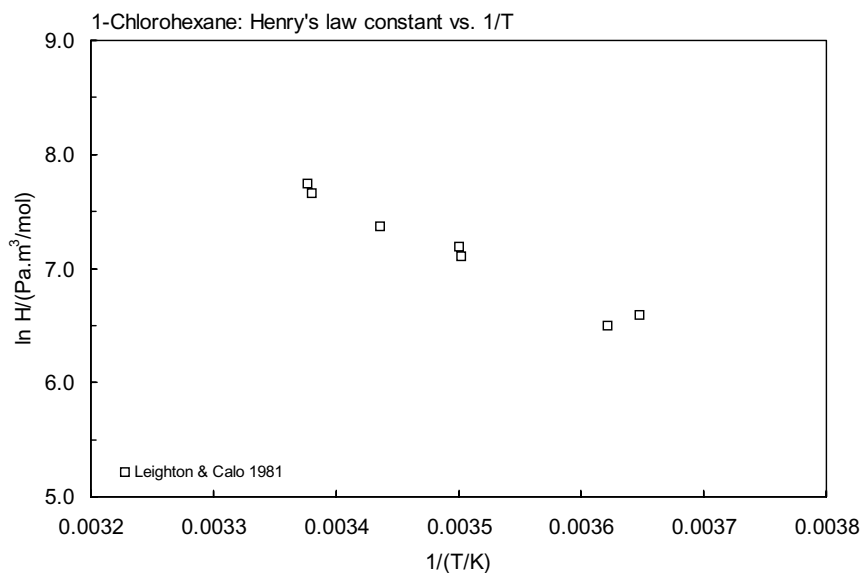


FIGURE 5.1.1.21.2 Logarithm of Henry's law constant versus reciprocal temperature for 1-chlorohexane.

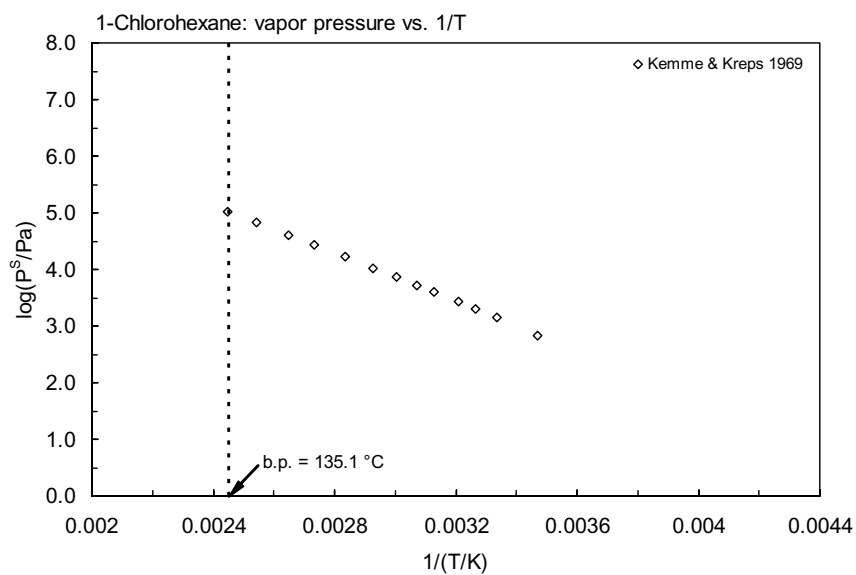
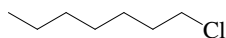


FIGURE 5.1.1.21.3 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorohexane.

5.1.1.22 1-Chloroheptane



Common Name: 1-Chloroheptane

Synonym: heptyl chloride

Chemical Name: 1-chloroheptane

CAS Registry No: 629-06-1

Molecular Formula: $C_7H_{15}Cl$

Molecular Weight: 134.647

Melting Point ($^{\circ}C$):

-69.5 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

160.4 (Lide 2003)

Density (g/cm^3):

0.8758, 0.8715 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

0.8758 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

153.7 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

183.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

48.19, 37.95 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

13.6 (generator column-GC/FID, Tewari et al. 1982; Miller et al. 1985)

13.6 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

404 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.0650 - 1539.35/(208.8 + t/^{\circ}C)$; temp range 67 – $206^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.0650 - 1539.35/(208.8 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

680* ($34.4^{\circ}C$, differential thermal analysis, measured range 34.4 – $160^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 6.83820 - 1410.064/(t/^{\circ}C + 195.639)$; temp range 34.4 – $160.1^{\circ}C$ (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

336.6 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.05057 - 1459.652/(t/^{\circ}C + 160.428)$; temp range 34.4 – $160^{\circ}C$ (Antoine eq. based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log(P_L/kPa) = 6.9631 - 1410.064/(T/K - 77.511)$; temp range 307–434 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 6.91670 - 1453.96/(t/^{\circ}C + 199.83)$; temp range 36 – $160^{\circ}C$ (Antoine eq., Dean 1992)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.08 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 5.1.1.22.1

Reported vapor pressures of 1-chloroheptane at various temperatures

Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
34.4	679.9	127.9	40343
46.6	1400	145.1	66994
53.5	2027	160.1	100445
59.1	2680		
67.5	4013	log P = A – B/(C + t/°C)	
73.6	5306		P/mmHg
81.1	7333	A	6.83820
90.9	10919	B	1410.064
101.1	16212	C	195.639
115.6	27064		

*DTA—differential thermal analyzer

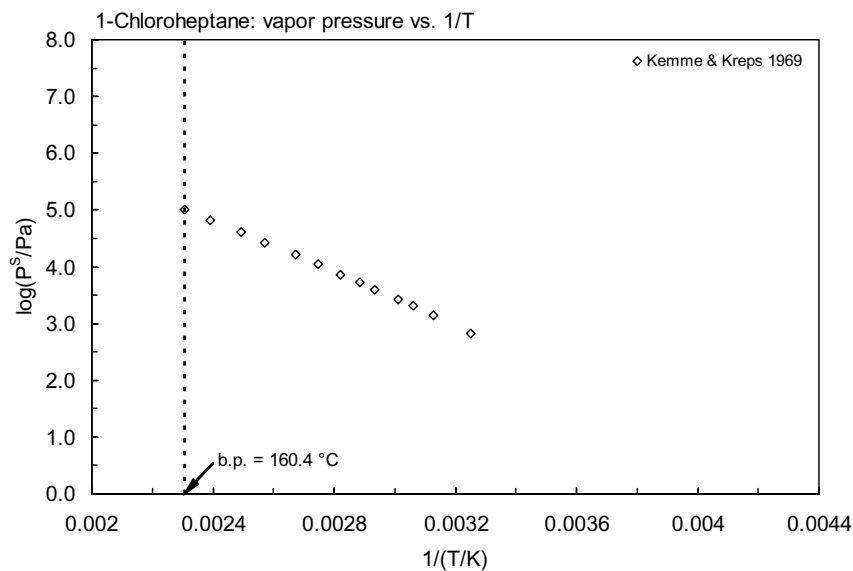
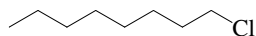


FIGURE 5.1.1.22.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chloroheptane.

5.1.1.23 1-Chlorooctane



Common Name: 1-Chlorooctane

Synonym: octyl chloride

Chemical Name: 1-chlorooctane

CAS Registry No: 111-85-3

Molecular Formula: $C_8H_{17}Cl$

Molecular Weight: 148.674

Melting Point ($^{\circ}C$):

-57.8 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

183.5 (Lide 2003)

Density (g/cm^3):

0.8738, 0.8695 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961; Weast 1982–83)

Molar Volume (cm^3/mol):

170.2 ($15^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

205.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

53.25, 41.09 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

3.67* (generator column-GC, measured range 5 – $40^{\circ}C$, Sarraute et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

127 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.1231 - 1639.2/(204.2 + t/^{\circ}C)$; temp range 86 – $231^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.1231 - 1369.20/(204.4 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

747* ($54.1^{\circ}C$, differential thermal analysis, measured range 54.1 – $184.1^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 6.84310 - 1469.829/(t/^{\circ}C + 187.157)$; temp range 54.1 – $184.1^{\circ}C$ (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

118.2 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.17348 - 1598.257/(t/^{\circ}C + 200.076)$ (Antoine eq. based on exptl. data of Kemme & Kreps 1969, temp range 54 – $184^{\circ}C$, Boublik et al. 1984)

$\log(P_L/kPa) = 5.968 - 1469.829/(T/K - 85.993)$; temp range 327 – $457 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 7.05152 - 1600.24/(t/^{\circ}C + 200.28)$; temp range 64 – $184^{\circ}C$ (Antoine eq., Dean 1992)

126.6* (calculated-Antoine eq. of Li & Rossini 1961, temp range 5 – $40^{\circ}C$, Saraute et al. 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$. Additional data at other temperatures designated * are compiled at the end of this section):

4437* (calculated-P/C, temp range 5 – $40^{\circ}C$, Sarraute et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.48 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 5.1.1.23.1

Reported aqueous solubilities, vapor pressures and Henry's law constants of 1-chlorooctane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Aqueous solubility		Vapor pressure				Henry's law constant	
Sarraute et al. 2004		Kemme & Kreps 1969		Sarraute et al. 2004		Sarraute et al. 2004	
generator column-GC		static method-DTA*		extrapolated -Antoine eq.#		calculated-P/C	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
5.0	3.38	54.1	746.6	5.0	26.30	5.0	925
9.9	3.52	63.9	1307	9.9	39.55	9.9	1365
9.9	3.49	72.4	2040	9.9	39.71	9.9	1365
9.9	3.36	78.2	2706	9.9	39.71	9.9	1435
10.0	3.29	87.1	4040	10.0	40.04	10.0	1460
19.1	3.78	93.4	5346	19.1	81.99	19.1	2721
25.0	3.67	101.1	7359	25.0	126.6	25.0	4437
25.1	3.90	110.7	10732	25.1	127.1	25.1	4215
25.2	3.84	121.8	16159	25.2	128.0	25.2	4291
30.0	4.03	136.7	27798	30.0	179.8	30.0	5847
34.8	4.01	149.8	40210	34.8	248.4	34.8	8103
35.1	4.0	167.4	66795	35.1	252.5	35.1	8406
35.1	4.16	184.1	103085	35.1	252.5	35.1	8073
40.0	4.09			40.0	347.5	40.0	11429
		eq. 2	P/mmHg				
		A	6.84310	Antoine eq.			
		B	1469.829	#see Li & Rossini 1961			
		C	187.157	eq. 2		P/mmHg	
				A		7.1231	
				B		1369.20	
				C		204.4	
pressure range 10–1500 torr mmHg							

*DTA—differential thermal analyzer

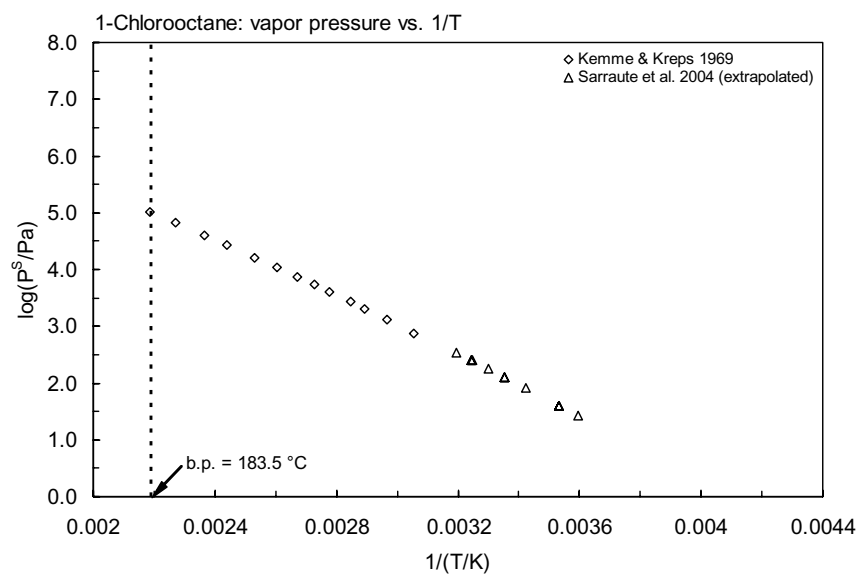
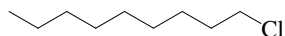


FIGURE 5.1.1.23.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorooctane.

5.1.1.24 1-Chlorononane



Common Name: 1-Chlorononane

Synonym: nonyl chloride

Chemical Name: 1-chlorononane

CAS Registry No: 2473-01-0

Molecular Formula: $C_9H_{19}Cl$

Molecular Weight: 162.700

Melting Point ($^{\circ}C$):

-39.4 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

205.2 (Lide 2003)

Density (g/cm^3):

0.7886 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

206.3 ($20^{\circ}C$, calculated-density)

228.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

58.27, 42.89 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

40.0 (extrapolated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.1802 - 1736.11/(200.4 + t/^{\circ}C)$; temp range $104\text{--}255^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.1802 - 1736.11/(200.4 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

680* ($69.1^{\circ}C$, differential thermal analysis, measured range $69.1\text{--}204.8^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 6.90463 - 1586.937/(t/^{\circ}C + 185.505)$; temp range $69.1\text{--}204.8^{\circ}C$ (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

35.9 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.17172 - 1655.007/(t/^{\circ}C + 205.166)$; temp range $69.1\text{--}204.8^{\circ}C$ (Antoine eq., based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log(P_L/kPa) = 6.09107 - 1332.89/(T/K - 54.65)$; temp range 289–409 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 7.04654 - 1665.57/(t/^{\circ}C + 192.26)$; temp range $69\text{--}205^{\circ}C$ (Antoine eq., Dean 1992)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.88 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 5.1.1.24.1

Reported vapor pressures of 1-chlorononane at various temperatures

Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
69.1	679.9	156.7	26731
70.8	733.3	170.3	40317
80.6	1280	188.6	66901
89.9	2013	204.8	100365
95.4	2613		
104.5	3933	$\log P = A - B/(C + t/^{\circ}\text{C})$	
111.5	5280		P/mmHg
119.8	7333	A	6.94063
129.5	10626	B	1586.937
141.3	16159	C	185.505

*DTA—differential thermal analyzer

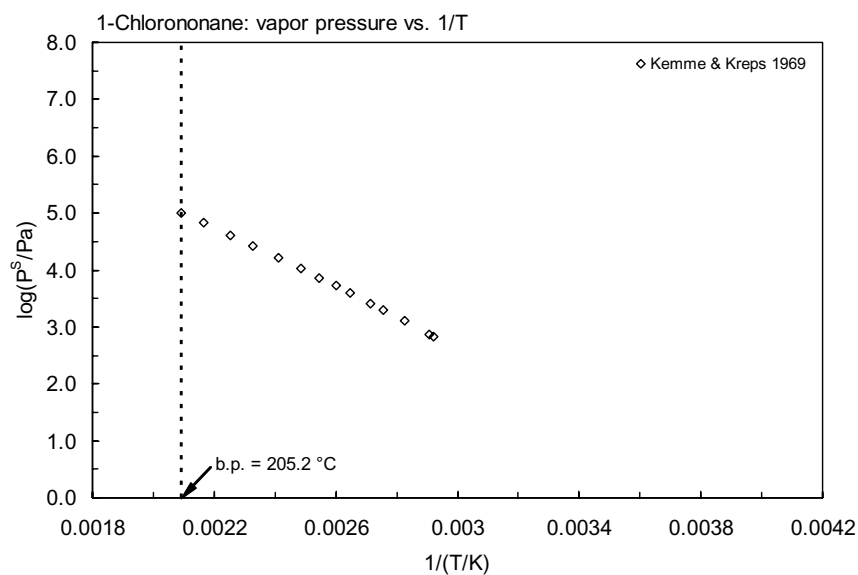
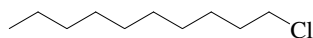


FIGURE 5.1.1.24.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorononane.

5.1.1.25 1-Chlorodecane



Common Name: 1-Chlorodecane

Synonym: decyl chloride

Chemical Name: 1-chlorodecane

CAS Registry No: 1002-69-3

Molecular Formula: $C_{10}H_{21}Cl$

Molecular Weight: 176.727

Melting Point ($^{\circ}C$):

-31.3 (Dreisbach 1961; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

225.9 (Lide 2003)

Density (g/cm^3):

0.8705, 0.8666 (20 $^{\circ}C$, 25 $^{\circ}C$, Dreisbach 1961)

Molar Volume (cm^3/mol):

203.0 (20 $^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

250.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

63.35, 45.2 (25 $^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

13.3 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.2372 - 1829.68/(196.6 + t/^{\circ}C)$; temp range 121–278 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.2372 - 1829.68/(196.6 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

733* (86.2 $^{\circ}C$, differential thermal analysis, measured range 86.2–225.6 $^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 6.99172 - 1676.793/(t/^{\circ}C + 182.017)$; temp range 86.2–225.6 $^{\circ}C$ (Antoine eq. on exptl. data, differential thermal analysis, Kemme & Kreps 1969)

9.85 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.07379 - 1645.521/(t/^{\circ}C + 178.639)$; temp range 86.2–225.6 $^{\circ}C$ (Antoine eq. based on exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log(P_L/kPa) = 6.11662 - 1676.793/(T/K - 91.133)$; temp range 359–499 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 6.93986 - 1639.06/(t/^{\circ}C + 177.04)$; temp range 86–225.9 $^{\circ}C$ (Antoine eq., Dean 1992)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25 $^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.29 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 5.1.1.25.1

Reported vapor pressures of 1-chlorodecane at various temperatures

Kemme & Kreps 1969			
static method-DTA*			
t/°C	P/Pa	t/°C	P/Pa
86.2	733.3	189.5	40183
98.9	1400	208.6	66861
106.2	2000	225.6	100618
112.8	2693		
122.7	4106	$\log P = A - B/(C + t/^{\circ}\text{C})$	
129.2	5346		P/mmHg
137.1	7293	A	6.99172
147.7	10666	B	1676.793
159.3	16065	C	182.017
175.7	26878		

*DTA—differential thermal analyzer

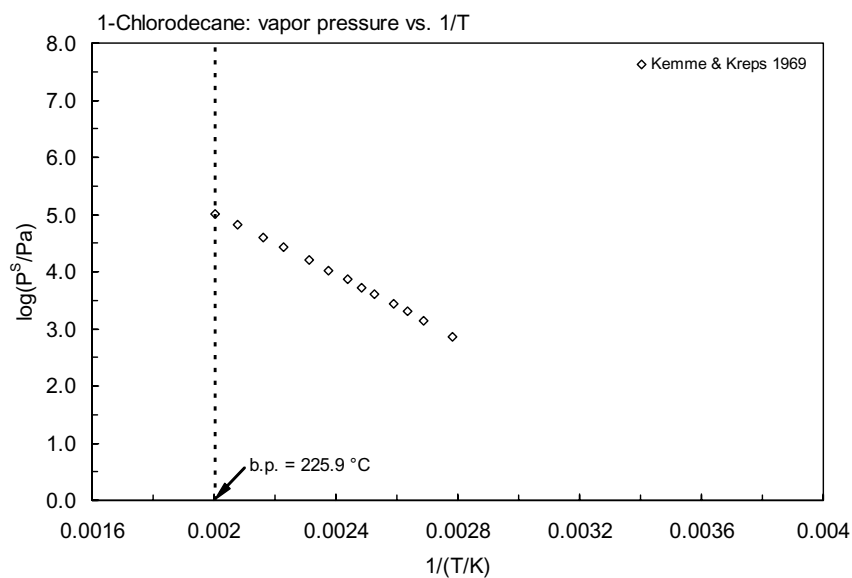


FIGURE 5.1.1.25.1 Logarithm of vapor pressure versus reciprocal temperature for 1-chlorodecane.

5.1.1.26 Chloroethene (Vinyl chloride)



Common Name: Vinyl Chloride

Synonym: chloroethene, chloroethylene, monochloroethylene, monovinylchloride, MVC

Chemical Name: chloroethylene, vinyl chloride, chloroethene

CAS Registry No: 75-01-4

Molecular Formula: C_2H_3Cl , $H_2C = CHCl$

Molecular Weight: 62.498

Melting Point ($^{\circ}C$):

−153.84 (Lide 2003)

Boiling Point ($^{\circ}C$):

−13.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9106 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

68.5 ($20^{\circ}C$, Stephenson & Malanowski 1987)

65.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

18.636, 20.799 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.745 (Dreisbach 1959; quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

8720, 9000 (15, $30^{\circ}C$, shake flask-interferometry, Gross & Saylor 1931)

2700* (continuous solvent flow system at 1 atmospheric pressure, measured range 0.2 – $75^{\circ}C$, Hayduk & Laudie 1974)

60 ($10^{\circ}C$, Pearson & Connell 1975)

60, 2700 (10, $25^{\circ}C$, selected, Dilling 1977)

1100 (Verschuereen 1977, 1983)

6800 ($20^{\circ}C$, selected, Nathan 1978)

8700* (restatement of Hayduk & Laudie 1974, temp range 0.2 – $75^{\circ}C$ at saturated pressure of vinyl chloride, DeLassus & Schmidt 1981)

8800* ($26^{\circ}C$, solubility bomb-headspace GC, measured range 15 – $85^{\circ}C$ at saturated pressure of vinyl chloride, DeLassus & Schmidt 1981)

2763* (recommended, temp range 0 – $175^{\circ}C$, Horvath 1982)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

538000* (Antoine eq. regression, temp range -105.6 to $-13.8^{\circ}C$, Stull 1947)

354600 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.49712 - 783.4/(230.0 + t/^{\circ}C)$, temp range -100 to $50^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

104698* ($-13.00^{\circ}C$, ebulliometry, measured range -64.9 to $-13.00^{\circ}C$, McDonald et al. 1959)

381600 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 6.88054 - 912.5/(242.0 + t/^{\circ}C)$; temp range -73 to $46^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 6.86108 - 892.757/(238.099 + t/^{\circ}C)$; temp range -64.9 to $13.0^{\circ}C$ (Antoine eq. from ebulliometric measurements, McDonald et al. 1959)

- 172719* (0°C, temp range -59.4 to 0°C, Huccura & Mathieu 1967)
 546800 (calculated-Antoine eq., Weast 1972-73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 6263.0/(T/K)] + 8.202782$; temp range -105.1 to -13.8°C (Antoine eq., Weast 1972-73)
 392800 (calculated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 6.89117 - 905.008/(239.475 + t/^\circ\text{C})$; temp range -64.9 to -13.0°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 309300 (Pearson & McConnell 1975)
 $\log (P/\text{mmHg}) = 6.89117 - 905.01/(239.48 + t/^\circ\text{C})$; temp range -657 to -13°C (Antoine eq., Dean 1985, 1992)
 $\log (P/\text{kPa}) = 5.98598 - 892.757/(238.099 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 387000 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.98598 - 892.757/(-35.051 + T/K)$; temp range 208-260 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.20198 - 556.26/(-85.385 + T/K)$; temp range 259-328 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 52.9654 - 2.5016 \times 10^3/(T/K) - 17.914 \cdot \log (T/K) + 1.0821 \times 10^{-2} \cdot (T/K) - 4.531 \times 10^{-14} \cdot (T/K)^2$; temp range 119-432 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 5680 (exptl.-1/K_{AW} = C_w/C_A, Hine & Mookerjee 1975)
 4723 (calculated-bond contribution method, Hine & Mookerjee 1975)
 117705 (10°C, Pearson & McConnell 1975)
 39660 (calculated-P/C, Neely 1976)
 106590 (calculated-P/C, Dilling 1977)
 2350 (calculated-P/C, Mackay & Shiu 1981)
 2817* (24.8°C, EPICS-GC/FID, measured range 10.3-34.6°C, Gossett 1987)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 7.385 - 3286/(T/K)$; temp range 10.3-34.6°C (EPICS measurements, Gossett 1987)
 2685* (EPICS-GC/FID, measured range 10-30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 6.138 - 2931/(T/K)$; temp range 10-30°C (EPICS measurements, Ashworth et al. 1988)
 2271 (computed value, Yaws et al. 1991)
 2172 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 4.119 - 1223/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.39 (calculated- π substituent const., Hansch et al. 1968)
 0.60 (Callahan et al. 1979; Mills et al. 1982)
 1.23 (calculated-fragment const., Mabey et al. 1982)
 2.79 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 0.845 (estimated-S, Lyman et al. 1982)
 0.756 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
 3.04, 1.60, < 1.0 (activated sludge, *Chlorella fusca*, golden ide, Freitag et al. 1984)
 0.068 (from USEPA 86, Yeh & Kastenbergs 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.9138 (sediment-water, calculated-K_{OW}, Mabey et al. 1982)
 1.748 (estimated-S, Lyman et al. 1982)
 0.477 (soil, selected, Jury et al. 1990)
 1.756 (quoted from USEPA 1986, Yeh & Kastenbergs 1991)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 25$ min from water, by rapidly stirring aqueous solutions in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

$t_{1/2}(\text{exptl}) = 27.6$ min, $t_{1/2}(\text{calc}) = 0.0054$ min, 16.1 min from water at 10°C (Dilling 1977)

$t_{1/2} \sim 0.805$ h for volatilization from a river of 1-m deep with a current of 3 m/s and wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989);

estimated $t_{1/2} \sim 2.5$ h from water (Thomas 1982);

volatilization $t_{1/2} = 0.2$ to 0.5 d from soil at 1 and 10 cm incorporation (Jury et al. 1984);

$t_{1/2} = 30$ d, estimated volatilization from soil (Jury et al. 1990).

Photolysis: degrade rapidly in air by reaction with photochemically produced hydroxyl radicals with an estimated $t_{1/2} = 1.5$ d (Perry et al. 1977; quoted, Howard 1989).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 26°C (Perry et al. 1977)

photooxidation $t_{1/2}$ was reported to be a few hours in the troposphere (Callahan et al. 1979)

$k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979, 1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{\text{O}_3} = 6.5 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Sanhueza et al. 1976; quoted, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.3 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Gay et al. 1976; quoted, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979, 1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 1.8 d, loss of 42.6% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}}(\text{calc}) = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{O}_3} = 1.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k < 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $3.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k_{\text{O}_3} = (2.45 \pm 0.45) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Zhang et al. 1983; quoted, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Tuazon et al. 1984)

$k_{\text{NO}_3} = (1.4 \pm 0.9) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 1 K (Andersson & Ljungström 1989)

photooxidation $t_{1/2} = 9.7\text{--}97$ h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k_{\text{OH}}(\text{calc}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{\text{NO}_3} = (2.3 \pm 1.1) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative to ethene at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)

$k_{\text{NO}_3} = 2.30 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculate atmospheric lifetime $\tau = 42$ d, and $k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 3.5$ d and $k_{\text{O}_3} = 2.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 66$ d at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = (3.30 \pm 1.66) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 1 K (quoted from Anderson & Ljungström 1989, Atkinson 1991)

$k_{\text{NO}_3} = 4.45 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sabljic & Güsten 1990)

$k_{\text{NO}_3} = 4.3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 5.25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (as per Atkinson 1987 and 1988, Müller & Klein 1991)

Hydrolysis: $t_{1/2} < 10$ yr (Callahan et al. 1979);

estimated acid-catalyzed rate constant of $3.30 \times 10^{-12} \text{ mol}^{-1} \text{ s}^{-1}$ at pH 5 with calculated $t_{1/2} = 2 \times 10^{11}$ d (Wolfe 1980; quoted, Ma et al. 1990)

abiotic hydrolysis or dehydrohalogenation $t_{1/2} < 120$ months (Olsen & Davis 1990).

Biodegradation: abiotic degradation rate constant of $k = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 26°C determined in laboratory experiments for the vapor phase reaction with hydroxyl radicals (Perry et al. 1977; quoted, Howard 1989)

$t_{1/2}(\text{aq. aerobic}) = 672\text{--}4320$ h, based on aqueous screening test data (Freitag et al. 1984; Helfgott et al. 1977; quoted, Howard et al. 1991)

greater than 99% degraded after 108 d under aerobic conditions and approximately 65% being mineralized to $^{14}\text{CO}_2$ under aerobic conditions (Davis & Carpenter 1990);

$t_{1/2}(\text{aq. anaerobic}) = 2688\text{--}17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} > 60$ d (Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 28$ d, $t_{1/2}(\text{anaerobic}) = 110$ d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 11$ wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 0.24\text{--}2.4$ h from air for the reaction with OH radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 4.3$ h with NO under simulated atmospheric conditions (Dilling et al. 1976);
estimated $t_{1/2} = 1.5$ d, based on its photochemical reaction with OH radical in air (Perry et al. 1977; quoted, Howard 1989);

residence time of 1.8 d, loss of 42.6% in 1 d or 12 sunlit hours at 300 K in urban environments estimated as toxic chemical for the reaction with OH radical (Singh et al. 1981)

$t_{1/2} = 9.7\text{--}97$ h, based on measured rate for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetimes $\tau = 42$ d for the reaction with NO_3 radical for a 12-h nighttime, average concn. of 2.4×10^9 molecule/ cm^3 , $\tau = 3.5$ d for the reaction with OH radical for a 12-h average concn. of 1.0×10^6 molecule/ cm^3 , and $\tau = 66$ d for the reaction with O_3 for a 24-h, average concn. of 7×10^{11} molecule/ cm^3 (Atkinson et al. 1987).

Surface water: estimated $t_{1/2} = 0.805$ h for volatilization from a river of 1 m deep with a current of 3 m/s and a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} = 672\text{--}4320$ h, based on aqueous screening test data (Freitag et al. 1984; Helfgott et al. 1977; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}69000$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and an estimated half-life for anaerobic biodegradation from a ground water field study of chlorinated ethenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} < 10$ d (Ryan et al. 1988);

$t_{1/2} = 0.2$ to 0.5 d for volatilization from soil at 1 and 10 cm incorporation (Jury et al. 1984; quoted, Howard 1989);

$t_{1/2} = 30$ d, estimated volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 30\text{--}180$ d (Howard et al. 1991; quoted, Jury et al. 1992);

$t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} < 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988; quoted, Jury et al. 1992).

TABLE 5.1.1.26.1
Reported aqueous solubilities of chloroethene (vinyl chloride) at various temperatures

Hayduk & Laudie 1974		DeLassus & Schmidt 1981		DeLassus & Schmidt 1981		Horvath 1982	
compressibility apparatus		“restatement” data#		solubility bomb-GC/FID		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
at 1.0 atm							
0.2	7537	0.2	9000	15	9500	0	5460.
25	2700	25	8700	16	9950	25	2764
50	1278	50	10100	20.5	9150	50	1421
75	507	75	12800	26	8800	75	780
at 1.36 atm				29.5	8900	100	538
0.2	8438	# “restatement” data		35	9400	150	337
at 3.06 atm		from Hayduk & Laudie 1974		41	8900	175	320
25	7153			46.5	8800		
50	3993			55	9500		
75	2125			65	9200		
at 6.12 atm				72.5	9800		
50	7674			80	10000		
75	4965			85	11200		
ΔH _{sol} /(kJ mol ⁻¹)							
25°C							

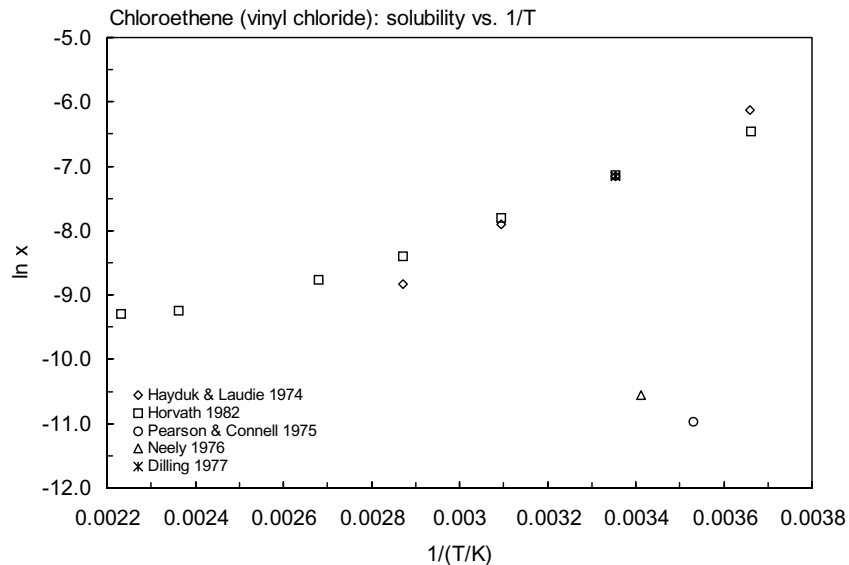


FIGURE 5.1.1.26.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for chloroethene.

TABLE 5.1.1.26.2

Reported vapor pressures of chloroethene (vinyl chloride) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot (T/K) + D \cdot (T/K)^2$	(5)		

Stull 1947		Huccura & Mathieu 1967		McDonald et al. 1959	
summary of literature data				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-103.6	133.3	-59.4	9870	-64.9	6769
-90.8	666.6	-54.3	13566	-56.4	12147
-83.7	1333	-49.4	18032	-43.37	25114
-75.7	2666	-44.5	23713	-29.09	51852
-66.8	5333	-39.5	31881	-14.83	97132
-61.1	7999	-34.5	39695	-13.64	102045
-53.2	13332	-29.65	50510	-13.00	104698
-41.3	26664	-24.9	63349		
-28.0	53329	-20.1	78440		
-13.8	101325	0.0	172719		
mp/°C	-153.7				

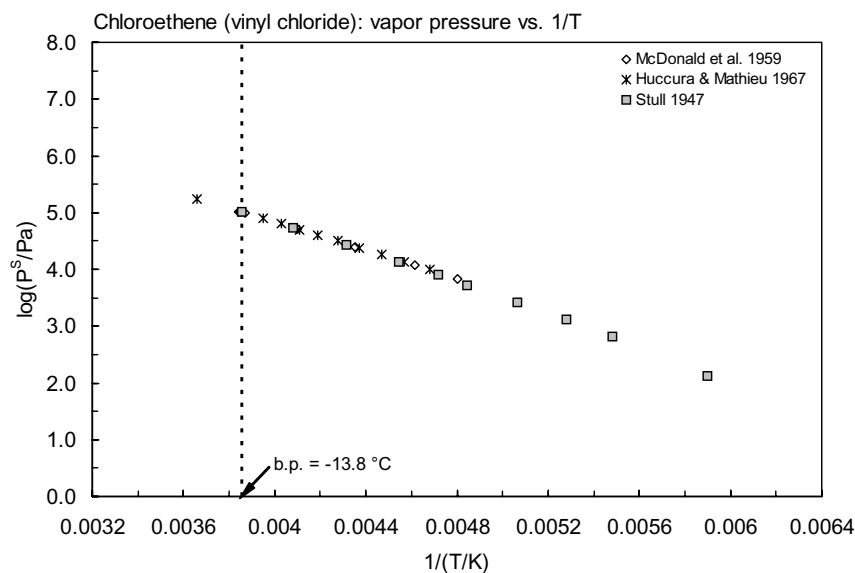


FIGURE 5.1.1.26.2 Logarithm of vapor pressure versus reciprocal temperature for chloroethene.

TABLE 5.1.1.26.3
Reported Henry's law constants of chloroethene (vinyl chloride) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/atm) = A - B/(T/K)$		(3)			
$\ln [H/(Pa \cdot m^3/mol)] = A - B/(T/K)$		(4)	$\ln [H/(atm \cdot m^3/mol)] = A - B/(T/K)$		(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
Hayduk & Laudie 1974		Gossett 1987	Ashworth et al. 1988		
compressibility measurement		EPICS-GC	EPICS-GC		
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
at 1 atm					
0.2	834	10.3	1489	10	1520
25	2342	17.5	1956	15	1702
50	4348	24.8	2819	20	2199
75	7751	34.6	3627	25	2685
at 1.36 atm					
0.2	1018	eq. 4a	H/(atm m³/mol)	30	3850
at 3.06 atm					
		A	7.385	eq. 4a	H/(atm m³/mol)
25	2685	B	3286	A	6.138
50	4669			B	2931
75	7988				

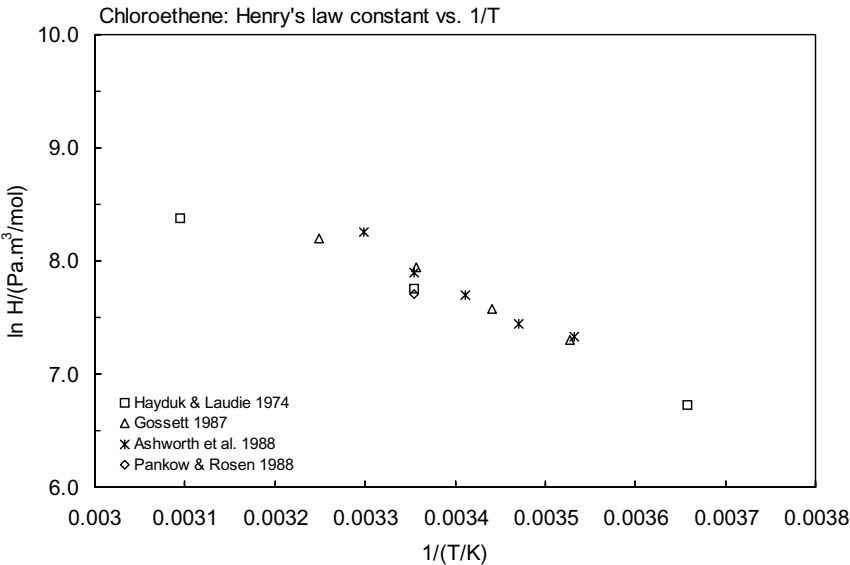


FIGURE 5.1.1.26.3 Logarithm of Henry's law constant versus reciprocal temperature for chloroethene.

5.1.1.27 1,1-Dichloroethene



Common Name: 1,1-Dichloroethene

Synonym: 1,1-dichloroethylene, vinylidene chloride, vinylidine chloride, 1,1-DCE

Chemical Name: 1,1-dichloroethene, 1,1-dichloroethylene

CAS Registry No: 75-35-4

Molecular Formula: $C_2H_2Cl_2$, $CH_2 = CCl_2$

Molecular Weight: 96.943

Melting Point ($^{\circ}C$):

-122.56 (Lide 2003)

Boiling Point ($^{\circ}C$):

31.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2180 (Horvath 1982; Weast 1982-83; Verschuereen 1983)

1.2132 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

79.9 ($20^{\circ}C$, calculated-density)

86.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

26.49, 28.18 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.514 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

400 ($20^{\circ}C$, shake flask-GC, McConnell et al. 1975; Pearson & McConnell 1975)

400 ($20^{\circ}C$, literature average, Dilling 1977)

2250* (solubility bomb-headspace GC, measured range $15-90.5^{\circ}C$, DeLassus & Schmidt 1981)

210* (summary of literature data, Horvath 1982)

2640, 3675 ($20^{\circ}C$, $30^{\circ}C$, saturation concn., Verschuereen 1983)

2232 ($30^{\circ}C$, headspace-GC, McNally & Grob 1984)

210 (Dean 1985; Riddick et al. 1986)

2843, 2790, 2782 (20 , 30 , $40^{\circ}C$, infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)

2420* (recommended, temp range $0-90^{\circ}C$, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 6.27413 - 3.8257 \times 10^{-2} \cdot (T/K) + 6.04607 \times 10^{-5} \cdot (T/K)^2$, temp range $288-363 K$ (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

86430* (Antoine eq. regression, temp range -77.2 to $31.7^{\circ}C$, Stull 1947)

97241* ($30.39^{\circ}C$, ebulliometry, measured range -28.36 to $32.50^{\circ}C$, Hildebrand et al. 1959)

84500 (calculated-Antoine eq., Weast 1972-73)

$\log (P/mmHg) = [-0.2185 \times 7211.8/(T/K)] + 8.087140$; temp range -77.2 to $31.7^{\circ}C$ (Antoine eq., Weast 1972-73)

80040 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 6.97215 - 1099.446/(237.184 + t/^{\circ}C)$; temp range -28 to $32.5^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

79710 (literature average, Dilling 1977)

78780 (Verschuereen 1977, 1983)

- 80040 (interpolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.09904 - 1100.431/(237.274 + t/^{\circ}\text{C})$; temp range -28 to 32.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = 6.9722 - 1099.4/(237.2 + t/^{\circ}\text{C})$; temp range -28 to 32°C (Antoine eq., Dean 1985, 1992)
 79860 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.10690 - 1104.29/(237.697 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 80060 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.10046 - 1100.67/(-35.9 + T/\text{K})$; temp range 244 – 306 K (Antoine eq., Stephenson & Malanowski 1987)
 66190, 95740, 134520 (20 , 30 , 40°C , quoted from DIPPR, Tse et al. 1992)
 $\log(P/\text{mmHg}) = -16.5419 - 1.6655 \times 10^3/(T/\text{K}) + 13.923 \cdot \log(T/\text{K}) - 4.0958 \times 10^{-2} \cdot (T/\text{K}) + 2.9995 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 151 – 482 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 3729 (20°C , batch stripping, Mackay et al. 1979)
 3127* (24.3°C , equilibrium cell-concn ratio, measured range 2.5 – 26.1°C , Leighton & Calo 1981)
 $\ln(k_H/\text{atm}) = 23.12 - 4618/(T/\text{K})$; temp range 2.5 – 26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
 2649 (20°C , EPICS-GC, Linoff & Gossett 1983; Gossett 1985)
 2645 (24.8°C , EPICS-GC, measured range 10 – 34.6°C , Gossett 1987)
 $\ln[H/(\text{atm m}^3/\text{mol})] = 8.845 - 3729/(T/\text{K})$; temp range 10.0 – 34.6°C (EPICS measurements, Gossett 1987)
 1520 (gas stripping-GC, Warner et al. 1987)
 7529 (20°C , EPICS-GC, Yurteri et al. 1987)
 2624* (EPICS-GC/FID, measured range 10 – 30°C , Ashworth et al. 1988)
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 6.123 - 2907/(T/\text{K})$; temp range 10 – 30°C (EPICS measurements, Ashworth et al. 1988)
 19249 (20 – 25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 2316 (computed value, Yaws et al. 1991)
 2320, 3415, 4813 (20 , 30 , 40°C , infinite dilution activity coeff. γ -GC, Tse et al. 1992)
 2376 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 5.397 - 1586/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.13 (shake flask, Log P Database, Hansch & Leo 1987)
 2.13 (recommended, Sangster 1993)
 2.13 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

- 1.72 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.176 (calculated- K_{OW} , Kenaga & Goring 1980)
 1.813 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2}(\text{exptl}) \sim 22$ min at 25°C for volatilization of 1 mg/L in water in an open container of 65 -mm in depth stirring at 200 rpm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)
 Evaporation $t_{1/2}(\text{exptl}) = 27.2$ min, $t_{1/2}(\text{calc}) = 0.029$ min, 20.1 min from water (Dilling 1977)
 $t_{1/2}(\text{calc}) = 5.9, 1.2$, and 4.7 d from a pond, river, and lake, respectively, using data for the oxygen reaeration rate of typical bodies of water (Mill et al. 1982; quoted, Howard 1989).

Photolysis:

- Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = (3.7 \pm 1.0) \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Hull et al. 1973; quoted, Atkinson & Carter 1984)
 Photooxidation $t_{1/2} \sim 50$ min reaction with NO_2 under UV irradiation (Gay, Jr. et al. 1976)
 $k < 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $3.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)
 $k_{OH} \sim 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 2.9 d, loss of 29.2% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)
 $k \sim 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1.5 mM *t*-BuOH as scavenger at pH 2 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)
 $k_{O_3} = 3.7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Tuazon et al. 1984)
 $k_{OH} = (14.9 \pm 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to *n*-butane at $22.3 \pm 1.2^\circ\text{C}$ with a lifetime of 0.75 d and $k_{OH} = 15.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to *n*-pentane at $24.4 \pm 0.4^\circ\text{C}$ (relative rate method, Edney et al 1986)
 photooxidation $t_{1/2} = 11$ h in relatively clean air or under 2 h in polluted air (Howard 1989)
 photooxidation $t_{1/2} = 9.9\text{--}98.7$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Goodman et al. 1986; quoted, Howard et al. 1991)
 $k_{NO_3} = (6.60 \pm 3.10) \times 10^{-16} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ relative to ethene at 298 ± 2 K (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)
 $k_{NO_3} = 6.6 \times 10^{-16} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime of 15 d, $k_{OH} = 8.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 3.4 d and $k_{O_3} = 3.7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 12 yr at room temp. (Atkinson et al. 1987; quoted, Sabljic & Güsten 1990)
 $k_{OH}(\text{calc}) = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 8.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
 $k_{NO_3} = 1.28 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)
 $k_{NO_3} = 1.23 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (Atkinson 1991)
 $k_{OH}(\text{calc}) = 2.04 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (as per Atkinson 1987 and 1988, Müller & Klein 1991)
 $k_{OH}(\text{calc}) = 2.67 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 10.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

Hydrolysis: estimated acid-catalyzed rate constant $k = 1.4 \times 10^{-13} \text{ mol}^{-1} \text{ s}^{-1}$ at pH 5 with $t_{1/2}(\text{calc}) = 6 \times 10^{12}$ d at pH 5 (Wolfe 1980);

estimated $t_{1/2} \sim 2.0$ yr at pH 7.0 (Schmidt-Bleek et al. 1982; quoted, Howard 1989);

$t_{1/2} = 6\text{--}9$ months has been observed with no significant difference in hydrolysis rate between pH 4.5 and 8.5 (Cline & Delfino 1987; quoted, Howard 1989);

abiotic hydrolysis or dehydrohalogenation half-life of 12 months (Olsen & Davis 1990).

Biodegradation: aerobic $t_{1/2}(\text{aq.}) = 672\text{--}4320$ h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); anaerobic $t_{1/2}(\text{aq.}) = 1944\text{--}4152$ h, based on anaerobic sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard 1989; Olsen & Davis 1990; Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 8.0$ wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 0.24\text{--}2.4$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

photodecomposition $t_{1/2} = 2.1$ h with NO under simulated atmospheric conditions (Dilling et al. 1976);

residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

photooxidation $t_{1/2} = 11$ h in relatively clean air (Edney et al. 1983; quoted, Howard 1989) or under 2 h in polluted air (Gay et al. 1976; quoted, Howard 1989);

lifetime of 0.75 d, based on measured rate data for the vapor phase reaction with OH radical in air at $(22.3 \pm 1.2)^\circ\text{C}$ (Edney et al. 1986);

$t_{1/2} = 9.9\text{--}98.7$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Goodman et al. 1986; quoted, Howard et al. 1991);

atmospheric lifetimes: 15 d for the reaction with NO_3 radical for a 12-h nighttime average concn. of $2.4 \times 10^9 \text{ molecule cm}^{-3}$, 3.4 d for the reaction with OH radical for a 12-h average concentration

of 1.0×10^6 molecule cm^{-3} , and 12 yr for the reaction with O_3 for a 24-h average concentration of 7×10^{11} molecule cm^{-3} at room temp. (Atkinson et al. 1987).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}3168$ h, based on estimated aqueous aerobic biodegradation half-life and anaerobic grab sample data for soil from ground water aquifer receiving landfill leachate (Wilson et al. 1986; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on acclimated aerobic soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2} < 10$ d (Ryan et al. 1988).

Biota: $t_{1/2} < 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.27.1

Reported aqueous solubilities of 1,1-dichloroethene at various temperatures

DeLassus & Schmidt 1981		Horvath 1982		Tse et al. 1992		Horvath & Getzen 1999a	
solubility bomb-GC/FID		summary of literature data		activity coefficient γ^∞ -GC		recommended, IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	2400	20	300	20	2843	5	3100
17	2550	25	350	30	2790	10	2890
20.5	2500			40	2782	15	2700
25	2250					20	2550
28.5	2400					25	2420
29.5	2550					30	2330
38.5	2200					35	2260
45	2100					40	2230
51	2300					45	2220
55	2100					50	2250
60	2400					55	2300
65	2250					60	2390
71	2950					65	2510
74.5	2500					70	2650
81	2950					75	2830
85.5	3700					80	3040
90.5	3500					85	3280
						90	3550
						eq. 1	S/wt%
						temp range 288–363 K	

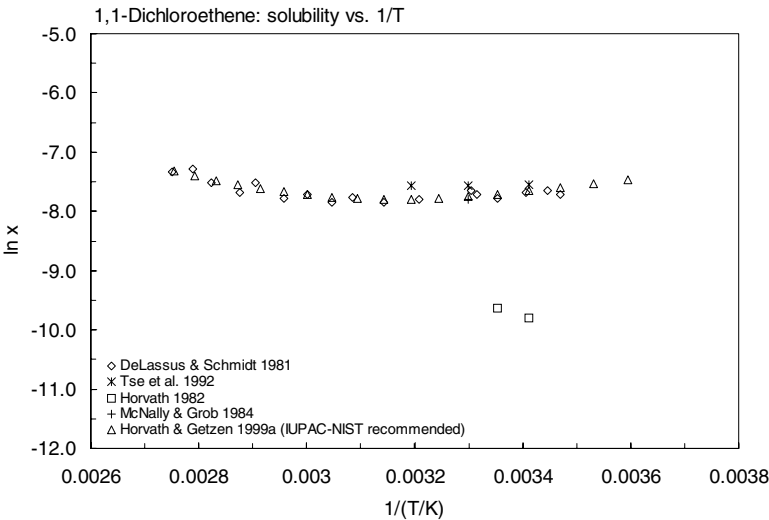


FIGURE 5.1.1.27.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1-dichloroethene.

TABLE 5.1.1.27.2
Reported vapor pressures of 1,1-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot (T/K) + D \cdot (T/K)^2$	(5)		

Stull 1947		Hildenbrand et al. 1959	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
-77.2	133.3	-28.36	6793
-60.0	666.6	-17.72	12204
-51.2	1333	-2.96	25279
-41.7	2666	13.75	51913
-31.1	5333	30.39	97241
-24.0	7999	31.56	101325
-15.0	13332	31.73	101986
-1.0	26664	32.50	104626
14.8	53329		
31.7	101325		
mp/°C	-122.5		

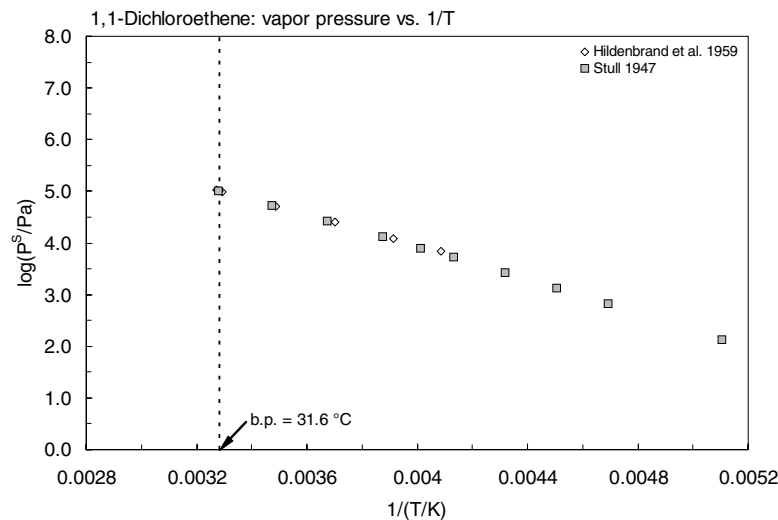


FIGURE 5.1.1.27.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1-dichloroethene.

TABLE 5.1.1.27.3
Reported Henry’s law constants of 1,1-dichloroethene at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$
$$\ln (1/K_{AW}) = A - B/(T/K)$$
$$\ln (k_H/\text{atm}) = A - B/(T/K)$$
$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$
$$\log (1/K_{AW}) = A - B/(T/K)$$
$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

$$(1)$$
$$(2)$$
$$(3)$$
$$(4)$$
$$(5)$$

$$(1a)$$
$$(2a)$$
$$(4a)$$

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tse et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		activity coefficient γ^∞ -GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
2.5	973	10.0	1287	10	1560	20	2320
7.0	1423	17.5	1935	15	2057	30	3415
12.9	2119	24.8	2645	20	2209	40	4813
18.0	2437	34.6	3708	25	2624		
19.5	3195			30	3222		
24.3	3127	eq. 4a	H/(atm m ³ /mol)				
26.1	3914	A	8.845	eq. 4a	H/(atm m ³ /mol)		
		B	3729	A	6.123		
eq. 3	H/atm			B	2907		
A	23.12						
B	4618						

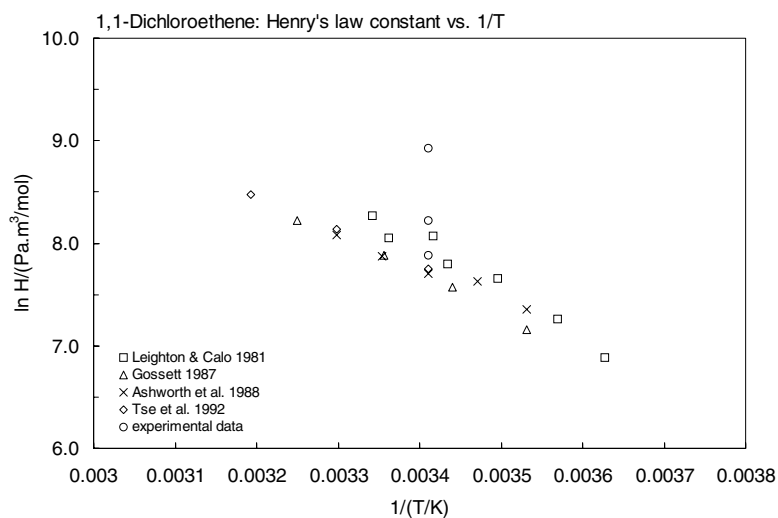
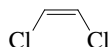


FIGURE 5.1.1.27.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1-dichloroethene.

5.1.1.28 *cis*-1,2-Dichloroethene

Common Name: *cis*-1,2-Dichloroethylene

Synonym: *cis*-acetylene dichloride, *cis*-1,2-dichloroethene, *cis*-1,2-dichloroethylene, (Z)-1,2-dichloroethene

Chemical Name: *cis*-1,2-dichloroethene, *cis*-1,2-dichloroethylene

CAS Registry No: 156-59-2

Molecular Formula: C₂H₂Cl₂, CHCl=CHCl

Molecular Weight: 96.943

Melting Point (°C):

−80.0 (Lide 2003)

Boiling Point (°C):

60.1 (Lide 2003)

Density (g/cm³ at 20°C):

1.2837 (Horvath 1982; Weast 1982–83; Riddick et al. 1986)

1.2818 (Dean 1985)

Molar Volume (cm³/mol):

75.52 (20°C, calculated-density)

86.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.57, 30.23 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.205 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3520 (Seidell 1940)

3500 (selected from literature or measured in DuPont laboratories, McGovern 1943)

5560 (37°C, shake flask-GC, Sato & Nakijima 1979)

3500 (summary of literature data, Horvath 1982)

7700 (Dean 1985)

6575, 6707, 6674 (20, 30, 40°C, infinite dilution activity coeff. γ[∞]-GC, Tse et al. 1992)

6292, 6092, 6220 (20, 30, 40°C, activity coeff. γ[∞]-differential pressure transducer, Wright et al. 1992)

6608 (20°C, limiting activity coeff. γ[∞] by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

6410* (tentative values, measured range 10–40°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

S/(wt%) = 27.7353 − 0.178316·(T/K) + 2.93282 × 10^{−4}·(T/K)², temp range 283–313 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

25571* (23.74°C, temp range 0.76–83.63°C, Ketelaar et al. 1947)

27260* (interpolated-Antoine eq. regression, temp range −58.4 to 59°C, Stull 1947)

28984* (dynamic-ebulliometry, measured range 19.2–62°C, Flom et al. 1951)

23540 (calculated-Antoine eq., Weast 1972–73)

log (P/mmHg) = [−0.2185 × 7420.6/(T/K)] + 7.685137; temp range −58.4 to 260°C (Antoine eq., Weast 1972–73)

27010 (calculated-Antoine eq., Boublik et al. 1973)

log (P/mmHg) = 7.0233 − 1105.436/(230.62 + t/°C); temp range 0.76–83°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

27010, 26740 (interpolated-Antoine equations; Boublik et al. 1984)

log (P/kPa) = 6.14603 − 1204.804/(230.55 + t/°C); temp range 0.76–83.63°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.03144 - 1153.738/(222.905 + t/^{\circ}\text{C})$; temp range 19.2–62°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 7.0223 - 1205.4/(230.6 + t/^{\circ}\text{C})$; temp range 0–84°C (Antoine eq., Dean 1985, 1992)
 26700 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.9771 - 1651.52/(T/\text{K})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 26980 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.30025 - 1293.95/(-32.41 + T/\text{K})$; temp range 273–334 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.22178 - 1271.55/(-30.557 + T/\text{K})$; temp range 332–495 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 21710, 33305, 49350 (20, 30, 40°C, estimated, Tse et al. 1992)
 $\log (P/\text{mmHg}) = 55.9403 - 3.1677 \times 10^3/(T/\text{K}) - 18.572 \cdot \log (T/\text{K}) + 9.8828 \times 10^{-3} \cdot (T/\text{K}) + 5.7644 \times 10^{-14} \cdot (T/\text{K})^2$;
 temp range 193–527 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

342.2 (exptl.- $1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975;)
 1970, 2370 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
 444 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
 413.4* (EPICS-GC, measured range 10.3–34.6°C, Gossett 1987)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 8.479 - 4192/(T/\text{K})$; temp range 10.3–34.6°C (EPICS measurements, Gossett 1987)
 441.1 (20°C, EPICS, Yurteri et al. 1987)
 460* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 5.164 - 3143/(T/\text{K})$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 745.5 (computed value, Yaws et al. 1991)
 324, 496, 740 (20, 30, 40°C, infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)
 331, 518, 751 (20, 30, 40°C, activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)
 319 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 674.5 (modified EPICS method-GC, Ryu & Park 1999)
 341 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 4.464 - 1559/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.86 (shake flask, Hansch & Leo 1985, 1987)
 1.86 (recommended, Sangster 1993)
 1.85 (infinite dilution activity coefficient-GC, Tse & Sandler 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.56 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

1.176 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.69 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2} = 18$ min from dilute aqueous solution (Dilling 1975);
 Evaporation $t_{1/2}(\text{exptl}) = 19.4$ min, $t_{1/2}(\text{calc}) = 0.75$ min, 20.7 min from water (Dilling 1977);
 $t_{1/2} = 19.4$ min from a slowly stirred beaker 6.5 cm deep equivalent to $t_{1/2} = 5.0$ h in a body of water 1 m deep (Dilling 1977; quoted, Verschueren 1983; Howard 1990)
 $t_{1/2} = 3.1$ h was estimated from Henry's law constant for a model river 1 m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{O}_3} = 6.2 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Blume et al. 1976; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{\text{OH}} = 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{O}_3} < 5.0 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{\text{O}_3} = 3.7 \times 10^{-14} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, was estimated at 300 K (Lyman 1982)

$k < 800 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{O}_3} = 6.2 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Tuazon et al. 1984)

photooxidation $t_{1/2} = 286 \text{ h}$, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{\text{NO}_3} = (7.5 \pm 3.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, relative to ethene at $298 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1987; quoted, Atkinson 1991)

$k_{\text{NO}_3} = 7.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime of 130 d, $k_{\text{OH}} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 12 d, and $k_{\text{O}_3} < 5 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of > 9 yr at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 2.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 2.38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{NO}_3} = 1.46 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{\text{OH}} = (2.38 \pm 0.14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Tuazon et al. 1988)

$k_{\text{NO}_3} = (1.39 \pm 0.13) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 2.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (as per Atkinson 1987 and 1988, Müller & Klein 1991)

$k_{\text{O}_3}(\text{aq.}) = (310 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2, with $t_{1/2} = 1.8 \text{ min}$ at pH 7 and 25°C (Yao & Haag 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); anaerobic $t_{1/2} = 2688\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} > 60 \text{ d}$ (Wood et al. 1985; quoted, Olsen & Davis 1990);

$k = 0.74 \text{ yr}^{-1}$ with $t_{1/2} = 88\text{--}339 \text{ d}$ (Barrio-Lage et al. 1986; quoted, Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

Photooxidation $t_{1/2} \sim 100 \text{ min}$ for reaction with NO_2 under UV irradiation, isomer not specified (Gay, Jr., et al. 1976)

photodecomposition $t_{1/2} = 3.0 \text{ h}$ with NO and 3.0 h with NO_2 under simulated atmospheric conditions (Dilling et al. 1976);

residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 129 \text{ d}$ resulting from the ozone attacking of the double bond (Tuazon et al. 1984; quoted, Howard 1990);

$t_{1/2} = 8.0 \text{ d}$ in the atmosphere for the reaction with photochemically produced OH radical (Goodman et al. 1986; quoted, Howard 1990);

$t_{1/2} = 286 \text{ h}$, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric lifetimes: 130 d for the reaction with NO_3 radical for a 12-h nighttime average concn. of $2.4 \times 10^9 \text{ molecule cm}^{-3}$, 12 d for the reaction with OH radical for a 12-h average concn. of $1.0 \times 10^6 \text{ molecule cm}^{-3}$, and > 9.0 yr for the reaction with O_3 for a 24-h average concn. of $7 \times 10^{11} \text{ molecule cm}^{-3}$, (Atkinson et al. 1987).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$k(\text{exptl}) = (310 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 25°C , with $t_{1/2} = 1.80$ min at pH 7 (Yao & Haag 1991).

Ground water: $1344\text{--}69000$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991) and an estimated half-life for anaerobic biodegradation from a ground water field studies of chlorinated ethylenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.1.28.1

Reported aqueous solubilities of *cis*-1,2-dichloroethene at various temperatures

Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999	
activity coefficient γ_∞		activity coefficient γ_∞		IUPAC-NIST recommended	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	6575	20	6292	10	7550
30	6707	30	6092	15	7050
40	6674	40	6220	20	6670
				25	6410
				30	6310
				35	6360
				40	6560

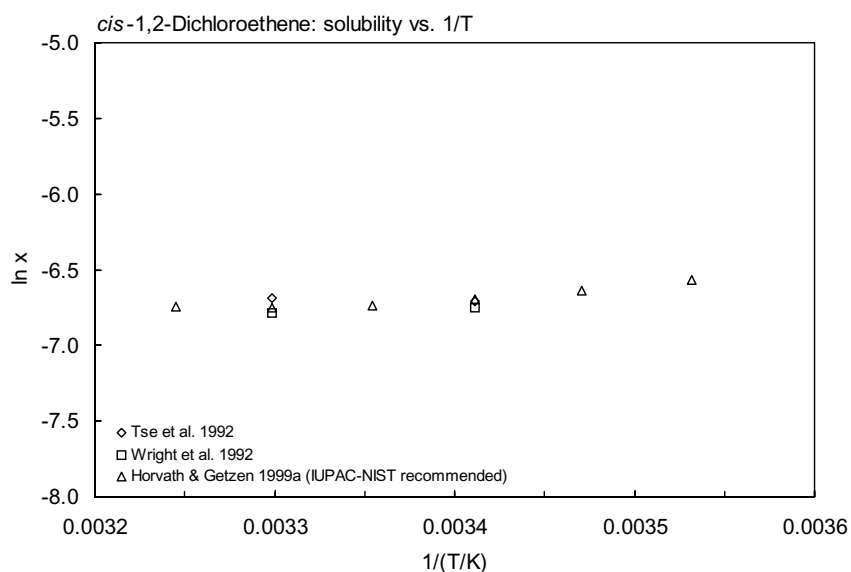


FIGURE 5.1.1.28.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *cis*-1,2-dichloroethene.

TABLE 5.1.1.28.2

Reported vapor pressures of *cis*-1,2-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log(T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Stull 1947		Ketelaar et al. 1947*163		Flom et al. 1951	
summary of literature data				static method-manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-58.4	133.3	0.76	8626	19.2	20732
-39.2	666.6	1.68	9066	26.9	28984
-29.9	1333	3.85	10186	34.1	38957
-19.4	2666	6.45	11572	39.3	48143
-7.90	5333	10.73	14172	44.4	58035
-0.50	7999	15.03	17425	47.8	66048
9.50	13332	20.19	21865	52.1	76833
24.6	26664	23.74	25571	55.0	85206
41.0	53329	26.73	29051	58.4	954-5
59.0	101325	30.11	33344	60.4	101578
		36.35	42823	62.0	107924
mp/°C	-80.5	40.02	49316		
		45.52	60728		
		50.34	71980		
		55.28	85193		
		59.97	98992		
		62.85	109631		
		66.56	123149		
		71.84	145094		
		76.76	168039		
		83.63	283929		

*for a complete data set, see [references](#).

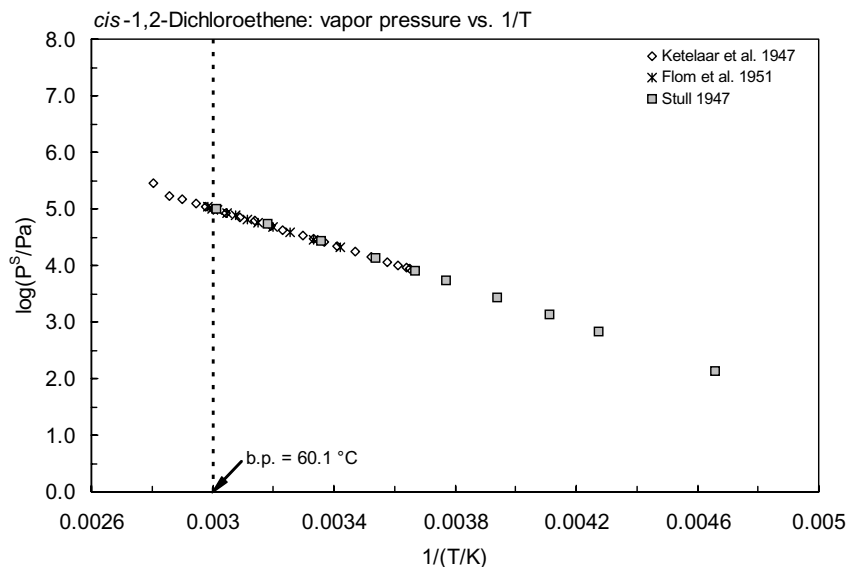


FIGURE 5.1.1.28.2 Logarithm of vapor pressure versus reciprocal temperature for *cis*-1,2-dichloroethene.

TABLE 5.1.1.28.3

Reported Henry's law constants of *cis*-1,2-dichloroethene at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1)$$

$$\log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2)$$

$$\log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4)$$

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K) \quad (4a)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

Gossett 1987		Ashworth et al. 1988		Tse et al. 1992		Wright et al. 1992	
EPICS-GC		EPICS-GC		activity coefficient γ_∞		activity coefficient γ_∞	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
10.3	174	10	273.6	20	324	20	331
17.5	268.5	15	330.3	30	496	30	518
24.8	413.4	20	364.8	40	740	40	751
34.6	552	25	460.0				
		30	582.6				
eq. 4a	H/(atm m ³ /mol)	eq. 4a	H/(atm m ³ /mol)				
A	8.479	A	5.164				
B	4192	B	3143				

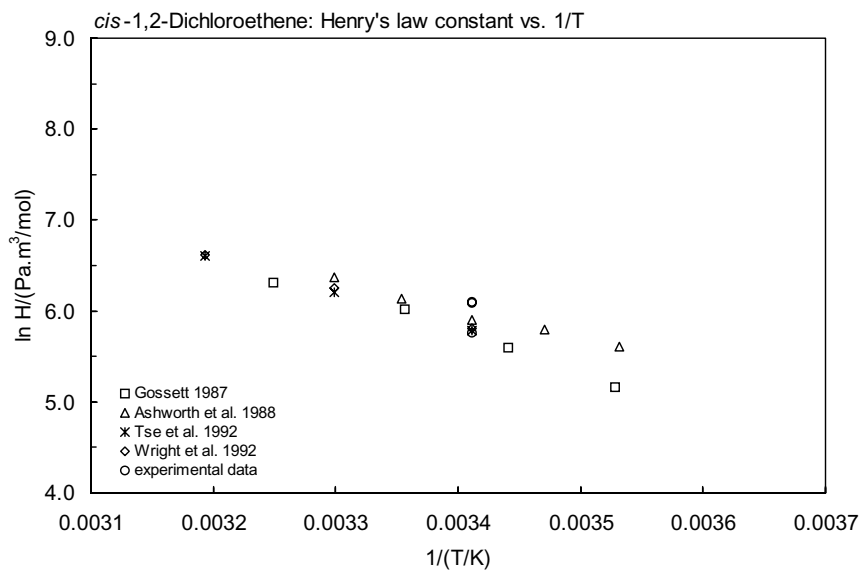
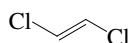


FIGURE 5.1.1.28.3 Logarithm of Henry's law constant versus reciprocal temperature for *cis*-1,2-dichloroethene.

5.1.1.29 *trans*-1,2-Dichloroethene

Common Name: *trans*-1,2-Dichloroethylene

Synonym: *trans*-1,2-dichloroethene, *trans*-1,2-dichloroethylene, *trans*-acetylene dichloride, Dioform, (E)-1,2-dichloroethene

Chemical Name: *trans*-1,2-dichloroethylene, *trans*-1,2-dichloroethene

CAS Registry No: 156-60-5

Molecular Formula: ClCH=CHCl

Molecular Weight: 96.943

Melting Point (°C):

−49.8 (Lide 2003)

Boiling Point (°C):

48.7 (Weast 1977, 1982–83)

Density (g/cm³ at 20°C):

1.2565 (Horvath 1982; Weast 1982–83)

Molar Volume (cm³/mol):

77.2 (20°C, calculated-density)

86.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

36.04, 28.89 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.98 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6260 (Seidell 1940)

6300 (selected from literature of measured in DuPont laboratories, McGovern 1943; Dilling 1977)

6260 (recommended, Horvath 1982)

4480, 4480, 4333 (20, 30, 40°C, infinite dilution activity coeff. γ^∞ -GC, Tse et al. 1992)

4488, 4111, 3931 (20, 30, 40°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)

4488 (20°C, limiting activity coeff. γ^∞ by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

4520* (tentative values, temp range 10–40°C, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 7.803906 - 4.5457 \times 10^{-2} \cdot (T/K) + 6.96755 \times 10^{-4} \cdot (T/K)^2$, temp range 283–313 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

44649* (25.32°C, temp range −38.19 to 84.84°C, Ketelaar et al. 1947)

43180* (interpolated-Antoine eq. regression, temp range −65.4 to 47.8°C, Stull 1947)

42970* (25.2°C, dynamic-ebulliometry, measured range 13.5–51.6°C, Flom et al. 1951)

43470 (Hardie 1964)

36743 (calculated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 7243.1/(T/K)] + 7.748400$; temp range −65.4 to 236.5°C (Antoine eq., Weast 1972–73)

44190 (calculated-Antoine eq., Boublik et al. 1973)

$\log (P/\text{mmHg}) = 6.96513 - 1141.984/(231.93 + t/^\circ\text{C})$; temp range −38 to 84°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

26660, 26660 (14, 20°C, Verschuereen 1977, 1983)

40792* (23.138°C, temp range −0.68 to 46.721°C, Machat 1983; quoted, Boublik et al. 1984)

44190, 43960 (interpolated-Antoine equations, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.09105 - 1142.553/(231.998 + t/^{\circ}\text{C})$; temp range -38.2 to 84.84°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.04724 - 1112.321/(227.56 + t/^{\circ}\text{C})$; temp range -0.68 to 46.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 6.9651 - 1141.9/(231.9 + t/^{\circ}\text{C})$; temp range -38.2 to 85°C (Antoine eq., Dean 1985, 1992)
 45300 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.68147 - 1498.42/(T/\text{K})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 44400 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.93307 - 1059.93/(-50.83 + T/\text{K})$; temp range 263 – 323 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.27465 - 1226.69/(-33.653 + T/\text{K})$; temp range 321 – 473 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 36250, 53970, 78100 (20, 30, 40°C , quoted from DIPPR, Tse et al. 1992)
 $\log (P/\text{mmHg}) = 48.4574 - 3.0496 \times 10^3/(T/\text{K}) - 14.694 \cdot \log (T/\text{K}) - 2.1262 \times 10^{-9} \cdot (T/\text{K}) + 7.3465 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 223 – 508 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

682.7 (calculated as $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
 1970, 2370 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
 669 (calculated-P/C, Dilling 1977)
 669 (calculated-P/C, Mackay & Shiu 1981)
 950.5 (20°C , EPICS, Lincoff & Gossett 1983; Gossett 1985)
 950* (EPICS-GC/FID, measured range 10 – 34.6°C , Gossett 1987)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.341 - 4182/(T/\text{K})$; temp range 10.0 – 34.6°C (EPICS measurements, Gossett 1987)
 914 (20°C , EPICS-GC, Yurteri et al. 1987)
 539 (gas stripping-GC, Warner et al. 1987)
 958* (EPICS-GC/FID, measured range 10 – 30°C , Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 5.333 - 2964/(T/\text{K})$; temp range 10 – 30°C (EPICS measurements, Ashworth et al. 1988)
 729 (20 – 25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 676 (computed value, Yaws et al. 1991)
 800, 1196, 1793 (20, 30, 40°C , infinite dilution activity coeff. γ -GC, Tse et al. 1992)
 768.7* (20°C , activity coeff. γ^{∞} -differential pressure transducer, measured range 20 – 40°C , Wright et al. 1992)
 1023* (26.2°C , EPICS-GC, measured range 26.2 – 46.1°C , Hansen et al. 1993)
 773 (20°C , equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 634.8 (modified EPICS method-GC, Ryu & Park 1999)
 875 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 5.247 - 1669/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.06 (Hansch & Leo 1985)
 2.09 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Hansch et al. 1995)
 2.09 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.34 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)
 1.68 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.56 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)
 1.77 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization: experimental $t_{1/2}(\text{exptl}) = 24$ min for 1 mg/L from water when stirred at 200 rpm at approximately 25°C in an open container of depth 65 mm (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982);

Evaporation $t_{1/2}(\text{exptl}) = 24$ min, $t_{1/2}(\text{calc}) = 0.85$ min, 20.8 min from water (Dilling 1977)

Volatilization $t_{1/2} = 3.0$ h from a model river 1 m deep with 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{O}_3} = 3.8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Blume et al. 1976; quoted, Atkinson & Carter 1984)

$k_{\text{OH}} = 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k_{\text{O}_3} = (1.8 \pm 0.29) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Zhang et al. 1983)

$k_{\text{O}_3} = 1.2 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Niki et al. 1983; quoted, Atkinson & Carter 1984; Tuazon et al. 1984)

$k_{\text{O}_3} = 2.0 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–323 K (quoted, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.3 \times 10^5 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, estimated at 300 K (Lyman 1982)

$k < 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $6.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radicals at 25°C (Mabey et al. 1982)

$k = (5.7 \pm 1.0) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{O}_3} = 1.8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Tuazon et al. 1984)

$k_{\text{OH}} = 1.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1986; quoted, Atkinson et al. 1987; Sabljic & Güsten 1990)

$k_{\text{NO}_3} = (5.7 \pm 2.7)5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{\text{NO}_3} = 5.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime of 179 d, $k_{\text{OH}} = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 5.1 d and $k_{\text{O}_3} = 1.5 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 110 d at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

photooxidation $t_{1/2} = 25.2$ h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{\text{NO}_3} = 1.11 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{\text{NO}_3} = (1.07 \pm 0.11) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative to ethene at 298 ± 2 K (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 2.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (as per Atkinson 1987 and 1988, Müller & Klein 1991)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672$ –4320 h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688$ –17280 h, based on estimated unacclimated aqueous aerobic degradation half-life (Howard et al. 1991);

$k = 0.1 \text{ yr}^{-1}$ with $t_{1/2} = 53$ d (Wood et al. 1985; quoted, Olsen & Davis 1990);

rate constant $k = 0.12$ –0.35 mini^{-1} in a fixed-film, packed-bed bioreactor containing a consortium of microorganisms (Strandberg et al. 1989);

$k = 1.8 \text{ yr}^{-1}$ with $t_{1/2} = 132$ –147 d (Barrio-Lage et al. 1986; quoted, Olsen & Davis 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 0.24$ –2.4 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

photodecomposition $t_{1/2} = 2.9$ h with NO and $t_{1/2} = 2.8$ h with NO_2 under simulated atmospheric conditions (Dilling et al. 1976);

Photooxidation $t_{1/2} \sim 100$ min for reaction with NO_2 under UV irradiation, isomer not specified (Gay, Jr., et al. 1976)

residence time of 2.9 d, loss of 29.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 44$ d resulting from ozone attacking of the double bond (Tuazon et al. 1984; quoted, Howard 1990);

$t_{1/2} = 3.6$ d in the atmosphere for the reaction with photochemically produced OH radical (Goodman et al. 1986; quoted, Howard 1990);

$t_{1/2} = 25.2$ h, based on estimated rate constant for reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric lifetimes, $\tau = 170$ d for the reaction with NO_3 radical for a 12-h nighttime average concn. of 2.4×10^9 molecule cm^{-3} , $\tau = 5.1$ d for the reaction with OH radical for a 12-h average concn. of 1.0×10^6 molecule $\cdot \text{cm}^{-3}$, and $\tau = 110$ d for the reaction with O_3 for a 24-h average concentration of 7×10^{11} molecule $\cdot \text{cm}^{-3}$ (Atkinson et al. 1987).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}69000$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and estimated half-life for anaerobic biodegradation of chlorinated ethylenes from a ground water field study (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on unacclimated aerobic aqueous screening test data (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2} < 10$ d (Ryan et al. 1988).

Biota: $t_{1/2} < 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.29.1

Reported aqueous solubilities of *trans*-1,2-dichloroethene at various temperatures

Tse et al. 1992		Wright et al. 1992		Horvath & Getzen 1999	
activity coefficient γ^∞		activity coefficient γ^∞		IUPAC-NIST recommended	
$t/^\circ\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$
20	4480	20	4488	10	5250
30	4480	30	4111	15	4970
40	4333	40	3931	20	4720
				25	4520
				30	4330
				35	4190
				40	4080

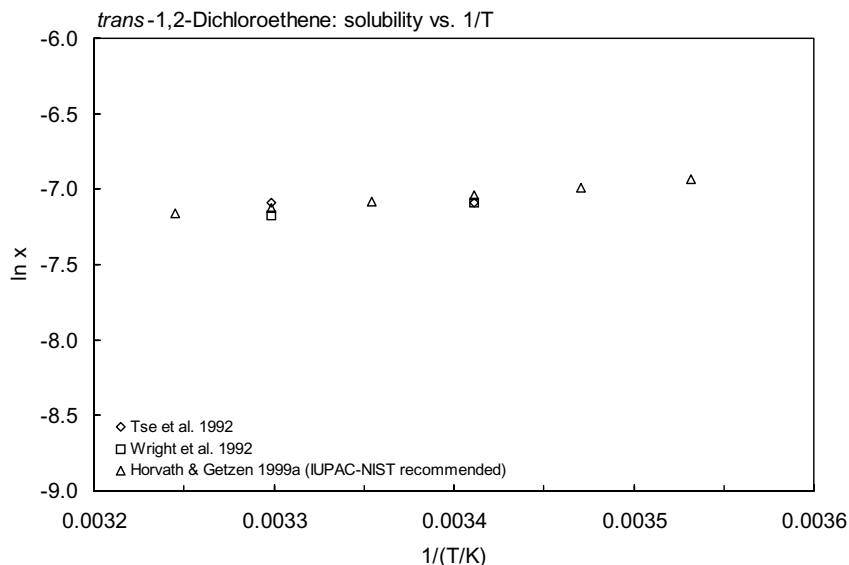


FIGURE 5.1.1.29.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *trans*-1,2-dichloroethene.

TABLE 5.1.1.29.2

Reported vapor pressures of *trans*-1,2-dichloroethene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		Ketelaar et al. 1947*		Flom et al. 1951		Machet 1983, Thesis	
summary of literature data		in Boublik et al. 1984		static method-manometer		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-65.4	133.3	-38.19	1387	13.5	26131	-0.68	13944
-47.4	666.6	-28.3	3000	20.5	35210	3.154	16825
-38.0	1333	-15.12	6733	25.3	42956	7.12	20300
-28.0	2666	-7.29	10092	29.7	50836	11.306	24599
-17.0	5333	0.52	15086	34.7	61835	15.344	29372
-10.0	7999	5.98	19438	38.6	71581	19.302	34777
-0.20	13332	11.12	24718	41.6	79300	23.138	40792
14.3	26664	16.91	31651	44.1	86513	27.017	47616
30.8	53329	19.06	34757	46.8	95099	33.103	60215
47.8	101325	25.32	44649	49.1	102165	38.951	74768
		28.23	50329	51.6	111151	45.27	93376

TABLE 5.1.1.29.2 (Continued)

Stull 1947		Ketelaar et al. 1947*		Flom et al. 1951		Machat 1983, Thesis	
summary of literature data				static method-manometer		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
mp/°C	-122.5	32.15	38448	$\Delta H_v/(\text{kJ mol}^{-1}) = 29.62$		46.721	98149
		35.84	66888				
		43.72	88272			bp/°C	47.655
		47.17	99365			Antoine eq	
		48.83	105591			eq. 2	P/kPa
		50.82	112737			A	6.04724
		56.12	133389			B	1112.321
		63.58	167812			C	227.560
		68.19	192917				
		77.16	248619				
		84.84	304561				

*for a complete data set, see [references](#).

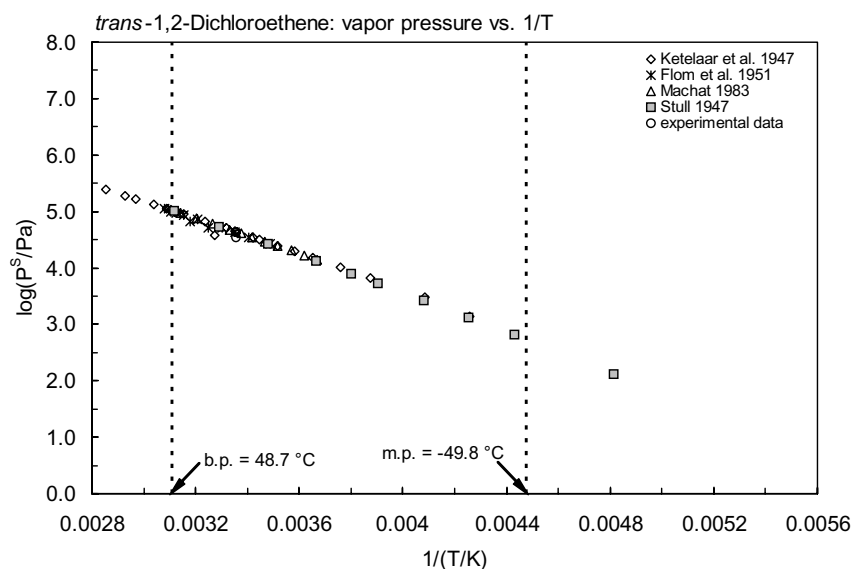


FIGURE 5.1.1.29.2 Logarithm of vapor pressure versus reciprocal temperature for *trans*-1,2-dichloroethene.

TABLE 5.1.1.29.3

Reported Henry's law constants of *trans*-1,2-dichloroethene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)		
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)		
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)					
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)		
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)					
Gossett 1987		Ashworth et al. 1988		Tse et al. 1992		Hansen et al. 1993	
EPICS-GC		EPICS-GC		activity coeff. γ^∞ -GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
10.0	425.6	10	597.8	20	800	26.2	1023
17.5	668.7	15	714.3	30	1196	35.0	1591
24.8	950.4	20	868.4	40	1793	46.1	2087
34.6	1398.3	25	957.5				
		30	1226.0				
eq. 4a	H/(atm m ³ /mol)			Wright et al. 1992		eq. 4a	H/(kPa m ³ /mol)
A	9.341	eq. 4a	H/(atm m ³ /mol)	activity coeff. γ^∞		A	11 ± 1.96
B	4182	A	10.65	t/°C	H/(Pa m ³ /mol)	B	3396 ± 602
		B	4368				
				20	768.7		
				30	1238		
				40	1854		

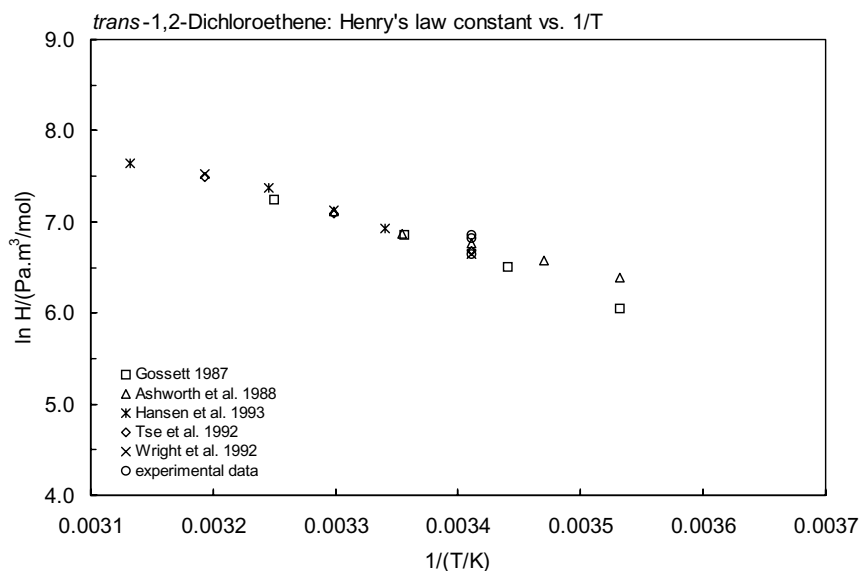
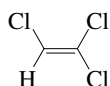


FIGURE 5.1.1.29.3 Logarithm of Henry's law constant versus reciprocal temperature for *trans*-1,2-dichloroethene.

5.1.1.30 Trichloroethylene



Common Name: Trichloroethylene

Synonym: TCE, acetylene trichloride, ethylene trichloride

Chemical Name: 1,1,2-trichloroethylene

CAS Registry No: 79-01-6

Molecular Formula: C_2HCl_3 , $CHCl=CCl_2$

Molecular Weight: 131.388

Melting Point ($^{\circ}C$):

-84.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

87.21 (Lide 2003)

Density (gm/cm^3 at $20^{\circ}C$):

1.4642 (Dreisbach 1959; Horvath 1982; Weast 1982-83)

1.4554 ($25^{\circ}C$, Dreisbach 1959)

Molar Volume (cm^3/mol):

89.02 (calculated-density, Miller et al. 1985)

107.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

34.27, 31.47 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0 (Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1818 (volumetric method, Wright & Schaffer 1932;)

1100 (data presented in graph, temp range $0-80^{\circ}C$, McGovern 1943)

1288* (temp range $10-50^{\circ}C$, Vallaud et al. 1957)

1100 ($20^{\circ}C$, McConnell et al. 1975; Pearson & McConnell 1975)

1780, 1500, 1470 (3, 20, $34^{\circ}C$, shake flask-GC/ECD, Chiou & Freed 1977)

1000, 1100, 1100 (1.5, 20, $25^{\circ}C$, literature average, Dilling 1977)

1000 (shake flask-titration/turbidity, Coca et al. 1980)

1472 (shake flask-LSC, Banerjee et al. 1980)

1474 (shake flask-LSC, Veith et al. 1980)

1100* (summary of literature data, temp range $0-80^{\circ}C$, Horvath 1982)

1366 (generator column-HPLC, Tewari et al. 1982)

743.1 ($30^{\circ}C$, headspace-GC, McNally & Grob 1984)

1370 (selected, Riddick et al. 1986)

1421 ($23-24^{\circ}C$, shake flask-GC, Broholm et al. 1992)

1350 ($20^{\circ}C$, calculated-activity coefficients, Wright et al. 1992)

1483, 1450, 1468 (20, 30, $40^{\circ}C$, infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)

1349, 1409, 1308 (20, 30, $40^{\circ}C$, activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)

1300-1500 ($9-71^{\circ}C$, generator column-GC, data presented in graph, Heron et al. 1998)

1330 ($20^{\circ}C$, limiting activity coeff. γ^{∞} by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

1280* (recommended, temp range $0-60^{\circ}C$, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 1.4049 - 8.2223 \times 10^{-3} \cdot (T/K) + 1.3218 \times 10^{-5} \cdot (T/K)^2$, temp range 273-333 K (equation derived from literature solubility data, Horvath & Getzen 1999a)

1417* ($21^{\circ}C$, batch equilibrium-GC, sample prepared at 1.0 MPa, measure range $21-117^{\circ}C$, Knauss et al. 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 19733* (temp range 25–87.15°C, Hertz & Rathmann 1912)
 9331 (extrapolated, data presented in graph, McGovern 1943)
 9645* (25.5°C, ebulliometry, measured range 18–86°C, McDonald 1944)
 $\log (P/\text{cmHg}) = 30.482609 - 2936.227/(T/K) - 7.999975 \cdot \log (T/K)$; temp range 18–86°C (ebulliometry, McDonald 1944)
 9735* (interpolated-Antoine eq. regression, temp range 25–87.2°C, Stull 1947)
 9906 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)
 $\log (P/\text{mmHg}) = 7.02808 - 1315.0/(230.0 + t/^{\circ}\text{C})$; temp range 7–155°C (Antoine eq. for liquid state, Dreisbach 1959)
 9723 (calculated-Antoine eq., Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 8314.7/(T/K)] + 7.956342$; temp range –43.8 to 86.7°C (Antoine eq., Weast 1972–73)
 9224 (calculated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 6.51827 - 1018.603/(192.731 + t/^{\circ}\text{C})$; temp range 17–86°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 8000 (20°C, Perry & Chilton 1973)
 7700 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
 3066, 7866, 9866 (1.5, 20, 25°C, interpolated from literature data, Dilling 1977)
 7998, 12660 (20°C, 30°C, Verschuereen 1983; Hewitt et al. 1992)
 9200, 9690 (interpolated-Antoine equations., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 5.59553 - 994.46/(189.705 + t/^{\circ}\text{C})$; temp range 17.8–86.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 4.70615 - 614.104/(140.089 + t/^{\circ}\text{C})$; temp range 25–87.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 6.5183 - 1018.6/(192.7 + t/^{\circ}\text{C})$; temp range 18–86°C (Antoine eq., Dean 1985, 1992)
 6307 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.15298 - 1315.04/(230.0 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 9911 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.15298 - 1315.0/(-43.15 + T/K)$; temp range 280–428 K (Antoine eq., Stephenson & Malanowski 1987)
 9691 (resistance measurement-Antoine eq., Foco et al. 1992)
 7753, 12350, 19080 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
 $\log (P/\text{mmHg}) = 23.6735 - 2.3763 \times 10^3/(T/K) - 5.8275 \cdot \log (T/K) + 1.9586 \times 10^{-3} \cdot (T/K) + 2.8882 \times 10^{-14} \cdot (T/K)^2$; temp range 188–571 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1186 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 248, 1186 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)
 967 (calculated-P/C, Neely 1976)
 388.2, 1215 (1.5, 25°C, calculated-P/C, Dilling 1977)
 890, 975 (20°C, exptl., calculated-P/C, Dilling 1977)
 1103 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
 $\log (H/\text{atm}) = 8.59 - 1716.16/(T/K)$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)
 985 (20°C, batch stripping-GC, Mackay et al. 1979)
 985* (25.2°C, equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)
 $\ln (k_H/\text{atm}) = 21.89 - 4647/(T/K)$; temp range 1.0–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
 999 (20°C, batch stripping-GC, Munz & Roberts 1987)
 970 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
 774; 683 (20°C, EPICS-GC; batch air stripping-GC, measured range 10–30°C, Lincoff & Gossett 1984)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 11.94 - 4929/(T/K)$; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.703 - 4308/(T/K)$; temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)

- 452, 795, 1348 (10, 20, 30°C, multiple equilibrium technique-GC, Munz 1985)
- 1185 (adsorption isotherm, Urano & Murata 1985)
- 970.7* (24.8°C, EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)
- $\ln [H/(\text{atm m}^3/\text{mol})] = 11.37 - 4780/(T/K)$; temp range 9.6–34.6°C (EPICS-GC, Gossett 1987)
- 816 (20°C, EPICS-GC, Munz & Roberts 1987)
- $\log K_{AW} = 6.026 - 1909/(T/K)$; temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)
- 1185 (gas stripping-P/C, Warner et al. 1987)
- 1048 (20°C, EPICS, Yurteri et al. 1987)
- 1034* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
- $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 7.845 - 3702/(T/K)$; temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)
- 922 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
- 768.4 (purge and trap method, Tancredi & Yanagisawa 1990)
- 768* (tap water, EPICS-GC, measured range 25–47.2°C, Tancredi & Yanagisawa 1990)
- $\log K_{AW} = 6.664 - 2141/(T/K)$; temp range 25–47.2°C (EPICS-GC, Tancredi & Yanagisawa 1990)
- 1182 (computed value, Yaws et al. 1991)
- 709, 1155, 1753 (20, 30, 40°C, determined from measured infinite dilution activity coeff. γ^∞ -GC, Tse et al. 1992)
- 756, 1152, 1908 (20, 30, 40°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
- 996 (activity coefficient γ^∞ from gas stripping-GC, Li et al. 1993)
- 1043* (static headspace-GC, measured range 25–50°C, Robbins et al. 1993)
- 794 (23°C, batch air stripping-IR, Nielsen et al. 1994)
- 870* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)
- 381, 1073 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
- $\ln K_{AW} = -3648/(T/K) + 0.00813 \cdot Z + 11.121$; with Z salinity 0–35.5‰, temp range 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)
- 775 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
- 1180 (vapor-liquid equilibrium-GC, Turner et al. 1996)
- $K_{AW} = 0.151 - 0.00597 \cdot (T/K) + 0.000680 \cdot (T/K)^2$; temp range 0–45°C (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)
- 751 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
- 885* (headspace equilibrium-GC, measured range 15–45°C, Peng & Wan 1997)
- $\ln (k_H/\text{atm}) = 8.19 - 1642/(T/K)$; temp range 15–45°C (headspace-GC measurements, Peng & Wan 1997)
- 709* (20°C, headspace equilibrium-GC, Peng & Wan 1998)
- 1195 (sea water 36‰, headspace-GC, measured range 15–45°C, Peng & Wan 1998)
- $\log (k_H/\text{atm}) = 8.62 - 1736/(T/K)$; sea water 36‰ NaCl, temp range: 15–45°C (headspace-GC measurements, Peng & Wan 1998)
- 1055 (modified EPICS method-GC, Ryu & Park 1999)
- $\ln [H/(\text{atm m}^3/\text{mol})] = 7.99 - 3736/(T/K)$; temp range 10–95°C (EPICS measurements, Heron et al. 1998)
- 1006; 981; 352 (EPICS-GC; quoted lit.; calculated-P/C, David et al. 2000)
- 703.4* (calculated from P and exptl measured solubility, temp range 21–117°C, Knauss et al. 2000)
- 823* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)
- $\ln K_{AW} = 9.9697 - 3287.5/(T/K)$; measured range 15–4 0°C (SPME-GC, Bierwagen & Keller 2001)
- 765 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
- $\log K_{AW} = 5.874 - 1871/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)
- 995* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
- $\ln K_{AW} = 12.13 - 3908.2/(T/K)$; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:

- 2.37 (Hansch & Elkins 1971)
- 2.29 (Leo et al. 1971; Hansch & Leo 1979; 1987)
- 2.61 (shake flask-GC/ECD, Chiou & Freed 1977)
- 2.42 (shake flask-LSC, Banerjee et al. 1980)
- 2.42 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982; Veith et al. 1983)
- 2.86 (HPLC- k' correlation, McDuffie 1981)

- 2.53 (generator column-HPLC, Tewari et al. 1982)
- 2.71, 2.79, 3.49, 3.57 (values used for OECD Lab. comparison tests, Harnisch et al. 1983)
- 2.84 (HPLC-RT correlation, Eadsforth 1986)
- 2.42 (recommended, Sangster 1993)
- 2.67 (calculated-activity coefficients γ° , Tse & Sandler 1994)
- 2.61 (recommended, Hansch et al. 1995)
- 2.27* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

- 2.99 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 1.59 (rainbow trout, Neely et al. 1974)
- 1.23–1.36 (calculated- K_{OW} , Veith et al. 1979; Veith et al. 1980)
- 1.23 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
- 1.23–1.59 (bluegill sunfish & rainbow trout, Barrows et al. 1980; Lyman 1981)
- 1.59 (rainbow trout, quoted, Bysshe 1982)
- 1.987 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.20 (calculated-MCI χ , Koch 1983)
- 2.996 (activated sludge, Freitag et al. 1984)
- 3.06, 2.39 (*Chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)
- 1.20, 1.05 (quoted, calculated, Sabljic 1987)
- 1.025 (quoted from USEPA 1986, Yeh & Kastenbergh 1991)
- 1.420 (calculated- K_{OW} , McCarty et al. 1992)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 2.10 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
- 2.20 (Pavlou & Weston 1983, 1984)
- 1.76, 2.20 (ICN humic acid-coated Al_2O_3 , ICN humic acid, Garbarini & Lion 1985)
- 1.66; 2.14, 2.40 (predicted-S, predicted- K_{OW} , Garbarini & Lion 1985)
- 1.76; 0.616 (Sapsucker Woods humic acid, Sapsucker Woods fulvic acid, Garbarini & Lion 1986)
- 1.238, 2.079, 2.045, 0.30, 1.827 (tannic acid, lignin, zein, cellulose, Aldrich humic acid, Garbarini & Lion 1986)
- 2.025, 2.086 (Sapsucker Woods soil, Sapsucker Woods ether-extracted soil, Garbarini & Lion 1986)
- 2.161, 2.458 (humic, oxidized humic, Garbarini & Lion 1986)
- 2.663 (fats, waxes, resins, Garbarini & Lion 1986)
- 2.54, 1.72 (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
- 2.00; 1.84 (quoted from Seip et al. 1986, calculated-MCI χ , Bahnick & Doucette 1988)
- 2.03 (soil, Chiou et al. 1988; quoted, Grathwohl 1990)
- 2.02, 2.11 (soil: quoted, HPLC-RT correlation, Hodson & Williams 1988)
- 1.79 (20°C, humic acid, Peterson et al. 1988; quoted, Grathwohl 1990)
- 1.53 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.61, 2.12 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.89, 2.50, 2.25 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.09; 2.56; 3.43 (20°C, soil, sand and loess; weathered shale and mudrock; unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 1.97, 2.15 (20°C, calculated- K_{OW} , Grathwohl 1990)
- 0.30–3.64 (cellulose anthracite, quoted, Grathwohl 1990)
- 2.01 (calculated average, Olsen & Davis 1990)
- 2.20, 1.78 (humic acid, humic acid-coated Al_2O_3 , Pavlostathis & Jaglal 1991)
- 2.03 (surface soil, Pavlostathis & Jaglal 1991)

- 3.39, 2.00 (organic carbon soil, Doust & Huang 1992)
 1.60, 1.60, 2.15 (bentonite, green & tan clay, Doust & Huang 1992)
 0.35, 1.40, 1.90, 2.20 (Barnwell, Congaree, McBean I & II sands, Doust & Huang 1992)
 1.66, 2.64, 2.83 (calculated-equilibrium desorption data, Pavlostathis & Mathavan 1992)
 2.23, 2.33, 2.35, 2.34, 2.34, 2.36, 2.41 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, Belgium, organic carbon $f_{OC} = 4.12\%$, EPICS-GC/FID, Dewulf et al. 1999)
 2.80; 2.00 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
 1.92, 2.00, 1.75 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM} :

- 1.23 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.42, 1.89 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.78, 2.36 (organic cations treated Marlette soil B_t horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil B_t horizon OM 4.38%; Oshtemo soil B_t horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 1.74 (Florida peat, OC 57.1%, batch equilibrium-sorption isotherm, Rutherford & Chiou 1992)

Environment Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2}$ (exptl.) = 21 min, calculated $t_{1/2}$ (calc) = 0.48 min from dilute aqueous solution of 1 ppm initial concn. in a 250 mL beaker with constant stirring at room temp (Dilling et al. 1975); volatilization $k = 2.79, 5.07 \text{ g cm}^{-2} \text{ s}^{-1}$ at $23.7 \pm 0.5^\circ\text{C}$ into the atmosphere (Chiou & Freed 1977); Evaporation $t_{1/2}$ (exptl) = 17.7, 18.5, 23.5 min, $t_{1/2}$ (calc) = : 0.47 min, 23.8 min at $20\text{--}25^\circ\text{C}$ and $t_{1/2}$ (exptl) = 31.9 min at 1.5°C from water (Dilling 1977)
 ratio of evaporation rate constant to that of oxygen reaeration rate constant: measured as 0.49 as compared to the predicted 0.44 (Smith et al. 1980);
 $t_{1/2}$ (exptl) = $1.42 \times 10^4 \text{ s}$ and $t_{1/2}$ (calc) = $5.1 \times 10^3 \text{ s}$ for water body of depth of 22.5 m (Klöpffer et al. 1982)
 estimated $t_{1/2} = 3.4 \text{ h}$ from water (Thomas 1982);
 $k = 0.025 \text{ d}^{-1}$, $t_{1/2} = 28 \text{ d}$ in spring at $8\text{--}16^\circ\text{C}$, $k = 0.052 \text{ d}^{-1}$, $t_{1/2} = 13 \text{ d}$ in summer at $20\text{--}22^\circ\text{C}$, $k = 0.045 \text{ d}^{-1}$, $t_{1/2} = 15 \text{ d}$ in winter at $3\text{--}7^\circ\text{C}$ for the periods when volatilization appears to dominate, and $k = 0.064 \text{ d}^{-1}$, $t_{1/2} = 10.7 \text{ d}$ with HgCl_2 , and $k = 0.081 \text{ d}^{-1}$, $t_{1/2} = 9.6 \text{ d}$ without HgCl_2 in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);
 $k = 7.22 \times 10^{-3} \text{ h}^{-1}$ (Mackay et al. 1985).

Photolysis: $t_{1/2} = 3.5 \text{ h}$ estimated from lab. simulated UV photolysis (light intensity about 6 times of natural sunlight at noon on a summer day in Freeport) for 10 ppm to react with 5 ppm NO at $27 \pm 1^\circ\text{C}$ (Dilling et al. 1976); probably would not occur (Callahan et al., 1979)
 photocatalyzed mineralization by the presence of TiO_2 with the rate of $830 \text{ ppm min}^{-1} \cdot \text{g}^{-1}$ of catalyst (Ollis 1985);
 $k = (4.08\text{--}6.27) \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

- $k_{OH} = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow system-LMR, Howard 1976)
 Photooxidation $t_{1/2} \sim 120 \text{ min}$ for reaction with NO_2 under UV irradiation (Gay, Jr. et al 1976)
 $k_{OH}^* = (2.37 \pm 0.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 234–420 K (discharge flow-resonance fluorescence, Chang & Kaufman 1977)
 $k_{OH} = (0.27 \pm 0.08) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ at 1 atm and $305 \pm 2 \text{ K}$ (relative rate method, Winer et al. 1978)
 $k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1979,1982; quoted, Tuazon et al. 1984; Atkinson et al. 1987)
 $k_{OH} = 2.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 5.3 d, loss of 17.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
 $k_{OH} = 1.2 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ estimated, and $k_{O_3} = 3.6 \times 10^3 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k_{O_3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with ozone at $296 \pm 2 \text{ K}$ (Atkinson et al. 1982; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k < 1000 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, $k = 6.0 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 radical (Mabey et al. 1982)

$k = (17 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{O_3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Tuazon et al. 1984)

$k_{OH}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.10 d^{-1} , $k_{O_3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.002 d^{-1} at room temp. (Atkinson et al. 1985)

$k_{OH} = (2.86 \pm 0.40) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to *n*-butane at $23.2 \pm 1.1^\circ\text{C}$ and a calculated atmospheric lifetime $\tau = 4.0 \text{ d}$ (Edney et al. 1986)

$k_{NO_3} = (1.5 \pm 0.7) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1987)

$k_{NO_3} = 1.5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime $\tau = 64 \text{ d}$, $k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with lifetime $\tau = 9.6 \text{ d}$ and $k_{O_3} < 3 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with lifetime $\tau > 1.5 \text{ yr}$ at room temp. (Atkinson et al. 1987)

$k_{OH}(\text{calc}) = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH}^* = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}(\text{calc}) = 6.92 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (as per Atkinson 1987 and 1988, Müller & Klein 1991)

$k_{NO_3} = (2.81 \pm 0.17) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative to ethene at $298 \pm 2 \text{ K}$ (Atkinson 1991)

$k(\text{aq.}) = (15 \pm 2) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $21 \pm 1^\circ\text{C}$, with a half-life of 37 min at pH 7 (Yao & Haag 1991).

Hydrolysis: not an important process (Mabey et al. 1982);

$k = 0.065 \text{ month}^{-1}$ at 25°C with $t_{1/2} = 10.7 \text{ months}$ (Dilling et al. 1975; quoted, Howard et al. 1991);

$k = 9.0 \times 10^{-5} \text{ h}^{-1}$ (Mackay et al. 1985);

abiotic hydrolysis or dehydrohalogenation $t_{1/2} = 10.7 \text{ months}$ (Olsen & Davis 1990)

$t_{1/2} = 320 \text{ d}$ at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: can be biodegraded by microorganisms in sea water;

$t_{1/2}(\text{aerobic}) = 6 \text{ months to } 1 \text{ yr}$ based on acclimated soil screening test data (Tabak et al. 1981; quoted, Howard et al. 1991)

$k = 1.1 \text{ yr}^{-1}$ with $t_{1/2} = 230 \text{ d}$ (Roberts et al. 1982; quoted, Olsen & Davis 1990)

$t_{1/2}(\text{anaerobic}) = 98 \text{ d to } 4.5 \text{ yr}$, based on sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard et al. 1991);

$k = 0.06 \text{ yr}^{-1}$ with biodegradation $t_{1/2} = 33 \text{ d}$, microcosm constructed with crushed rock and water containing low microbial biomass depleted all TCE in 21 months of incubation (Barrio-Lage et al. 1987, quoted, Olsen & Davis 1990)

$k \sim 0.02 \text{ min}^{-1}$ in a fixed-film, packed-bed bioreactor containing a consortium of microorganisms (Strandberg et al. 1989);

$k = 0.08 \text{ yr}^{-1}$ with $t_{1/2} = 43 \text{ d}$ (Olsen & Davis 1990)

$t_{1/2}(\text{aerobic}) = 180 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 98 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant of $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 10.5 \text{ h}^{-1}$ (flagfish, calculated-BCF $\times k_2$, McCarty et al. 1992)

$k_2 = 0.398 \text{ h}^{-1}$ (flagfish, estimated-one compartment first-order kinetics, McCarty et al. 1992)

Environmental Half-Lives:

Air: tropospheric $t_{1/2} = 6.0 \text{ wk}$, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

photodecomposition $t_{1/2}$ = of 3.5 h with NO and $t_{1/2} = 2.9 \text{ h}$ with NO_2 under simulated atmospheric conditions (Dilling et al. 1976);

photooxidation $t_{1/2} \sim 120 \text{ min}$ for reaction with NO_2 under UV irradiation (Gay, Jr. et al. 1976)

residence time of 5.3 d , loss of 17.2% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 27\text{--}272$ h, based on photooxidation half-life in air (Atkinson 1985; quoted, Howard et al. 1991);
atmospheric lifetime $\tau = 4.0$ d, based on the photooxidation rate constant in the gas phase at $23.2 \pm 1.1^\circ\text{C}$ (Edney et al. 1986);

atmospheric lifetimes $\tau = 64$ d for the reaction with NO_3 for a 12-h nighttime average concn. of 2.4×10^9 molecule/ cm^3 , $\tau = 9.6$ d for the reaction with OH radical for a 12-h average concn. of 1.0×10^6 molecule cm^{-3} , and $\tau > 1.5$ yr for the reaction with O_3 for a 24-h average concn. of 7×10^{11} molecule/ cm^3 (Atkinson et al. 1987);

$t_{1/2} \sim 3.7$ d (Yeh & Kastenberg 1991).

Surface water: estimated $t_{1/2} = 1.2\text{--}90$ d in surface waters at various locations in the Netherlands in case of a first order reduction process (Zoeteman et al. 1980)

half-lives from marine mesocosm: $t_{1/2} = 28$ d in the spring at $8\text{--}16^\circ\text{C}$, $t_{1/2} = 13$ d in the summer at $20\text{--}22^\circ\text{C}$ and $t_{1/2} = 15$ d in the winter at $3\text{--}7^\circ\text{C}$ when volatilization dominates, and $t_{1/2} = 10.7$ d and 8.6 d for experiments with and without HgCl_2 as poison, respectively, in September 9–15 (Wakeham et al. 1983)

Biodegradation $t_{1/2}$ (aerobic) = 100 d, $t_{1/2}$ (anaerobic) = 400 d; hydrolysis $t_{1/2} = 320$ d at pH 7 in natural waters (Capel & Larson 1995)

$t_{1/2} = 4320\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} \sim 90$ d (Yeh & Kastenberg 1991);

measured rate constant $k = (15 \pm 2) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $21 \pm 1^\circ\text{C}$, with $t_{1/2} = 37$ min at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 7704\text{--}39672$ h, based on hydrolysis half-life (Dilling et al. 1975; quoted, Howard et al. 1991) and anaerobic sediment grab sample data (Barrio-Lage et al. 1986; quoted, Howard et al. 1991)

$t_{1/2} \sim 2.0$ yr in the ground water in the Netherlands (estimated, Zoeteman et al. 1981);

$t_{1/2} \sim 86$ d (Yeh & Kastenberg 1991).

Soil: $t_{1/2} < 10$ d (Ryan et al. 1988);

$t_{1/2} = 4320\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} \sim 43$ d in upper soil and $t_{1/2} \sim 86$ d in lower soil (Yeh & Kastenberg 1991).

Sediment: $t_{1/2} \sim 43$ d (estimated, Yeh & Kastenberg 1991).

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{1/2} < 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988).

TABLE 5.1.1.30.1

Reported aqueous solubilities of trichloroethylene at various temperatures

$$S/(\text{wt}\%) = 0.10494 + 4.9038 \times 10^{-5} \cdot (t/^\circ\text{C}) + 6.4541 \times 10^{-6} \cdot (t/^\circ\text{C})^2 - 1.8808 \times 10^{-8} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 1.4049 - 8.2223 \times 10^{-3} \cdot (T/\text{K}) + 1.3218 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Vallaud et al. 1957		Horvath 1982		Tse et al. 1992		Wright et al. 1992	
in Horvath 1982		summary of literature data		activity coefficient		activity coefficient	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
10	1280	0	1049	20	1483	20	1340
20	1285	10	1061	30	1450	30	1409
25	1288	20	1083	40	1468	40	1308
30	1290	25	1099				
40	1305	30	1117				
50	1330	40	1160				
		50	1212				
		60	1271				
		70	1335				
		80	1405				
		eq. 1	$S/\text{wt}\%$				

(Continued)

TABLE 5.1.1.30.1 (Continued)

2.

Horvath & Getzen 1999a				Knauss et al. 2000	
summary of literature data				batch equilibrium-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
at 1.0 MPa					
0	1450	40	1260	21	1417
5	1410	45	1270	50	1450
10	1370	50	1280	75	1878
15	1330	55	1300	99	2872
20	1310	60	1330	117	5268
25	1280				
30	1279	eq. 2	S/wt%		
35	1260	temp range 273–333 K			

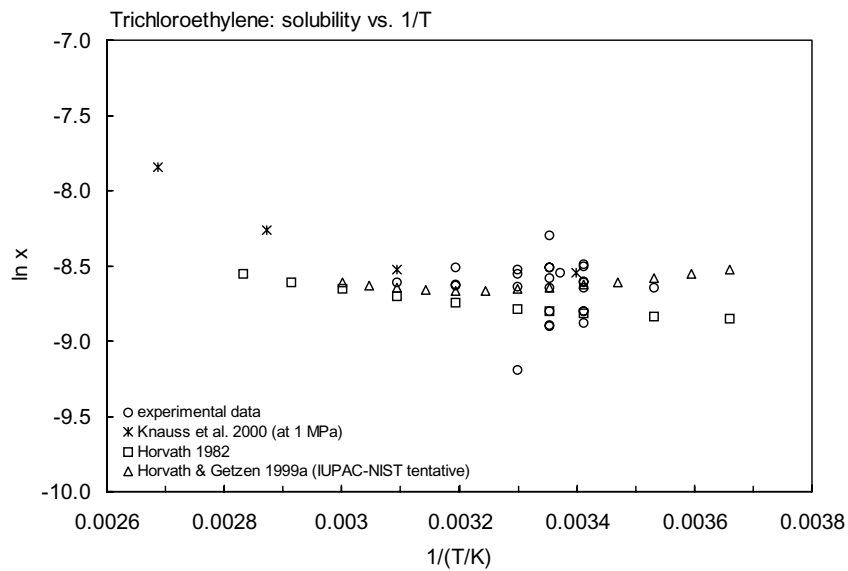


FIGURE 5.1.1.30.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.2

Reported vapor pressures of trichloroethylene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

Hertz & Rathmann 1912		McDonald 1944		Stull 1947	
		ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
25.0	9733	17.8	4239	-43.8	133.3
30.0	12266	19.85	7226	-22.8	666.6
38.0	18532	20.99	7506	-12.4	1333
44.15	23598	24.4	8813	-1.0	2666
45.0	24398	25.5	9546	11.9	5333
51.0	31197	27.4	10319	20.0	7999
65.0	31329	30.2	11999	31.4	13332
77.0	74927	31.2	12426	48.0	26664
87.15	101325	34.39	14292	67.0	53329
		38.49	17305	86.7	101325
		39.29	18025		
		42.41	20545	mp/°C	-73
		44.51	22425		
		46.44	24318		
		51.05	29264		
		55.8	35210		
		60.5	41876		
		65.07	48889		
		71.44	61115		
		76.93	72988		
		80.38	81966		
		85.82	97018		
		86.47	98992		

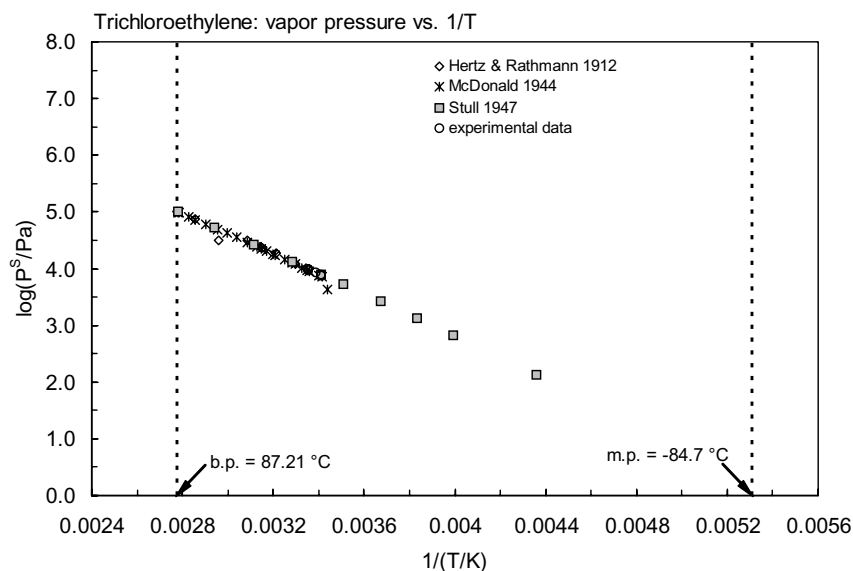


FIGURE 5.1.1.30.2 Logarithm of vapor pressure versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.3

Reported Henry's law constants of trichloroethylene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)	$\log (k_H/\text{atm}) = A - B/(T/K)$	(3a)
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

1.

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancredi & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
1.0	240	9.6	383	10	545.1	25	768
1.0	254.4	17.5	324.2	15	675.8	26.5	797.2
1.2	231.2	24.8	970.7	20	853.2	27.4	999.5
2.5	307.1	34.6	1510	25	1034	28.9	979.4
7.0	366.4			30	1297	28.9	828.7
10.0	424.4	eq. 4	H/(atm m ³ /mol)			29.7	881.2
12.0	464.7	A	11.37	eq. 4	H/(atm m ³ /mol)	29.9	1159
12.0	484.8	B	4780	A	7.845	33.3	1019
12.9	523.4			B	3702	35.6	1386
14.0	565.2					38.3	1554
18.0	683.9					40	1484
18.0	692.3					44.7	1638
18.0	683.9					45	2724
19.0	717.7					47.2	2504
19.2	761.1						

TABLE 5.1.1.30.3 (Continued)

Leighton & Calo 1981		Gossett 1987		Ashworth et al. 1988		Tancréde & Yanagisawa 90	
equilibrium cell-GC		EPICS-GC		EPICS-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
19.5	723.2					eq. 1a	K _{AW}
24.3	979.6					A	6.664
25.2	984.7					B	2141
25.3	995.3						
26.0	1005						
26.0	1028						
26.1	1018						
eq. 3	k _H /atm						
A	22.68						
B	4735						

2.

Tse et al. 1992		Wright et al. 1992		Robbins et al. 1993		Dewulf et al. 1995	
activity coefficient		activity coefficient		headspace-GC		EPICS-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
20	709	20	756	25	1043	2.0	231.05
30	1155	30	1152	30	1330	6.0	290.1
40	1753	40	1753	40	1672	10.0	327.2
				45	2270	18.2	615.3
				50	2665	25.0	870.1
						eq. 1	K _{AW}
						A	11.121
						B	3648

3.

Peng & Wan 1997		Knauss et al. 2000		Bierwagen & Keller 2001		Görgényi et al. 2002	
static headspace-GC		calculated-P/C(measured)		SPME-GC		EPICS-SPME method	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/Pa m ³ /mol
15	575	21	703.4	15	585	2.0	246
20	709	50	2552	25	823	6.0	348.6
25	885	75	4934	30	1114	10	447
30	1167	99	6854	40	1523	18	718
35	1309	117	6127			25	995
40	1650			eq 1	K _{AW}	30	1308
45	2005			A	9.9697	40	1871
				B	3287.5	50	2765
eq. 3	k _H /atm					60	3601
A	8.62					eq. 1	K _{AW}
B	1736					A	12.13
						B	3908.2

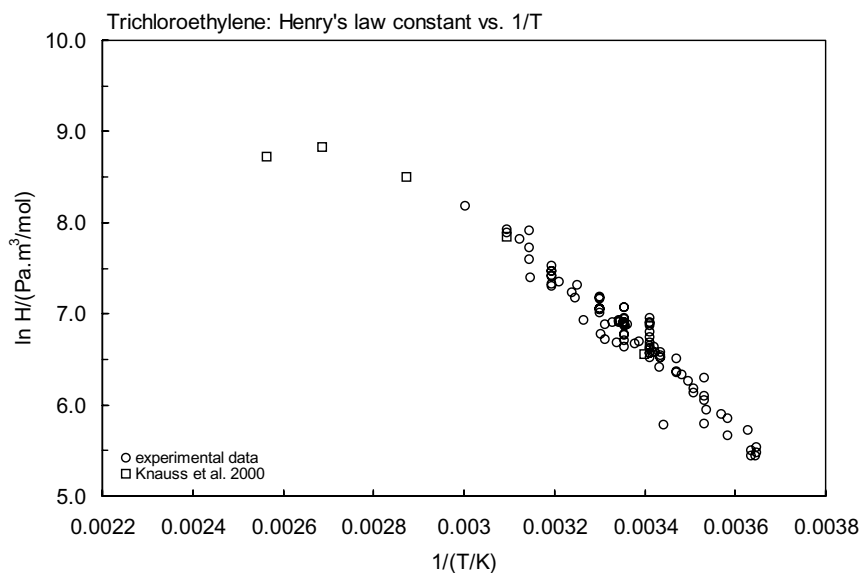


FIGURE 5.1.1.30.3 Logarithm of Henry's law constant versus reciprocal temperature for trichloroethylene.

TABLE 5.1.1.30.4
Reported octanol-water partition coefficients of
trichloroethylene at various temperatures

Dewulf et al. 1999

EPICS-GC

t/°C	log K _{OW}
2.2	2.18
6.0	2.18
10.0	2.28
14.1	2.24
18.7	2.29
24.8	2.20

change in enthalpy:

$$\Delta H_{OW}/(\text{kJ mol}^{-1}) = 3.4$$

(-8.4 to 15.2)

enthalpy of transfer

$$\Delta H_{oct}/(\text{kJ mol}^{-1}) = 2.7$$

(-9.0 to 14.5)

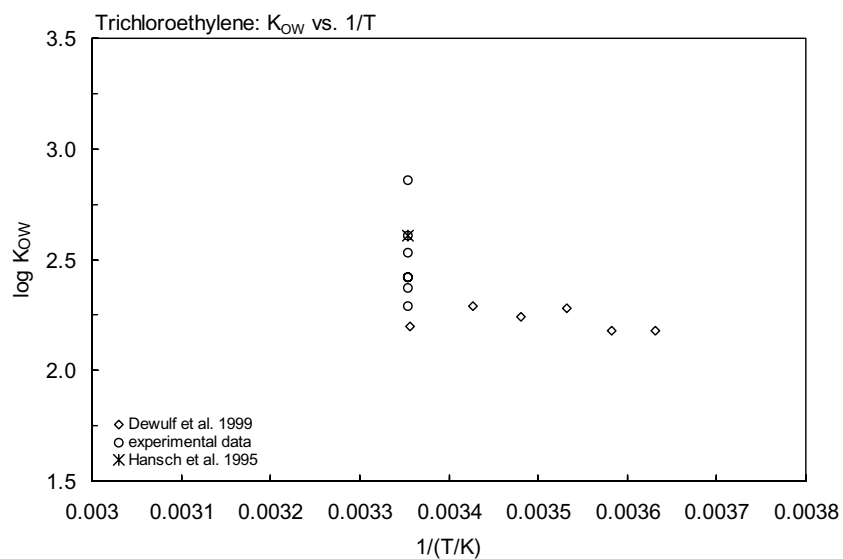
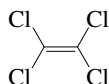


FIGURE 5.1.1.30.4 Logarithm of K_{OW} versus reciprocal temperature for trichloroethylene.

5.1.1.31 Tetrachloroethylene



Common Name: Tetrachloroethylene

Synonym: ethylene tetrachloride, perchloroethene, perchloroethylene, tetrachloroethene, 1,1,2,2-tetrachloro-ethylene

Chemical Name: tetrachloroethylene

CAS Registry No: 127-18-4

Molecular Formula: C_2Cl_4 , $CCl_2=CCl_2$

Molecular Weight: 165.833

Melting Point ($^{\circ}C$):

-22.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

121.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.62272, 1.61446 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

1.6227 (Horvath 1982; Weast 1982-83)

1.62283, 1.61431 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

102.0 ($20^{\circ}C$, calculated-density)

128.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.61, 34.72 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.56 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

150 (selected from literature or measured in DuPont laboratories, data also presented in graph, temp range $0-80^{\circ}C$, McGovern 1943)

150 ($20^{\circ}C$, McConnell et al. 1975; Pearson & McConnell 1975)

130, 120, 140 (1.5, 20, $25^{\circ}C$, selected from literature, Dilling 1977)

200 ($20^{\circ}C$, shake flask-GC, Chiou et al. 1977)

400 (shake flask-GC, Freed et al. 1979)

136 ($37^{\circ}C$, shake flask-GC, Sato & Nakijima 1979)

486 (shake flask-LSC, Banerjee et al. 1980)

200 (shake flask-titration/turbidity, Coca & Diaz 1980, Coca et al. 1980)

478 (shake flask-LSC, Veith et al. 1980)

150* (summary of literature data, temp range $0-80^{\circ}C$, Horvath 1982)

242 ($23-24^{\circ}C$, shake flask-GC, Broholm et al. 1992)

286* ($19.5^{\circ}C$, shake flask-GC/TC, measured range $0-91.8^{\circ}C$, Stephenson 1992)

256 (activity coeff. by inert gas stripping-GC, Li et al. 1993)

258.8 ($20^{\circ}C$, limiting activity coeff. by inert air stripping-GC, Hovorka & Dohnal 1997)

206* (tentative value, temp range $0-70^{\circ}C$, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 0.26479 - 1.5487 \times 10^{-3} \cdot (T/K) + 2.4477 \times 10^{-6} \cdot (T/K)^2$, temp range 273-343 K (equation derived from reported solubility data, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

192.3* ($22^{\circ}C$, batch equilibrium-GC, sample prepared at 1.0 MPa, measure range $22-161^{\circ}C$, Knauss et al. 2000)

215 (deionized water, batch equilibrium, Ladaa et al. 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 2666 (extrapolated, data presented in graph, McGovern 1943)
 2397* (Antoine eq. regression, temp range -20.6 to 120.8°C, Stull 1947)
 2462 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)
 $\log(P/\text{mmHg}) = 7.02003 - 1415.5/(221.0 + t/^\circ\text{C})$; temp range 34–187°C (Antoine eq. for liquid state, Dreisbach 1959)
 2453* (vapor-liquid equilibrium VLE data, measured range 27.887–108°C, Polák et al. 1970)
 $\log(P/\text{mmHg}) = 7.05854 - 1438.947/(233.368 + t/^\circ\text{C})$; temp range 27.887–108°C (ebulliometry, Polák et al. 1970)
 4524* (37.088°C, temp range 37.088–119.650°C, Boublik & Aim 1972; quoted, Boublik et al. 1984)
 2394 (calculated-Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 9240.5/(T/\text{K})] + 8.026207$; temp range -20.6 to 120.8°C (Antoine eq., Weast 1972–73)
 2388 (calculated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 6.97183 - 1386.915/(217.526 + t/^\circ\text{C})$; temp range 37–119°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 1866 (20°C, McConnell et al. 1975; Pearson & McConnell 1975)
 640, 1893, 2480 (1.5, 20, 25°C, interpolated from literature data, Dilling 1977)
 2417, 2456 (calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.10343 - 1387.956/(217.64 + t/^\circ\text{C})$, temp range: 37–120°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.19467 - 1445.722/(224.074 + t/^\circ\text{C})$, temp range: 26.9–108°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 2465 (Daubert & Danner 1986; quoted, Howard 1990)
 2462 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.10170 - 1386.90/(217.52 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 2415 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.1017 - 1386.9/(-55.63 + T/\text{K})$, temp range: 310–393 K, (Antoine eq., Stephenson & Malanowski 1987)
 2479, 4319 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 30.4038 - 1.5265 \times 10^3/(T/\text{K}) - 8.783 \cdot \log(T/\text{K}) - 2.6364 \times 10^{-9} \cdot (T/\text{K}) + 9.4381 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 142–306 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 2718 (exptl.-1/K_{AW} = C_w/C_A, Hine & Mookerjee 1975)
 248, 581 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)
 1621 (20°C, batch stripping-GC, Mackay et al. 1979)
 2006 (20°C, calculated-P/C, Kavanaugh & Trussell 1980)
 $\log(H/\text{atm}) = 10.38 - 2159.0/(T/\text{K})$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)
 1635* (equilibrium cell-concn ratio-GC/FID, measured range 1–26.1°C, Leighton & Calo 1981)
 $\ln(k_H/\text{atm}) = 16.05 - 3539/(T/\text{K})$; temp range 1.0–26.1°C (equilibrium cell-concn ratio, Leighton & Calo 1981)
 1528 (20°C, gas stripping-GC, Munz & Roberts 1982)
 1316 (20°C, EPICS-GC, Lincoff & Gossett 1983; Gossett 1985)
 1317; 1175 (20°C, EPICS-GC; gas stripping-GC, measured range 10–30°C, Lincoff & Gossett 1984)
 $\ln[H/(\text{atm m}^3/\text{mol})] = 13.12 - 5119/(T/\text{K})$; temp range 10–30°C (EPICS measurements, Lincoff & Gossett 1984)
 $\ln[H/(\text{atm m}^3/\text{mol})] = 11.32 - 4622/(T/\text{K})$; temp range 10–30°C (batch air stripping measurements, Lincoff & Gossett 1984)
 2908 (adsorption isotherm, Urano & Murata 1985)
 1445 (20°C, multiple equilibration, Munz & Roberts 1986)
 1852* (EPICS-GC, measured range 9.6–34.6°C, Gossett 1987)
 $\ln[H/(\text{atm m}^3/\text{mol})] = 12.45 - 4918/(T/\text{K})$; temp range 9.6–34.6°C (EPICS measurements, Gossett 1987)
 1445 (20°C, EPICS-GC, Munz & Roberts 1987)
 $\log K_{AW} = 5.92 - 1802/(T/\text{K})$; temp range 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

- 2908 (gas stripping-GC, Warner et al. 1987)
 1304 (20°C, EPICS-GC, Yurteri et al. 1987)
 1733* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 10.65 - 4368/(T/K)$; temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)
 1363* (tap water, EPICS-GC, temp range 25–47.2°C, Tancréde & Yanagisawa 1990)
 $\log K_{AW} = 7.481 - 2279/(T/K)$; temp range 25–47.2°C (EPICS-GC, Tancréde & Yanagisawa 1990)
 2721 (computed value, Yaws et al. 1991)
 1759* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 $\ln (1/K_{AW}) = -5.13 + 1736/(T/K)$; temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
 1599 (γ^∞ from gas stripping-GC, Li et al. 1993)
 1723* (static headspace-GC, temp range 25–45°C, Robbins et al. 1993)
 1490* (EPICS-GC/FID, temp range 2–25°C, Dewulf et al. 1995)
 717, 1914 (6.0, 25°C, EPICS-GC, natural sea water with salinity of 35‰, Dewulf et al. 1995)
 $\ln K_{AW} = -4528/(T/K) + 0.01080\cdot Z + 14.655$; with Z salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)
 1319 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 1200 (20°C, inert air stripping-GC, Hovorka & Dohnal 1997)
 1710* (equilibrium headspace-GC, temp range 15–45°C, Peng & Wan 1997)
 $\log (k_H/\text{atm}) = 9.06 - 1822/(T/K)$, temp range 15–45°C (headspace-GC measurements, Peng & Wan 1997)
 1260 (20°C, headspace equilibrium-GC, Peng & Wan 1998)
 2200* (sea water 36‰ NaCl, headspace-GC, temp range 15–45°C, Peng & Wan 1998)
 $\log (k_H/\text{atm}) = 9.09 - 1795/(T/K)$; sea water 36‰ NaCl, temp range 15–45°C (headspace-GC measurements, Peng & Wan 1998)
 1159.2 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 2890 (modified EPICS method-GC, Ryu & Park 1999)
 1781* (calculated-P/C(exptl. measured), temp range 22–161°C, Knauss et al. 2000)
 1690 (static headspace method, Ladaa et al. 2001)
 1299 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)
 $\log K_{AW} = 6.394 - 1955/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C. Additional data at other temperatures designated * are compiled at the end of this section:

- 2.60 (shake flask-GC, Chiou et al. 1977)
 2.60 (shake flask, Hansch & Leo 1979)
 2.53 (shake flask-LSC, Banerjee et al. 1980)
 2.53 (shake flask-LSC, Veith et al. 1980,1983; Veith & Kosian 1982)
 2.67 (RP-HPLC-RT correlation, Veith et al. 1980)
 3.78 (HPLC-RT correlation, McDuffie 1981)
 3.30, 2.72–3.57 (shake flask method: mean, range of mean values, OECD 1981)
 3.40 (shake flask, Hansch & Leo 1985, 1987)
 3.40 (correction of Ball & Roberts 1991 selection, Ball & Roberts 1992)
 3.40 (recommended, Sangster 1993)
 3.40 (recommended, Hansch et al. 1995)
 2.27* (24.8°C, EPICS-GC, measured range 2.2–24.8°C Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 3.48 (head-space GC/FID, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 1.59 (trout, Neely et al. 1974)
 1.598 (trout muscle, calculated-ratio of rate const. k_1/k_2 , Neely et al. 1974)
 1.45–1.88 (calculated- K_{OW} , Veith et al. 1979; Veith et al. 1980)
 –1.70 (male Albino rats, Geyer et al. 1980)
 1.69 (bluegill sunfish, Barrows et al. 1980)

- 1.49 (calculated-S, Kenaga 1980)
- 1.69 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
- 2.35 (calculated- K_{OW} , Lyman et al. 1982)
- 2.40 (microorganisms-water, Mabey et al. 1982)
- 2.06 (rainbow trout, Veith & Kosian 1982)
- 1.70 (calculated-MCI χ , Koch 1983)
- 1.70, 2.30 (quoted, calculated, Sabljic 1987)
- 1.60 (calculated-solvatochromic parameters, Hawker 1990)
- 2.40 (calculated- K_{OW} , McCarty et al. 1992)
- 1.79 (rainbow trout, Saito et al. 1992)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 2.38 (calculated, Kenaga & Goring 1980, Kenaga 1980)
- 2.32 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
- 2.14; 2.54, 2.89; 2.35, 2.57 (calculated- K_{OW} ; calculated-S and mp; calculated-S, Karickhoff 1981)
- 2.23 (average of 3 sediments and 5 soils, batch equilibrium, Schwarzenbach & Westall 1981)
- 2.04 (Schwarzenbach & Westall 1981)
- 3.23 (calculated- K_{OW} , Lyman et al. 1982)
- 2.38 (peaty soil, calculated- K_{OM} , Friesel et al. 1984)
- 2.56 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
- 2.56 (soil, Chiou et al. 1988)
- 2.00 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.76, 2.53 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 1.75 (untreated Marlette soil B_t horizon, OC 0.30%, batch equilibrium, Lee et al. 1989)
- 2.87, 2.78 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.64 (20°C, soil, sand and loess, sorption isotherm-headspace method, Grathwohl 1990)
- 3.29 (20°C, weathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 4.03 (20°C, unweathered shale and mudrock, sorption isotherm-headspace method, Grathwohl 1990)
- 2.39, 2.57 (20°C, calculated- K_{OW} , Grathwohl 1990)
- 2.14 (calculated-molecular conductivity index, Olsen & Davis 1990)
- 2.45 (2.57% organic carbon in surface soil, Pignatello 1990,1991)
- 1.81–2.95 (calculated- K_{OW} , Ball & Roberts 1991)
- 3.60 (Borden organic phase with no mineral sorption, Ball & Roberts 1991)
- 2.90 (Borden organic phase with no mineral sorption but with Curtis et al. 1986 correlation, Ball & Roberts 1992)
- 2.62, 2.79, 2.74, 2.80, 2.85, 2.78, 2.83 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon f_{OC} = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)
- 0.393–1.943 (19 soils from U.S. and China with polar organic carbon POC ranging from 2.89–59.9% and organic carbon OC ranging from 1.08–50.8%, batch sorption equilibrium, Kile et al. 1999)
- 1.13–2.11 (9 freshwater sediments from U.S. and China with polar organic carbon POC ranging from 5.36–52.5% and organic carbon OC ranging from 0.58–5.62%, batch sorption equilibrium, Kile et al. 1999)
- 2.32, 2.45, 2.22 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, 0.1 \leq OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM} :

- 1.70 (untreated A horizon Marlette soil, Lee et al. 1989)
- 2.56, 2.30(A horizon Marlette soil treated with HDTMA, DDTMA, Lee et al. 1989)
- 1.64 (untreated B_t horizon Marlette soil, Lee et al. 1989)
- 2.75, 2.64 (treated B_t horizon Marlette soil with HDTMA, DDTMA, Lee et al. 1989)
- 2.32, 1.90 (quoted, calculated-molecular conductivity index, Olsen & Davis 1990)
- 3.20; 2.40 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2}(\text{exptl}) = (27 \pm 3)$ min for 1 mg/L in water when stirred at 200 rpm at approximately 25°C in an open container of 65 mm deep and $t_{1/2}(\text{calc}) = 0.56$ min (Dilling et al. 1975; quoted, Callahan et al. 1979; Mills et al. 1982)

Evaporation $t_{1/2}(\text{exptl}) = 20\text{--}27.1$ min, $t_{1/2}(\text{calc}) = 0.20, 26.5$ min at 20–25°C, and $t_{1/2}(\text{exptl}) = 37.5$ min, $t_{1/2}(\text{calc}) = 27$ min at 15°C from water (Dilling 1977)

ratio of evaporation rate constant to that of oxygen reaeration: a measured value of 0.44 to that of 0.40 as predicted (Smith et al. 1980);

$t_{1/2} = 5\text{--}12$ d from pond, $t_{1/2} = 3$ h–7 d from river, $t_{1/2} = 3.6\text{--}14$ d from lake were estimated using representative reaeration rates (Lyman et al. 1982; quoted, Howard 1990);

estimated $t_{1/2} \sim 4.2$ h from water (Thomas 1982);

rate constants: $k = 0.028$ d⁻¹, $t_{1/2} = 25$ d in spring at 8–16°C, $k = 0.051$ d⁻¹, $t_{1/2} = 14$ d in summer at 20–22°C, $k = 0.056$ d⁻¹, $t_{1/2} = 12$ d in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.057$ d⁻¹, $t_{1/2} = 12.1$ d with HgCl₂, and $k = 0.058$ d⁻¹, $t_{1/2} = 12.0$ d without HgCl₂ as poison in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Photolysis: photocatalyzed mineralization by the presence of TiO₂ with the rate of 6.8 ppm/min per gram of catalyst (Ollis 1985); rate constant of 3.09×10^{-3} h⁻¹ with H₂O₂ under photolysis at 25°C in F-113 solution and with HO⁻ in the gas (Dilling et al. 1988).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{O}_3} < 2 \times 10^{-23}$ cm³ molecule⁻¹ s⁻¹ at 297 K (Mathias et al. 1974; quoted, Atkinson & Carter 1984; Tuazon et al. 1984; Atkinson et al. 1987)

$k_{\text{OH}} = 1.3 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ with a lifetime about 10 d (Yung et al. 1975; quoted, Callahan et al. 1979)

$k_{\text{OH}} = 1.7 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at 296 K (discharge flow system-LMR, Howard 1976)

$k_{\text{OH}}^* = (1.69 \pm 0.07) \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at 297 K, measured range 297–420 K with calculated lifetime of 0.4–0.6 yr in troposphere (discharge flow system-RF, Chang & Kaufman 1977)

$k_{\text{OH}} = (0.13 \pm 0.04) \times 10^{10}$ cm³ M⁻¹ s⁻¹ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1978)

$k_{\text{OH}} = 1.70 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson et al. 1979, 1982; quoted, Tuazon et al. 1984; Atkinson et al. 1987)

$k_{\text{OH}} = 1.7 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹, residence time of 68 d, loss of 1.5% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$k_{\text{OH}} = 1.0 \times 10^{11}$ cm³ mol⁻¹ s⁻¹, and $k_{\text{O}_3} = 1.0 \times 10^3$ cm³ mol⁻¹ s⁻¹ at 300 K (estimated, Lyman 1982)

$k \ll 100$ M⁻¹ h⁻¹ for singlet oxygen 25°C (Mabey et al. 1982)

completely degraded in an hour (Dimitriades et al. 1983; quoted, Howard 1990)

$k < 0.1$ M⁻¹ s⁻¹ for reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{O}_3} < 2 \times 10^{-23}$ cm³ molecule⁻¹ s⁻¹, $k_{\text{OH}} = 1.7 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Tuazon et al. 1984)

$k_{\text{OH}}^* = 1.67 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 4.2 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹, $k_{\text{OH}}(\text{obs.}) = 1.7 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{\text{NO}_3} < 4.0 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{\text{NO}_3} < 4.0 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ with a calculated atmospheric lifetime $\tau > 240$ d, $k_{\text{OH}} = 1.7 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ with lifetime $\tau = 140$ d, and $k_{\text{O}_3} < 2 \times 10^{-23}$ cm³ molecule⁻¹ s⁻¹ with a lifetime $\tau > 2 \times 10^3$ yr at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 1.8 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹, $k_{\text{OH}}(\text{obs.}) = 1.66 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}} = 2.34 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K, $k_{\text{NO}_3} = 9.7 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ at 296 K (Atkinson 1990)

$k_{\text{NO}_3} < 5.20 \times 10^{-17}$ cm³ molecule⁻¹ s⁻¹ relative to ethene at 298 ± 2 K (Atkinson 1991)

Hydrolysis: $k = 0.079$ month⁻¹ at 25°C with $t_{1/2} = 8.8$ months (Dilling et al. 1975; quoted, Callahan et al. 1979); abiotic hydrolysis or dehydrohalogenation $t_{1/2} = 8.8$ months (Olsen & Davis 1990)

Biodegradation: aqueous aerobic $t_{1/2} = 4320\text{--}8640$ h, based on aerobic river die-away test data (Mudder 1981; quoted, Howard et al. 1991) and saltwater grab sample test data (Jensen & Rosenberg 1975; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2352\text{--}39672$ h, based on anaerobic screening test data (Bouwer et al. 1981; quoted, Howard et al. 1991);

first-order $k = 1.1$ yr⁻¹ with $t_{1/2} = 230$ d (Roberts et al. 1982; quoted, Olsen & Davis 1990)

$t_{1/2} = 34$ d (Wood et al. 1985; quoted, Olsen & Davis 1990).

$t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 98$ d in natural waters (Capel & Larson 1995)

Biotransformation: estimated rate constant for bacteria $k = 1 \times 10^{-10}$ ml cell⁻¹ h⁻¹ (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 3.323$ h⁻¹; $k_2 = 0.0823$ h⁻¹ (trout muscle, Neely et al. 1974)

$k_1 = 11.4$ h⁻¹ (flagfish, calculated-BCF $\times k_1$, McCarty et al. 1992)

$k_2 = 0.0454$ h⁻¹ (flagfish, estimated-one compartment first-order kinetic, McCarty et al. 1992)

$k_1 = 3.30$ h⁻¹; $k_2 = 0.0833$ h⁻¹ (trout, Hawker & Connell 1985)

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} = 12$ wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

disappearance $t_{1/2} > 10$ d for the reaction with OH radical (Darnall et al. 1976);

lifetime ~ 10 d, based on reaction with OH radical (Yung et al. 1975; quoted, Callahan et al. 1979);

photodecomposition $t_{1/2} = 14.2$ h with NO and $t_{1/2} = 8.3$ h with NO₂ under simulated atmospheric conditions (Dilling et al. 1976);

estimated N. troposphere residence time of 150 d by one compartment nonsteady state model (Singh et al. 1978);

lifetime of 1.0 yr in troposphere (Altshuller 1980);

residence time of 68 d, loss of 1.5% in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

estimated troposphere residence time of 200–390 d (Lyman 1982);

$t_{1/2} = 384$ – 3843 h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric lifetimes: $\tau > 240$ d for the reaction with NO₃ for a 12-h nighttime average concentration of 2.4×10^9 molecule/cm³, $\tau = 140$ d for the reaction with OH radical for a 12-h average concentration of 1.0×10^6 molecule/cm³, and $\tau > 2000$ yr for the reaction with O₃ for a 24-h average concentration of 7×10^{11} molecule/cm³ (Atkinson et al. 1987).

Surface water: estimated $t_{1/2} = 9.9$ – 32 d in surface waters at various locations in case of a first order reduction process; $t_{1/2} = 3$ – 30 d in rivers, $t_{1/2} = 30$ – 300 d in lakes and ground waters (Zoeteman et al. 1980)

$t_{1/2} = 25$ d in spring at 8–16°C, 14 d in summer at 20–22°C and 12 d in winter at 3–7°C when volatilization dominates, and $t_{1/2} = 12.1$ d and 12.0 d for experiments with and without HgCl₂ as poison respectively in September 9–15 in marine mesocosm (Wakeham et al. 1983)

$t_{1/2} = 4320$ – 8640 h, based on aerobic river die-away test data (Mudder 1981; quoted, Howard et al. 1991) and saltwater sample grab data (Jensen & Rosenberg 1975; quoted, Howard et al. 1991);

calculated $t_{1/2} = 10$ d and 32 d concentration reduction between sampling points on the Rhine River and a lake in the Rhine basin, respectively (Zoeteman et al. 1980; quoted, Howard 1990)

$t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 98$ d in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2} = 8640$ – 17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} < 10$ d (Ryan et al. 1988);

$t_{1/2} = 4320$ – 8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $t_{1/2} < 1$ d in tissues of bluegill sunfish (Barrows et al. 1980);

$t_{1/2} = 14$ h, clearance from fish in simulated ecosystem (Neely 1980);

$t_{1/2} < 10$ d, subject to plant uptake via volatilization (Ryan et al. 1988);

$t_{1/2} = 0.4$ – 0.5 d to eliminate from small fish (McCarty et al. 1992).

TABLE 5.1.1.31.1

Reported aqueous solubilities of tetrachloroethylene at various temperatures

$$S/(\text{wt}\%) = 1.49696 \times 10^{-2} - 7.8009 \times 10^{-6} \cdot (t/^{\circ}\text{C}) - 5.1403 \times 10^{-7} \cdot (t/^{\circ}\text{C})^2 + 3.6938 \times 10^{-8} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 0.26479 - 1.5487 \times 10^{-3} \cdot (T/\text{K}) + 2.4477 \times 10^{-6} \cdot (T/\text{K})^2 \quad (2)$$

Horvath 1982		Stephenson 1992		Horvath & Getzen 1999a		Knauss et al. 2000	
summary of literature data		shake flask-GC		summary of literature data		batch equilibrium-GC	
t/ $^{\circ}\text{C}$	S/g·m ⁻³	t/ $^{\circ}\text{C}$	S/g·m ⁻³	t/ $^{\circ}\text{C}$	S/g·m ⁻³	t/ $^{\circ}\text{C}$	S/g·m ⁻³
at 1.0 MPa							
0	149.7	0	273	0	244	23	192.3
10	148.8	9.5	270	5	234	51	247.4
20	149	19.5	286	10	224	75	313.8
25	150.3	31.1	221	15	218	101	519
30	152.7	40.0	213	20	211	124	1006
40	162	50.1	273	25	206	150	1895
50	179.1	61.3	304	30	202	161	2513
60	206.3	71	377	35	200		
70	245.7	80.2	380	40	198		
80	299.7	91.8	523	45	198		
				50	199		
eq. 1	S/wt%			55	202		
				60	205		
				65	210		
				70	216		
				eq. 2	S/wt%		
				temp range 273–343 K			

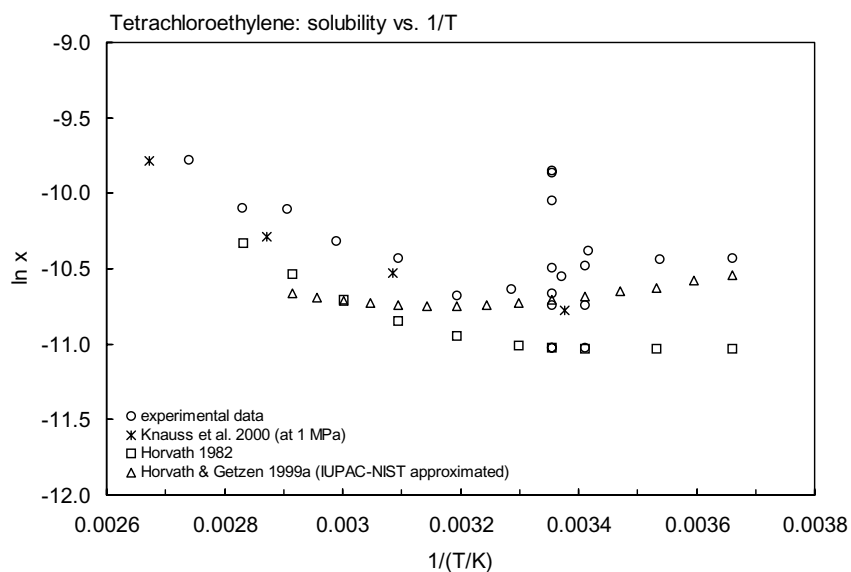
FIGURE 5.1.1.31.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.2

Reported vapor pressures of tetrachloroethylene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Polak et al. 1970		Boublik & Aim 1972	
summary of literature data		vapor-liquid equilibrium		in Boublik et al. 1984	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-20.6	133.3	27.887	2869	37.088	4524
2.40	666.6	35.758	4274	46.239	6967
13.8	1333	41.702	5689	52.671	9306
26.3	2666	46.502	7101	58.697	12046
40.1	5333	57.065	11276	63.270	14549
49.2	7999	61.254	15412	68.545	17921
61.3	13332	68.065	17620	73.064	21314
79.8	26664	74.529	22541	78.165	25780
100.0	53329	81.957	29555	82.292	29923
120.8	101325	88.055	36557	87.183	35493
		94.568	45465	91.791	41470
mp/ $^{\circ}\text{C}$	-19.0	98.917	52316	97.291	49704
		104.269	61875	103.930	61295
		107.692	68694	111.548	77125
				119.650	97337
				eq. 2	P/kPa
				A	6.10343
				B	1387.956
				C	217.640
				bp	121.074

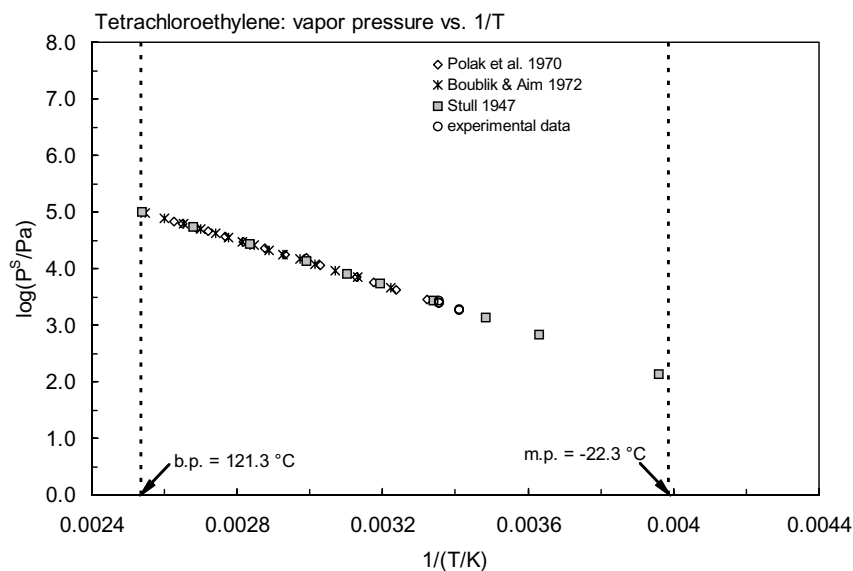


FIGURE 5.1.1.31.2 Logarithm of vapor pressure versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.3

Reported Henry's law constants of tetrachloroethylene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)	$\log (k_H/\text{atm}) = A - B/(T/K)$	(3a)
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

1.

Leighton & Calo 1981		Gossett 1987		Tancredi & Yanagisawa 1990		Kolb et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		equilibrium headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
1.0	377.4	9.6	691	25	1363	40	1759
1.0	413.5	17.5	1186	26.5	1694	60	2080
1.2	430.6	24.8	1793	27.4	2224	70	3658
2.5	474.9	34.6	2857	28.9	2160	80	3375
7.0	572.9			28.9	2034		
10.0	675.2			29.7	2770	eq. 2	1/K _{AW}
12.0	731.4	eq. 4	H/(atm m ³ /mol)	29.9	2998	A	-5.13
12.0	797.6	A	12.45	33.3	3057	B	-1736
12.9	826.0	B	4918	35.6	2413		
14.0	914.7			38.3	2745		
18.0	1122			40	4895		
18.0	1144	Ashworth et al. 1988		44.7	5549		
18.0	1145	EPICS-GC		45	6004		
19.0	1176	t/°C H/(Pa m ³ /mol)		47.2	5886		
19.2	1156						
19.5	1182	10	857.2	eq. 1a	K _{AW}		

TABLE 5.1.1.31.3 (Continued)

Leighton & Calo 1981		Gossett 1987		Tancredi & Yanagisawa 1990		Kolb et al. 1992	
equilibrium cell-GC		EPICS-GC		EPICS-GC		equilibrium headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
24.3	1583	15	1125	A	7.481		
25.2	1623	20	1429	B	2279		
25.3	1651	25	1733				
26.0	1636	30	2482				
26.0	1712						
26.1	1679	eq. 4	H/(atm m ³ /mol)				
		A	10.65				
eq. 3	k _H /atm	B	4368				
A	22.68						
B	4735						

2.

Robbins et al. 1993		Dewulf et al. 1995		Peng & Wan 1997		Knauss et al. 2000	
headspace-GC		EPICS-GC		equilibrium headspace-GC		calculated-P/C	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
25	1723	2.0	359.2	15	1016	22	1781
30	2340	6.0	2492	20	1272	51	5837
40	3070	10.0	602.7	25	1710	75	10328
45	2847	18.2	995.6	30	2160	101	18540
		25.0	1490	35	2713	124	19157
				40	3283	150	20200
		eq. 1	K _{AW}	45	4108	161	19844
		A	14.655	eq. 3a	k _H /atm		
		B	4528	A	9.06		
				B	1822		

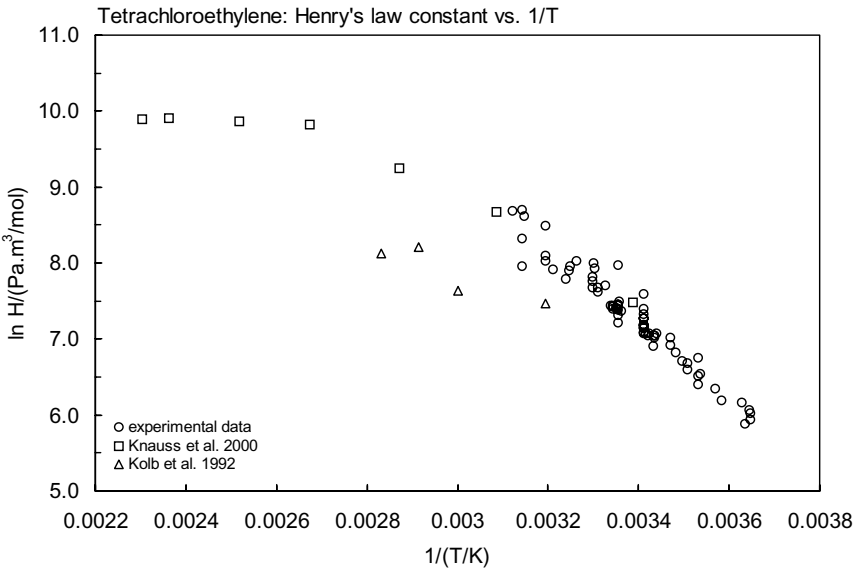


FIGURE 5.1.1.31.3 Logarithm of Henry's law constant versus reciprocal temperature for tetrachloroethylene.

TABLE 5.1.1.31.4

Reported octanol-water partition coefficients of tetrachloroethylene at various temperatures

Dewulf et al. 1999

EPICS-GC	
t/°C	log K _{OW}
2.2	2.25
6.0	2.27
10.0	2.38
14.1	2.32
18.7	2.36
24.8	2.27

change in enthalpy:

$$\Delta H_{OW}/(\text{kJ mol}^{-1}) = 2.6$$

(-11.1 to 16.3)

enthalpy of transfer

$$\Delta H_{\text{oct}}/(\text{kJ mol}^{-1}) = 4.7$$

(-9.0 to 18.4)

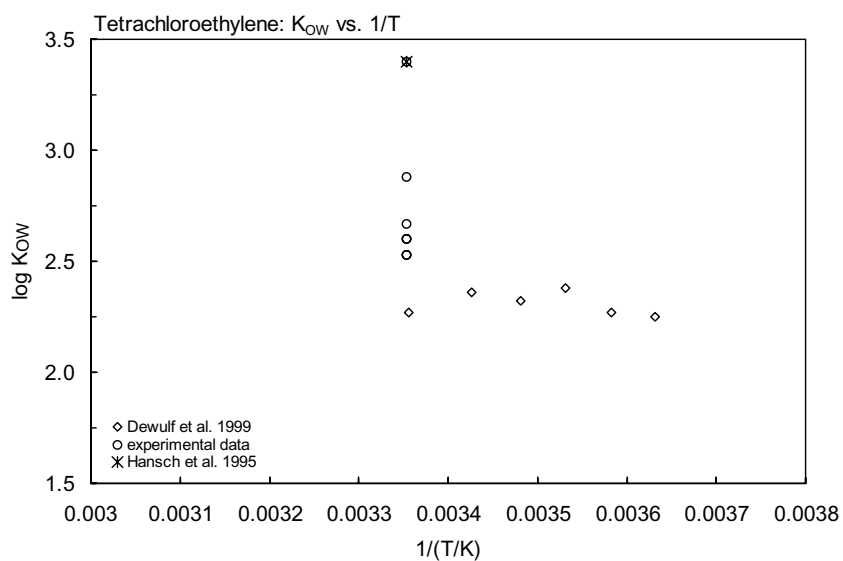
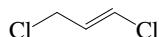


FIGURE 5.1.1.31.4 Logarithm of K_{OW} versus reciprocal temperature for tetrachloroethylene.

5.1.1.32 1,3-Dichloropropene



Common Name: 1,3-Dichloropropene

Synonym: 1,3-dichloropropylene, 1,3-dichloro-1-propene, Telone II

Chemical Name: 1,3-dichloropropene

CAS Registry No: 542-75-6

Molecular Formula: $C_3H_4Cl_2$, $CH_2ClCH=CHCl$

Molecular Weight: 110.970

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

112.0 (*trans*-stereoisomer I, Horvath 1982; McNally & Grob 1984; Dean 1985; Lide 2003)

104.3 (*cis*-stereoisomer II, Horvath 1982; McNally & Grob 1984; Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.224 (*trans*-stereoisomer I, Horvath 1982; McNally & Grob 1984)

1.217 (*cis*-stereoisomer II, Horvath 1982; McNally & Grob 1984)

Molar Volume (cm^3/mol):

91.2 (*trans*-stereoisomer I, $20^{\circ}C$, calculated-density)

90.7 (*cis*-stereoisomer II, $20^{\circ}C$, calculated from density)

108.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2800 (*trans*-stereoisomer I, Dilling 1977)

2700 (*cis*-stereoisomer II, Dilling 1977)

2723 (recommended, Horvath 1982)

1071 (*trans*-stereoisomer I, headspace-GC, McNally & Grob 1983)

1088 (*cis*-stereoisomer II, headspace-GC, McNally & Grob 1983)

1020 ($30^{\circ}C$, *trans*-stereoisomer I, headspace-GC, McNally & Grob 1984)

911 ($30^{\circ}C$, *cis*-stereoisomer II, headspace-GC, McNally & Grob 1984)

1000 ($20^{\circ}C$, Wauchope et al. 1992)

2250 (Wauchope et al. 1992)

4533, 4311, 4223 ($20, 30, 40^{\circ}C$, activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

4533, 5733 (*trans*-, *cis*-stereoisomer, data from Dow Chemicals, Dilling 1977)

435, 569 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

3333 ($20^{\circ}C$, selected, Mills et al. 1982)

3334 ($20^{\circ}C$, quoted, Warner et al. 1987)

3866 ($20^{\circ}C$, Wauchope et al. 1992)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

232 (calculated-P/C, Dilling 1977)

137 (calculated-P/C, Warner et al. 1987)

122, 198, 302 ($20, 30, 40^{\circ}C$, activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.98 (selected, Mills et al. 1982)

1.41 (quoted, Verhaar et al. 1992)

1.84 (*cis/trans*, calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

1.505 (soil, selected, Wauchope et al. 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 31$ min in water from stirring in an open container of depth 65 mm at 200 rpm (Dilling et al. 1975)

$t_{1/2}(\text{exptl}) = 29.6$ min, $t_{1/2}(\text{calc}) = 2.4$ min, 23.8 min for *cis*-stereoisomer, and $t_{1/2}(\text{calc}) = 3.2$ min, 24.6 min for *trans*-stereoisomer from water (Dilling 1977)

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (7.74 \pm 0.2) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ *cis*-isomer, $k_{OH} = (1.31 \pm 0.05) \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ for *trans*-isomer at $22 \pm 2^\circ\text{C}$, calculated $t_{1/2} = 12$ h and 7 h for the *cis*- and *trans*-isomer, respectively (relative rate method, Tuazon et al. 1984)

$k_{O_3} = 1.5 \times 10^{-19}$ cm³ molecule⁻¹ s⁻¹ *cis*-isomer, $k_{O_3} = 6.7 \times 10^{-19}$ cm³ molecule⁻¹ s⁻¹ for *trans*-isomer at room temp., calculated $t_{1/2} = 52$ d and 12 d for *cis*- and *trans*-isomer, respectively (relative rate method, Tuazon et al. 1984)

$k_{OH}(\text{calc}) = 1.1 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(\text{obs.}) = 7.5 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for *cis*-isomer; $k_{OH}(\text{calc}) = 1.3 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(\text{obs.}) = 1.26 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ for *trans*-isomer at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH}(\text{calc}) = 8.8 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(\text{obs.}) = 8.45 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for *cis*-isomer; $k_{OH}(\text{calc}) = 10.0 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(\text{obs.}) = 14.4 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for *trans*-isomer at room temp. (SAR [structure-activity relationship], Atkinson 1987)

Hydrolysis: $t_{1/2} = 133$ –271 h, based on measured rate constants for hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991); rate of hydrolysis is, however, independent of pH over the range of pH 5 to pH 10 (McCall 1987).

Biodegradation: aqueous aerobic $t_{1/2} = 168$ –672 h, based on unacclimated aqueous aerobic biodegradation screening studies (Tabak et al. 1981; Krijgheld & Van der Gen 1986; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ –2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 0.24$ –2.4 h from air for the reaction with OH radicals (Darnall et al. 1976);

$t_{1/2}(\text{calc}) = 12$ h and 7 h for the *cis*- and *trans*-isomer, respectively, for reactions with OH radical; $t_{1/2}(\text{calc}) = 52$ d and 12 d for *cis*- and *trans*-isomer, respectively, for reactions with O_3 at room temp. (Tuazon et al. 1984).

$t_{1/2} = 4.66$ –80.3 h, based on measured rate constants for reaction with OH radical and ozone (Howard et al. 1991)

Surface water: $t_{1/2} = 133$ –271 h, based on measured rate of hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 133$ –271 h, based on measured rate of hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 133$ –271 h, based on measured rate of hydrolysis at pH 7 and 25°C (Mill et al. 1985; quoted, Howard et al. 1991) and at pH 5 and 20°C (McCall 1987; quoted, Howard et al. 1991).

Biota:

5.1.1.33 Chloroprene



Common Name: Chloroprene

Synonym: 2-chloro-1,3-butadiene

Chemical Name: 2-chloro-1,3-butadiene

CAS Registry No: 126-99-8

Molecular Formula: C_4H_5Cl , $CH_2=CClCH=CH_2$

Molecular Weight: 88.536

Melting Point ($^{\circ}C$):

-130 (Kirk-Othmer 1985; Verschueren 1983; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

59.4 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

69.145 (Boublik et al. 1984)

Density (g/cm^3 at $20^{\circ}C$):

0.9583 (Weast 1982–83; Dean 1985)

0.9580 (Verschueren 1983)

Molar Volume (cm^3/mol):

92.4 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

102.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

964000 ($20^{\circ}C$, saturation concentration, Verschueren 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

26660, 36660 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

28740 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.30955 - 793.85/(181.137 + t/^{\circ}C)$, temp range: 20 – $60^{\circ}C$ (Antoine eq. from reported exptl. data Boublik et al. 1984)

28780 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.16150 - 783.45/(197.7 + t/^{\circ}C)$; temp range 20 – $60^{\circ}C$ (Antoine eq., Dean 1985, 1992)

29450 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.652 - 1545.3/(T/K)$; temp range: 279 – $333\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.6519 - 1545.0/(T/K)$; temp range 243 – $263\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

23200 (quoted, Howard 1989)

$\log(P/mmHg) = 8.9353 - 1.9176 \times 10^3/(T/K) + 0.73836 \cdot \log(T/K) - 8.4743 \times 10^{-3} \cdot (T/K) + 6.0224 \times 10^{-6} \cdot (T/K)^2$; temp range 143 – $525\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

3242 (estimated by bond contribution method, Howard 1989)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.03 (Howard 1989)

Bioconcentration Factor, $\log BCF$:

1.342 (estimated- K_{ow} , Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, $\log K_{oc}$:

2.498 (soil, estimated- K_{ow} , Lyman et al. 1982)

1.699 (soil, molecular topology and QSAR, Sabljic 1984)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 3$ h from a model river 1 m deep with a current velocity of 1 m/s and a wind speed of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.9\text{--}27.8$ h, based on estimated rate constants for the reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on aqueous aerobic screening test data for vinyl chloride (Helfgott et al. 1977; Freitag et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 0.24\text{--}2.4$ h from air for the reaction with OH radicals (Darnall et al. 1976);

$t_{1/2} = 1.8$ h for the reaction with photochemically produced hydroxyl radicals and $t_{1/2} = 12$ h for the reaction with ozone in atmosphere (Cupitt 1980; quoted, Howard 1989);

$t_{1/2} = 2.9\text{--}27.8$ h, based on estimated rate constants for reaction with hydroxyl radicals and ozone in air (Atkinson & Carter 1984; Atkinson 1987; quoted, Howard et al. 1991).

Surface water: estimated $t_{1/2} = 6.7\text{--}53$ d in surface waters at various locations in case of a first order reduction process; and $t_{1/2} = 3\text{--}30$ d in rivers, $t_{1/2} = 30\text{--}300$ d in lakes and ground waters (Zoeteman et al. 1980)

$t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

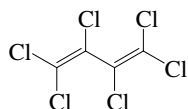
Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

5.1.1.34 Hexachlorobutadiene



Common Name: Hexachlorobutadiene

Synonym: HCBd, perchloro-1,3-butadiene

Chemical Name: 1,1,2,3,4,4-hexachloro-1,3-butadiene

CAS Registry No: 87-68-3

Molecular Formula: C_4Cl_6 , $Cl_2C=CClC=CCl_2$

Molecular Weight: 260.761

Melting Point ($^{\circ}C$):

-21.0 (Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

215 (Horvath 1982; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.682 (Horvath 1982)

Molar Volume (cm^3/mol):

155.2 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

206.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.20 (Melnikov 1971)

2.00 ($20^{\circ}C$, Pearson & McConnell 1975)

3.23 (shake flask-HPLC, Banerjee et al. 1980)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

20.0 ($20^{\circ}C$, Pearson & McConnell 1975)

$\log(P/kPa) = 6.06503 - 1520.873/(163.685 + t/^{\circ}C)$; temp range 70 – $200^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.4781 - 1783.8/(-84.48 + T/K)$; temp range 343 – $484\ K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

2604 (calculated-P/C, Warner et al. 1987)

1044 (batch stripping, Warner et al. 1987)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.74 (HPLC-RT correlation, Konemann et al. 1979)

4.78 (shake flask-HPLC, Banerjee et al. 1980)

4.63 (calculated-fragment const., Könemann 1981)

4.90 (shake flask-GC, both phases, Chiou 1985)

4.78 (recommended, Sangster 1993)

4.78 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

4.70 (Thomann 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2965\text{--}28650$ h, based on an estimated rate constant for vapor phase reaction with OH radicals (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: no hydrolyzable groups, rate constant at pH 7 is zero (Kollig et al. 1987).

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on monitoring data and acclimated aqueous screen test data (Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}17280$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: tropospheric $t_{1/2} \sim 1.0$ wk, when exposed outdoors to diurnal and climatic variations of incident radiation and temperature (Pearson & McConnell 1975)

$t_{1/2} = 2865\text{--}28650$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

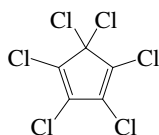
Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

5.1.1.35 Hexachlorocyclopentadiene



Common Name: Hexachlorocyclopentadiene

Synonym: 1,2,3,4,5,5-hexachlorocyclopentadiene, perchlorocyclopentadiene, HCCPD

Chemical Name: 1,2,3,4,5,5-hexachloro-1,3-cyclopentadiene

CAS Registry No: 77-47-4

Molecular Formula: C_5Cl_6

Molecular Weight: 272.772

Melting Point ($^{\circ}C$):

-9 (Lide 2003)

Boiling Point ($^{\circ}C$):

239 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$): 1.702

Molar Volume (cm^3/mol):

160.3 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

210.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.805 (Shake flask-LSC Lu et al. 1974)

1.80 (Zepp et al. 1979)

0.805 (Callahan et al. 1979; Dobbs et al. 1980; Geyer et al. 1981; Warner et al. 1987; Isnard & Lambert 1988)

1.80 ($28^{\circ}C$, vapor saturation or shake flask-GC, Wolfe et al. 1982)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

10.84 (Verschuereen 1977; Warner et al. 1987)

10.67 (Wolfe et al. 1982)

11.90 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.4813 - 2804.32/(T/K)$; temp range 335–512 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -9.7942 - 3.3161 \times 10^3/(T/K) + 10.171 \cdot \log(T/K) - 2.1115 \times 10^{-2} \cdot (T/K) + 9.2045 \times 10^{-6} \cdot (T/K)^2$; temp range 284–746 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$):

2736 (concentration ratio-GC, Wolfe et al. 1982)

1662 (batch stripping; Warner et al. 1987)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.04 (HPLC-RT correlation, McDuffie 1981)

5.04 ($28^{\circ}C$, concentration ratio-GC, Wolfe et al. 1982)

5.26 (HPLC-RT correlation, Eadsforth 1986)

5.04 (recommended, Sangster 1993)

5.04 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.53, 2.97, 3.21, 2.65 (algae, snail, mosquito, fish, Lu et al. 1975)

1.47 (fathead minnow, Veith et al. 1979)

3.04, 3.21 (*Chlorella*, calculated-solubility, Geyer et al. 1981)

- 1.47, 4.19 (quoted, calculated- K_{OW} , Mackay 1982)
 3.18, 3.89 (estimated-S and K_{OW} , Isnard & Lambert 1988)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.08 (sediment organic carbon, calculated- K_{OW} , Wolfe et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: appears to be important in flowing waters (Callahan et al. 1979).

Photolysis: near-surface photolysis is an important process with a rate constant $k = 4.9 \text{ d}^{-1}$ with $t_{1/2} = 11 \text{ min}$ (Callahan et al. 1979);

direct photolysis in natural waters in midday sunlight of Athens, Georgia at latitude 34°N and 83°W with $t_{1/2} < 10 \text{ min}$, and near-surface photolysis rate constant $k(\text{calc}) = 3.9 \text{ h}^{-1}$ on cloudless days averaged over both light and dark periods for a year (Wolfe et al. 1982);

photolysis $t_{1/2} = 1.0 \text{ min}$ to 10.7 min , based on photolysis studies in aqueous solutions (Butz et al. 1982; Wolfe et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 1.0$ to 8.9 h , based on calculated rate constants for the vapor phase reactions with OH radicals and O_3 in air (Cupitt 1980; quoted, Howard et al. 1991).

Hydrolysis: appears to be an important fate process with a rate constant $k = 5.6 \times 10^{-7} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 14 \text{ d}$ (Callahan et al. 1979);

reaction rate constant was independent of pH range of about 3 to 10 under most environmental conditions and an extrapolated rate constant $k = 4 \times 10^{-3} \text{ s}^{-1}$ was found at 25°C with $t_{1/2} = 173 \text{ h}$ (Wolfe et al. 1982; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 168$ to 672 h , based on aerobic aqueous screening test data (Tabak et al. 1981; Freitag et al. 1982; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ to 2688 h , based on aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 1.0$ to 8.9 h , based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 1.0 \text{ min}$ to 173 h , based on photolysis and hydrolysis half-lives (Howard et al. 1991); measured rate constant $k = (90 \pm 40) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $25 \pm 2^\circ\text{C}$, with $t_{1/2} = 6 \text{ min}$ at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 173$ to 1344 h , based on aerobic aqueous biodegradation and hydrolysis half-lives (Howard et al. 1991).

Sediment: hydrolysis rate constant in the sediment was assumed to be the same as that of water and decay rate constant $k = 1.5$ to $5.4 \times 10^{-5} \text{ s}^{-1}$ for natural pond sediment-water system (Wolfe et al. 1982).

Soil: $t_{1/2} = 168$ to 672 h , based on aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biota:

5.1.2 BROMOALKANES AND BROMOALKENES

5.1.2.1 Bromomethane



Common Name: Methyl bromide

Synonym: bromomethane, monobromomethane, Embafume, Terabol

Chemical Name: bromomethane, methyl bromide

CAS Registry No: 74-83-9

Molecular Formula: CH_3Br

Molecular Weight: 94.939

Melting Point ($^{\circ}\text{C}$):

-93.68 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

3.5 (Lide 2003)

Density (g/cm^3 at 20°C):

1.6755, 1.6617 (20°C , 25°C , Dreisbach 1961)

Molar Volume (cm^3/mol):

56.7 (20°C , calculated-density)

52.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

23.26, 24.098 (25°C , at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

13410* (vapor saturation-gravitational method, measured range 10 – 32°C , Haight 1951)

20700, 24140 (20°C , 25°C , gravitational method, Glew & Moelwyn-Hughes 1953)

14400 (Irmann 1965; Hine & Mookerjee 1975)

13400 (Jolles 1966; Günther et al. 1968)

12930 (Korenman et al. 1971)

900 (20°C , Verschueren 1977, 1983)

15223* (summary of literature data, temp range 5 – 80°C , Horvath 1982)

17500 (20°C , Windholz et al. 1983)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

256550 (interpolated-Antoine eq. regression, temp range -96.3 to 3.6°C , Stull 1947)

217700 (calculated-Antoine eq., Dreisbach 1959, 1961)

$\log(P/\text{mmHg}) = 6.95965 - 986.59/(238.32 + t/^{\circ}\text{C})$; temp range -58 to 53°C (Antoine eq. for liquid state, Dreisbach 1959, 1961)

$\log(P/\text{mmHg}) = 6.95965 - 986.590/(238.32 + t/^{\circ}\text{C})$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

183900 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 5925.9/(T/\text{K})] + 7.482362$; temp range -96.3 to 190°C (Antoine eq., Weast 1972–73)

218930 (calculated-Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 7.08823 - 1044.42/(244.684 + t/^{\circ}\text{C})$ (Antoine eq., Kudchadker et al. 1979)

187000 (20°C , Thomas 1982)

216900, 219000 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.20369 - 1041.723/(244.36 + t/^{\circ}\text{C})$; temp range -69.9 to 4.5°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.2243 - 1049.898/(245.319 + t/^{\circ}\text{C})$; temp range -70 to 3.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.21313 - 1044.42/(224.684 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
217680 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.08455 - 986.59/(-34.83 + T/\text{K})$; temp range 201–296 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 29.3988 - 2.0406 \times 10^3/(T/\text{K}) - 7.9966 \cdot \log (T/\text{K}) - 4.1899 \times 10^{-10} \cdot (T/\text{K}) + 5.0174 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 179–467 K (vapor pressure eq., Yaws 1994)

218630 (selected and summary of literature data, temp range 179.48–318.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

631*; 621 (exptl.-concn ratio, measured range 5 – 80°C ; calculated-P/C, Glew & Moelwyn-Hughes 1953)

$\log \{H/(\text{mmHg} \cdot \text{L}/\text{mol})\} = 73.022 - 22.261 \cdot \log (T/\text{K}) - 4254.8/(T/\text{K})$; temp range 278.16–253.16 K (Glew & Moelwyn-Hughes 1953)

733* (29.43°C , concentration ratio, measured range 29.44 – 49.59°C , Swain & Thornton 1962)

652 (calculated as $1/K_{\text{AW}} \cdot C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

533 (20°C , calculated-P/C, Mackay & Shiu 1981)

19958 (20°C , calculated-P/C, Mabey et al. 1982)

1317 (calculated-P/C, Thomas 1982)

20260 (20 – 25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

10690 (calculated-P/C, Mackay & Shiu 1990)

687.4 (computed value, Yaws et al. 1991)

204, 515 (0 , 22°C , distilled water, headspace-GC, Elliott & Rowland 1993)

596* (gas-liquid equilibrator-GC, measured range 1.1 – 30.5°C , De Bruyn & Saltzman 1997)

490 (20°C , selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 3.468 - 1221/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.19 (shake flask-GC, Leo et al. 1975)

1.19 (Hansch & Leo 1979; Hansch & Leo 1985)

1.19 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.11 (calculated-infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

0.623 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

0.672 (calculated- K_{OW} , Lyman et al. 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.236, 2.241, 2.215 (Naaldwijk loamy sand, Aalsmeer loam, Boskoop peaty clay, Howard 1989)

0.771 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

2.10 (calculated-S, Lyman et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated experimental $t_{1/2} = 27$ min 1 mg/L when stirred at 200 rpm in water at approximately 25°C in an open container (Dilling et al. 1975; quoted, Callahan et al. 1979);

$t_{1/2} \sim 30$ min (Mills et al. 1982);

$t_{1/2} = 3.0$ h in a model river (estimated, Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} \sim 0.2$ and 0.5 d for the volatilization from 1 and 10 cm of soil, respectively (Jury et al. 1984; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}^* = (4.14 \pm 0.43) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 245–375 K with lifetime of 1.32 yr in the troposphere (flash photolysis-RF, Davis et al. 1976)

$k_{OH} = 3.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow system, Howard & Evenson 1976)

$k_{OH} = 4.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 289 d, loss of 0.4% in one day or 12 sunlit hour at 300 K (Singh et al. 1981)

$k_{OH} = 2.4 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (estimated, Lyman 1982)

$k_{OH}^* = 3.93 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 0.1 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation $t_{1/2} = 1633\text{--}16327 \text{ h}$ in air, based on measured rates for reaction with OH radicals in air (Atkinson 1985; quoted, Howard et al. 1991)

Hydrolysis: first-order $k = 4.0 \times 10^{-7} \text{ s}^{-1}$ with a maximum $t_{1/2} = 20 \text{ d}$ at pH 7 and 25°C (Radding et al. 1977; Mabey & Mill 1978; quoted, Callahan et al. 1979);

$k = 4.09 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 20 \text{ d}$ at pH 7 and 25°C (Mabey & Mill 1978)

$t_{1/2} = 470\text{--}912 \text{ h}$, based on measured first-order hydrolysis rate constants (Mabey & Mill 1978; Ehrenberg et al. 1974; quoted, Vogel & Reinhard 1986; Howard 1989; Howard et al. 1991);

$k = 1.44 \times 10^{-3} \text{ h}^{-1}$ at pH 7 and 25°C (Callahan et al. 1979; quoted, Mabey et al. 1982)

$k = 3 \times 10^{-7} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 26.7 \text{ d}$ (Castro & Belser 1981; quoted, Howard 1989).

Biodegradation: aerobic $t_{1/2}(\text{aq.}) = 168\text{--}672 \text{ h}$, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991);

anaerobic $t_{1/2}(\text{aq.}) = 672\text{--}2688 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Tabak et al. 1981; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

lifetime of 3.8 yr in the troposphere (Altshuller 1980);

$t_{1/2} = 0.29 \text{ y}$ in the atmosphere for the reaction with $2 \times 10^6 \text{ OH radicals/cm}^3$ at 25°C (Dilling 1982; quoted, Howard 1989);

$t_{1/2} = 289 \text{ d}$ estimated as toxic chemical residence time with rate constant of $4 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radicals at 300 K (Singh et al. 1980,1981; quoted, Howard 1989);

$t_{1/2} = 1633\text{--}16327 \text{ h}$, based on measured rates for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 20 \text{ d}$ at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{1/2} = 168\text{--}672 \text{ h}$, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 336\text{--}912 \text{ h}$, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic waste water inoculum and hydrolysis half-life (Tabak et al. 1981; Mabey & Mill 1978; Ehrenberg et al. 1974; quoted, Vogel & Reinhard 1986; Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672 \text{ h}$, based on unacclimated aerobic aqueous screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.2.1.1**Reported aqueous solubilities of bromomethane at various temperatures**

$$S/(\text{wt}\%) = 1.4019 - 6.3562 \times 10^{-2} \cdot (t/^{\circ}\text{C}) + 1.71977 \times 10^{-3} \cdot (t/^{\circ}\text{C})^2 - 2.8262 \times 10^{-5} \cdot (t/^{\circ}\text{C})^3 + 2.5268 \times 10^{-7} \cdot (t/^{\circ}\text{C})^4 - 9.3470 \times 10^{-10} \cdot (t/^{\circ}\text{C})^5 \quad (1)$$

Haight 1951		Horvath 1982	
gravitational method		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	26790	5	35000
17	18300	10	27997
25	13410	20	18401
32	11490	25	15223
		30	12804
		40	9517
		50	7430
		60	5919
		70	4757
		eq. 1	S/wt%

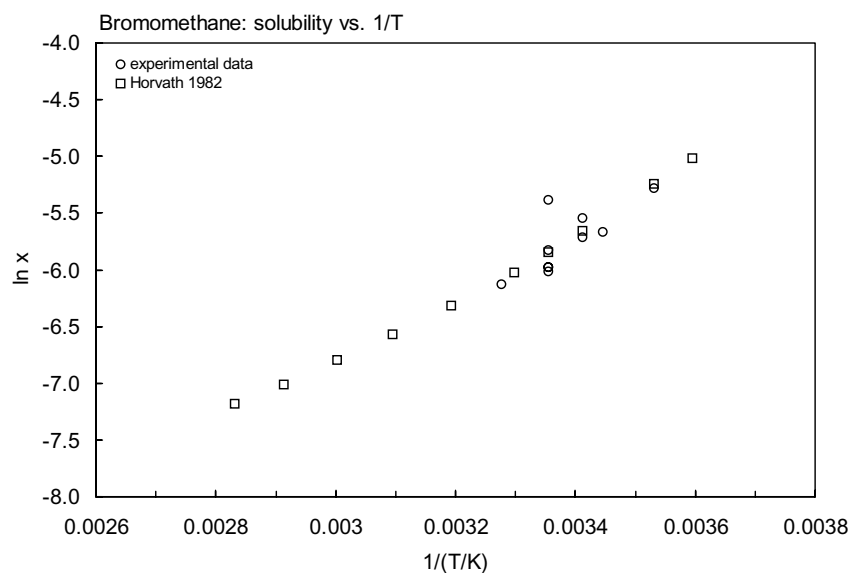
**FIGURE 5.1.2.1.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for bromomethane.

TABLE 5.1.2.1.2
Reported Henry's law constants of bromomethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)			
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
$\log H = A - B \cdot \log (T/K) - C/(T/K)$		(6)			
Glew & Moelwyn-Hughes 1953		Swain & Thornton 1962	De Bruyn & Saltzman 1997		
concentration ratio		concentration ratio	gas-liquid membrane equilibrators-GC		
t/°C	H/(Pa m³/mol)	t/°C H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	
				pure water	seawater 35‰ NaCl
5.0	276	29.43 729	1.1	205.5	253.9 255.2
10.0	340	29.43 733	5.0	261.8	321.7 320.6
14.98	427	29.44 744	10.0	334.4	424.0 417.0
20.0	532	40.35 980	13.4	380.9	471.3 460.6
24.97	631	40.35 992	18.0	440.5	536.1 -
30.0	744	40.35 1005	19.4	458.5	- 539.0
40.05	1005	49.59 1253	21.2	494.3	- 566.1
50.04	1301		25.0	596.0	708.6 666.1
60.03	1653		30.5	666.6	810.6 761.8
70.0	1987				
80.0	2400				
25.0	622				
eq 6	P/(mmHg·L/mol)				
A	73.022				
B	22.261				
C	4254.8				

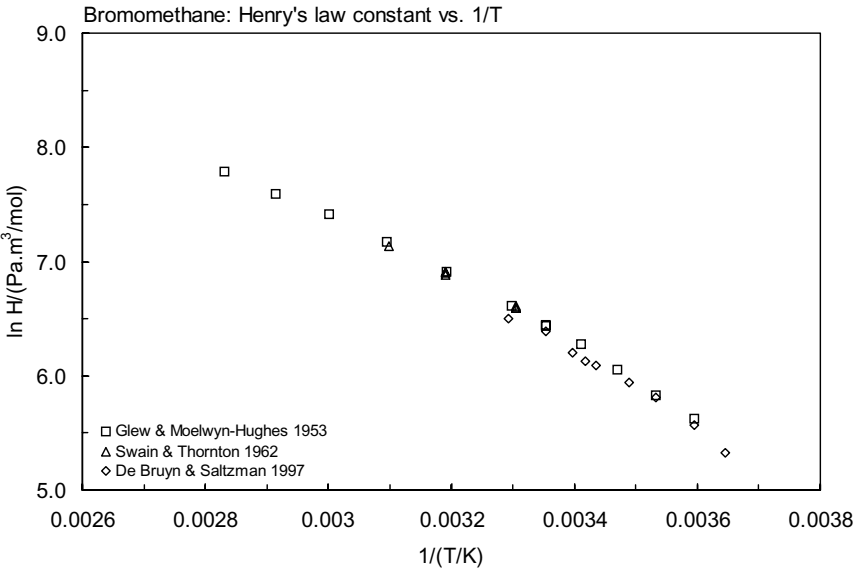
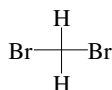


FIGURE 5.1.2.1.2 Logarithm of Henry's law constant versus reciprocal temperature for bromomethane.

5.1.2.2 Dibromomethane



Common Name: Dibromomethane

Synonym: methylene bromide

Chemical Name: dibromomethane, methylene bromide

CAS Registry No: 74-95-3

Molecular Formula: CH_2Br_2

Molecular Weight: 173.835

Melting Point ($^{\circ}\text{C}$):

-52.5 (Weast 1982-83; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

97.0 (Horvath 1982; Weast 1982-83; Lide 2003)

Density (g/cm^3 at 20°C):

2.4970, 2.4842 (20°C , 25°C , Dreisbach 1961)

2.4970 (Horvath 1982; Weast 1982-83)

Molar Volume (cm^3/mol):

70.1 (Stephenson & Malanowski 1987)

76.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

11480* (20°C , volumetric method, measured range 0 – 30°C , Rex 1906)

11700, 11930 (15°C , 30°C , shake flask-interferometer, Gross & Saylor 1931)

11486 (Seidell 1940; quoted, Deno & Berkheimer 1960)

17500 (shake flask-residue volume method, Booth & Everson 1948)

11000 (O'Connell 1963; Jolles 1966)

11442* (summary of literature data, Horvath 1982)

11500 (Dean 1985)

12800*, 11400 (19.3°C , 29.5°C , shake flask-GC/TC, measured range 0 – 90.1°C , Stephenson 1992)

11420, 12030, 12270, 12580 (20 , 30 , 35 , 40°C , infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)

11114, 12060, 13052 (20 , 30 , 40°C , activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)

12300 (20°C , limiting activity coeff. γ^{∞} by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4626, 7518 (20°C , 30°C , Rex 1906)

5775* (Antoine eq. regression, temp range -35.1 to 98.6°C , Stull 1947)

6034 (calculated by formula, Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.0625 - 1327.8/(220.58 + t/^{\circ}\text{C})$; temp range 17 – 236°C (Antoine eq. for liquid state, Dreisbach 1961)

5767 (calculated-Antoine eq., Weast 1972-73)

$\log(P/\text{mmHg}) = [-0.2185 \times 8722.0/(T/\text{K})] + 8.028019$; temp range -35.1 to 98.6°C (Antoine eq., Weast 1972-73)

5922 (Antoine eq. regression, Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 7.82594 - 1784.9/(263.73 + t/^{\circ}\text{C})$ (Antoine eq., Kudchadker et al. 1979)

6034 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.1874 - 1327.8/(-52.57 + T/\text{K})$; temp range 290 – 409 K (Antoine eq., Stephenson & Malanowski 1987)

4650, 7730, 9840, 12383 (20, 30, 35, 40°C, quoted from DIPPR, Tse et al. 1992)
 $\log(P/\text{mmHg}) = 35.3525 - 3.0445 \times 10^3/(T/K) - 9.5792 \cdot \log(T/K) + 5.8258 \times 10^{-10} \cdot (T/K) + 2.9443 \times 10^{-6} \cdot (T/K)^2$;
 temp range 221–611 K (vapor pressure eq., Yaws 1994)
 6084.6 (selected and summary of literature data, temp range 220.61–413.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

90.0 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 73.16 (calculated-bond method, Hine & Mookerjee 1975)
 86.13 (batch stripping-GC, Nicholson et al. 1984)
 86.03 (Munz & Roberts 1989)
 70.9, 111.5, 142, 172 (20, 30, 35, 40°C, infinite dilution activity coeff. γ^∞ -GC, Tse et al. 1992)
 72.7, 141, 252 (20, 30, 40°C, activity coeff. γ^∞ -differential pressure transducer, Wright et al. 1992)
 281, 513 (35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 25.4, 48.3, 81.9 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
 $\ln K_{AW} = 11.70 - 4418/(T/K)$; seawater of salinity of 30.4‰, temp range 0–20°C (Moore et al. 1995)
 66.8 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 68.94 (20°C, exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated:

2.50 (Hansch et al. 1968)
 1.70 (recommended, Sangster 1993)
 1.70 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)
 1.70, 1.65, 1.64 (25, 35, 50°C, from infinite dilution activity coefficient determined by relative GC technique, Bhatia & Sandler 1995)
 1.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

3.07 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 4.1 ppm/min-g of catalyst (Ollis 1985).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k(\text{aq.}) = (6.1 \pm 0.61) \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$ was measured in 66.7% dioxane-water at 35.7°C (Hine et al. 1956; quoted, Roberts et al. 1992)

$k_{OH} = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and estimated residence time of 46 d at 300 K (Singh et al. 1980)

$k_{OH} = 5 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, estimated at 300 K (Lyman 1982)

$k(\text{aq.}) = 4.0 \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution with reference to CH_3CCl_3 (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{O_3}(\text{aq.}) \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with $t_{1/2} \geq 80$ d at pH 7 (Yao & Haag 1991).

$k_{OH}(\text{aq.}) = (9.0 \pm 3.0) \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

Hydrolysis: rate constant $k = 1.2 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 183$ yr at pH 7 and 25°C (Mabey & Mill 1978)

$t_{1/2} = 183$ yr at pH 7 and 25°C, based on overall hydrolysis rate constant (Mill et al. 1982; quoted, Howard et al. 1991).

Biodegradation:

$k = 2.1 \times 10^{-4} \text{ min}^{-1}$ with $t_{1/2} = 24$ min in anoxic sediment-water suspension (Jafvert & Wolfe 1987)

$t_{1/2}$ (aq. aerobic) = 168–672 h, based on unacclimated aerobic screening test data for bromoform from experiments utilizing settled domestic wastewater inoculum (Tabak et al. 1981; quoted, Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 672–2688 h, based on unacclimated aqueous aerobic half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2}$ = 2.4–24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

estimated as toxic chemical residence time of 46 d with rate constant of $2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radical at 300 K (Singh et al. 1980);

photooxidation $t_{1/2}$ = 851–8510 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2}$ = 183 yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{1/2}$ = 55 h in anoxic sediment-water suspension (Jafvert & Wolfe 1987);

$t_{1/2}$ = 168–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured $k \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with $t_{1/2} \geq 80 \text{ d}$ at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2}$ = 336–1344 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2}$ = 55 h in anoxic Bar-H sediment-water suspension (Jafvert & Wolfe 1987)

Soil: $t_{1/2}$ = 168–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.2.2.1

Reported aqueous solubilities of dibromomethane at various temperatures

$$S/(\text{wt}\%) = 1.1594 - 4.3267 \times 10^{-3} \cdot (t/^\circ\text{C}) + 1.8201 \times 10^{-4} \cdot (t/^\circ\text{C})^2 - 1.3335 \times 10^{-6} \cdot (t/^\circ\text{C})^3 \quad (1)$$

1.

Rex 1906		Horvath 1982		Stephenson 1992		Tse et al. 1992	
volumetric method		summary of literature data		shake flask-GC		activity coefficient	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	11730	5	11594	0	11700	20	11420
10	11460	10	11330	9.7	11300	30	12030
20	11480	20	11350	19.3	12800	35	12270
30	11760	25	11442	29.5	11400	40	12580
		30	11574	39.5	12000		
				49.5	12700		
				59.9	13600		
				69.9	13600		
				79.8	16100		
				90.1	15100		
Gross & Saylor 1931						Wright et al. 1992	
shake flask-interferometer						activity coefficient	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$					$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
15	11700					20	11114
30	11930					30	12060
						40	13052

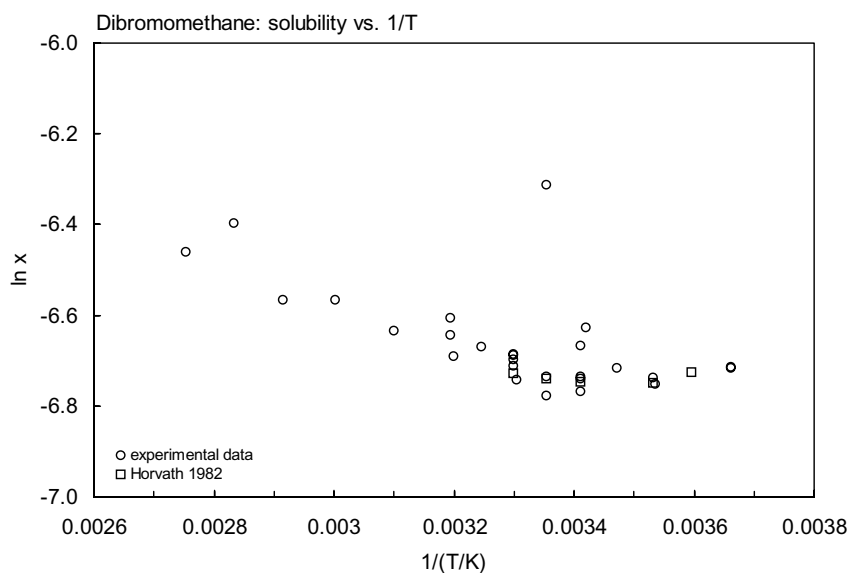


FIGURE 5.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for dibromomethane.

TABLE 5.1.2.2.2

Reported vapor pressures of dibromomethane at various temperatures

Stull 1947

summary of literature data

t/°C	P/Pa
-35.1	133.3
-13.2	666.6
-2.40	1333
9.70	2666
23.3	5333
31.6	7999
42.3	13332
58.5	26664
79.0	53329
98.6	101325
mp/°C	-52.8

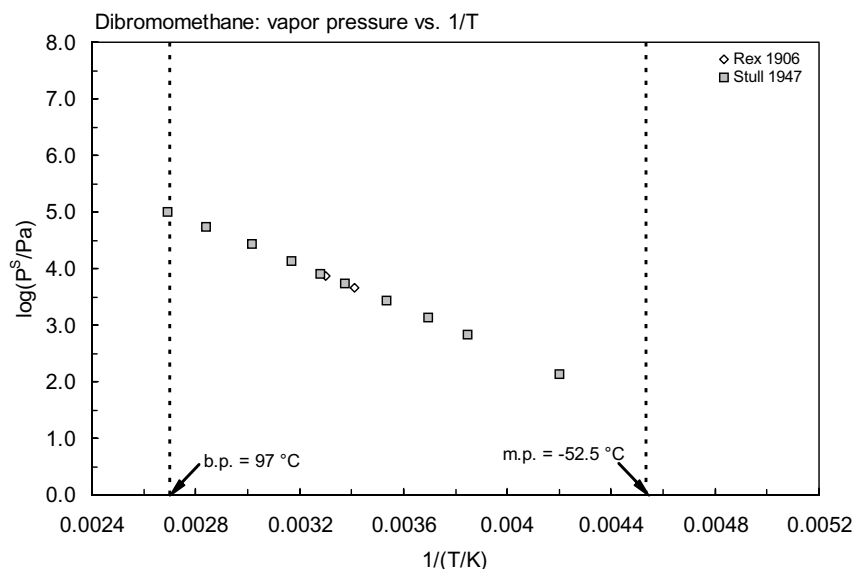


FIGURE 5.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for dibromomethane.

TABLE 5.1.2.2.3

Reported Henry's law constants of dibromomethane at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

Tse et al. 1992		Wright et al. 1992		Bhatia & Sandler 1995		Moore et al. 1995	
activity coefficient		activity coefficient		activity coefficient		gas stripping-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
20	70.9	20	72.7	35	281	seawater, salinity 30.4‰	
30	111.5	30	141	50	513	0	25.4
35	142	40	252			10	48.3
40	172					20	81.9
						eq. 1	K_{AW}
						A	11.70 ± 0.03
						B	4418 ± 154

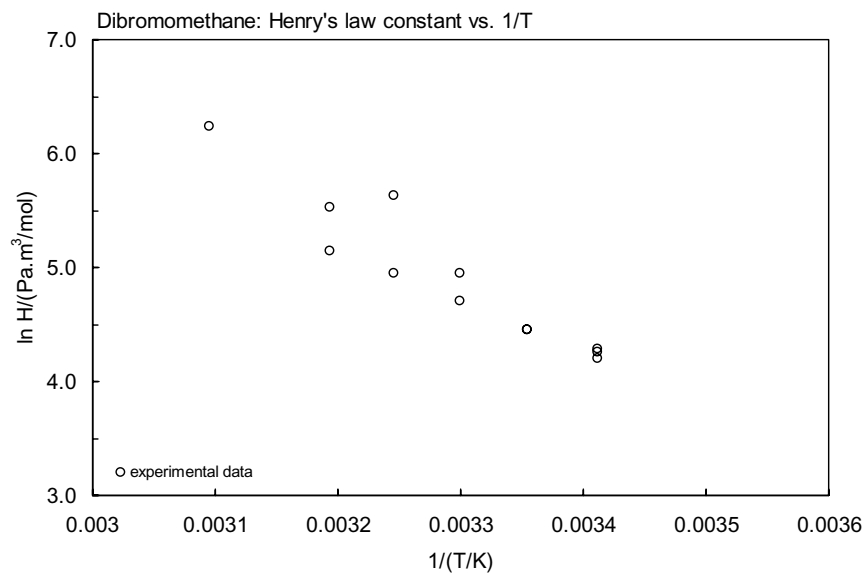
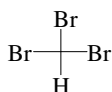


FIGURE 5.1.2.2.3 Logarithm of Henry's law constant versus reciprocal temperature for dibromomethane.

5.1.2.3 Tribromomethane



Common Name: Tribromomethane

Synonym: bromoform, methenyl tribromide

Chemical Name: tribromomethane

CAS Registry No: 75-25-2

Molecular Formula: CHBr_3

Molecular Weight: 252.731

Melting Point ($^{\circ}\text{C}$):

8.69 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

149.1 (Lide 2003)

Density (g/cm^3 at 20°C):

2.8910 (Kahlbaum & Arndt 1898; Riddick et al. 1986)

2.8917, 2.8909 (Kudchadker et al. 1979)

Molar Volume (cm^3/mol):

87.42 (20°C , calculated-density)

99.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

3010, 3190 (15°C , 30°C , shake flask-interferometer, Gross & Saylor 1931)

3110 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

3190 (30°C , Seidell 1941)

3033 (Verschuereen 1977)

3100 (recommended, Horvath 1982)

3931 (30°C , headspace-GC, McNally & Grob 1984)

3200 (30°C , Dean 1985)

3180 (30°C , selected, Riddick et al. 1986)

3235, 3452, 3695 (20, 30, 40°C , infinite dilution activity coeff. γ -GC, Tse et al. 1992)

3978, 4555, 3467 (20, 35, 50°C , activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)

3163 (20°C , equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

987* (30°C , temp range 30 – 110°C , Kireev & Simnikow 1941; quoted, Boublik et al. 1984)

667* (22°C , summary of literature data, temp range 22 – 150.5°C , Stull 1947)

2453* (47.207°C , temp range 47.207 – 139.055°C , Boublik & Aim 1972; quoted, Boublik et al. 1984)

815 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 9673.3/(T/K)] + 7.875367$; temp range 22 – 150°C (Antoine eq., Weast 1972–73)

715 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/\text{mmHg}) = 6.82182 - 1376.748/(200.966 + t/^{\circ}\text{C})$; temp range 30 – 100°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

720 (calculated-Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 7.03141 - 1511.50/(214.21 + t/^{\circ}\text{C})$ (Antoine eq., Kudchadker et al. 1979)

717 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 5.97839 - 1294.382/(202.729 + t/^{\circ}\text{C})$; temp range 30 – 100.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- $\log (P/\text{mmHg}) = 6.8218 - 1376.7/(201.0 + t/^{\circ}\text{C})$; temp range 30–101°C (Antoine eq., Dean 1985, 1992)
 790 (quoted, Riddick et al. 1986)
 727 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.20911 - 1544.81/(-54.77 + T/\text{K})$; temp range 320–412 K (Antoine eq., Stephenson & Malanowski 1987)
 543, 981, 1704 (20, 30, 40°C, quoted from DIPPR, Tse et al. 1992)
 $\log (P/\text{mmHg}) = -10.2943 - 2.170 \times 10^3/(T/\text{K}) + 9.1193 \cdot \log (T/\text{K}) - 1.6495 \times 10^{-2} \cdot (T/\text{K}) + 7.4917 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 281–696 K (vapor pressure eq., Yaws 1994)
 685.5 (selected and summary of literature data, temp range 281.2–478.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 68.3 (calculated- $1/K_{AW}$, C_W/C_A , Hine & Mookerjee 1975)
 7.66 (calculated-bond method, Hine & Mookerjee 1975)
 62.3, 62.0 (calculated-P/C, recommended, Mackay & Shiu 1981, 1990)
 56.7 (20°C, calculated-P/C, Mabey et al. 1982)
 43.6, 43.6; 58.8 (20°C, batch stripping-GC, calculated-P/C, distilled water, Nicholson et al. 1984)
 46.6, 41.54, 43.6 (20°C, batch stripping-GC, natural potable water samples, Nicholson et al. 1984)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 116.0 - 5670/(T/\text{K})$; temp range 10–30°C (air stripping-GC, Nicholson et al. 1984)
 54.2 (EPICS-LSC, Munz & Roberts 1987, 1989)
 $\log K_{AW} = 4.729 - 1905/(T/\text{K})$; temp range 10–30°C (EPICS-LSC measurements, Munz & Roberts 1987)
 53.9 (gas stripping-GC, Warner et al. 1987)
 56.7 (20–25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)
 40.5, 70.9, 122 (20, 30, 40°C, infinite dilution activity coeff. γ^{∞} -GC, Tse et al. 1992)
 34.0, 71.6, 207 (20, 35, 50°C, activity coeff. γ^{∞} -differential pressure transducer, Wright et al. 1992)
 43.6 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 182, 536 (10, 20°C, gas stripping-GC, Moore et al. 1995)
 14.3, 29.2, 52.9 (0, 10, 20°C, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)
 $\ln K_{AW} = 13.16 - 4973/(T/\text{K})$; seawater of salinity of 30.4‰, temp range: 0–20°C (Moore et al. 1995)
 42.65 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 5.476 - 2120/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)
 104.4 (37°C, equilibrium headspace-GC, Batterman et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.30 (calculated as per Tute 1971, Callahan et al. 1979)
 2.38 (calculated-f const., Mabey et al. 1982; Valsaraj 1988)
 2.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

- 1.80 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.07 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization: calculated $t_{1/2} = 63$ min to 24.2 d (using Langbein & Durum 1967 published O_2 reaeration values) and $t_{1/2} = 65.6$ d both from rivers and streams (Kaczmar et al. 1984).
 Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 6.2 ppm/min per gram of catalyst (Ollis 1985).
 Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
 $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 0.5 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

photooxidation $t_{1/2} = 1299\text{--}12989$ h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k = 4.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with OH radical in water with reference to CH_3CCl_3 (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k_{\text{OH}}(\text{aq.}) = (1.3 \pm 0.6) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution at pH 8.5 (Haag & Yao 1992)

Hydrolysis: a maximum $t_{1/2} = 686$ yr has been estimated at pH 7 and 25°C from experimental data at $100\text{--}150^\circ\text{C}$ (Radding et al. 1977) which corresponds to a first-order rate constant $k = 3.2 \times 10^{-11} \text{ s}^{-1}$ (Radding et al. 1977; Mabey & Mill 1978; quoted, Mabey et al. 1982; Howard et al. 1991);

rate constant $k = 3.2 \times 10^{-11} \text{ s}^{-1}$ with $t_{1/2} = 686$ yr at pH 7 and 25°C (Mabey & Mill 1978)

rate constant $k = 2.5 \times 10^{-9} \text{ h}^{-1}$ assigned by analogy to trichloromethane (Mabey et al. 1982).

Biodegradation: $t_{1/2} = 672\text{--}4320$ h in soil, based on unacclimated aerobic aqueous screening test data from experiments utilizing settled domestic wastewater inoculum (Bouwer et al. 1984; quoted, Howard et al. 1991); anaerobic $t_{1/2} = 2688\text{--}17280$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated rate constant $k \sim 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 1299\text{--}12989$ h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 686$ yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on unacclimated aerobic aqueous screening test data from experiments utilizing settled domestic wastewater inoculum (Bouwer et al. 1984; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.2.3.1

Reported aqueous solubilities of tribromomethane at various temperatures

Gross & Saylor 1931		Tse et al. 192		Wright et al. 1992	
shake flask-interferometer		activity coefficient		activity coefficient	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
15	3010	20	3235	20	3978
30	3190	30	3452	35	4555
		40	3695	50	3467

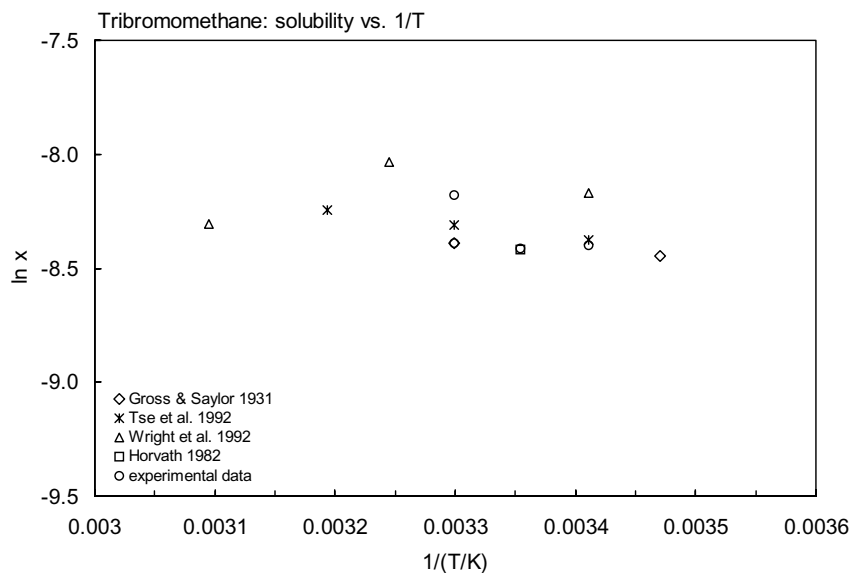


FIGURE 5.1.2.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tribromomethane.

TABLE 5.1.2.3.2

Reported vapor pressures of tribromomethane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Kireev & Simnikow 1941		Stull 1947		Boublik & Aim 1972			
in Boublik et al. 1984		summary of literature data		in Boublik et al. 1984			
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
30.0	987	-	133.3	47.207	2453	123.929	49704
35.0	1267	22.0	666.6	59.767	4524	130.982	61295
40.0	1747	34.0	1333	69.518	6967	139.055	77125
50.0	2946	48.0	2666	76.389	9306	bp/ $^{\circ}\text{C}$	78.177
60.0	4693	63.6	5333	82.821	12046		at 10 mmHg
70.0	7399	73.4	7999	87.709	14549	Antoine eq.	
80.0	11306	85.9	13332	93.356	17921	eq. 2	P/kPa
90.0	16852	106.1	26664	98.173	21314	A	6.20467
110.0	24198	127.9	53329	103.595	25780	B	1541.946
		150.5	101325	108.003	29923	C	218.084
				113.216	35493		
		mp/ $^{\circ}\text{C}$	8.5	118.078	41470		

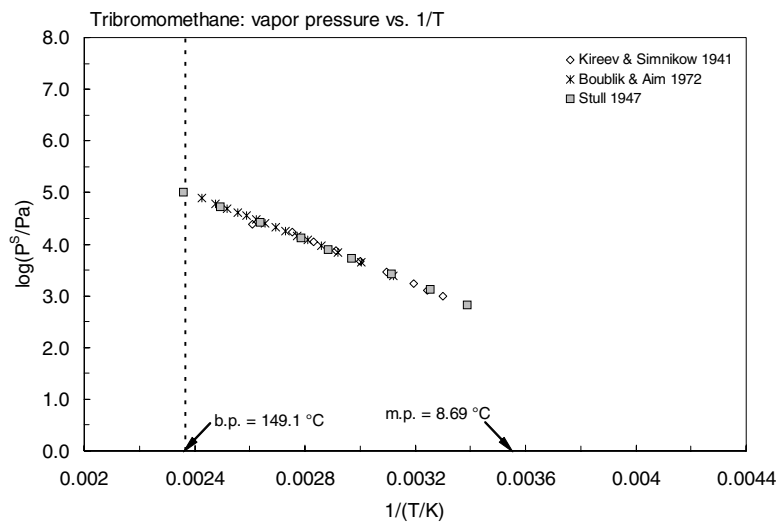


FIGURE 5.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for tribromomethane.

5.1.2.4 Bromoethane (Ethyl bromide)



Common Name: Ethyl bromide

Synonym: bromoethane, monobromoethane

Chemical Name: ethyl bromide, bromoethane

CAS Registry No: 74-96-4

Molecular Formula: C_2H_5Br , CH_3CH_2Br

Molecular Weight: 108.965

Melting Point ($^{\circ}C$):

-118.60 (Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

38.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4594, 1.4492 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

1.4505 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

75.12 (calculated from density)

75.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.55, 26.48 ($25^{\circ}C$, at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.858 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

9140* ($20^{\circ}C$ volumetric method, measured range $0-30^{\circ}C$, Rex 1906)

9600 ($17.5^{\circ}C$, volumetric method, Fühner 1924)

8880 ($30^{\circ}C$, van Arkel & Vles 1936)

9064 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

9000 (shake flask-interferometry, Donahue & Bartell 1952)

8939* (summary of literature data, temp range $0-30^{\circ}C$, Horvath 1982)

9100 (Dean 1985; Riddick et al. 1986)

9000* (tentative value, temp range $0-^{\circ}C$, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 13.2481 - 8.0012 \times 10^{-2} \cdot (T/K) + 1.29448 \times 10^{-4} \cdot (T/K)^2$, temp range $273-303 K$ (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

51440, 75140 ($20^{\circ}C$, $30^{\circ}C$, Rex 1906)

70095* ($28.145^{\circ}C$, temp range $28.145-75.365^{\circ}C$, Zmaczynski 1930)

53329* ($21^{\circ}C$, summary of literature data, temp range -74.3 to $38.4^{\circ}C$, Stull 1947)

62460 (calculated-Antoine eq., Dreisbach 1959)

$\log (P/mmHg) = 6.91995 - 1090.81/(231.71 + t/^{\circ}C)$; temp range -32 to $110^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

$\log (P/mmHg) = 6.91995 - 1090.81/(231.71 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log (P/mmHg) = [-0.2185 \times 6843.1/(T/K)] + 7.635277$; temp range 74.3 to $229.5^{\circ}C$ (Antoine eq., Weast 1972-73)

62230 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.11352 - 1121.957/(234.741 + t/^{\circ}C)$; temp range $28.145-75.4^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.9886 - 1121.9/(234.7 + t/^{\circ}\text{C})$; temp range 28–75°C (Antoine eq., Dean 1985, 1992)

62470 (lit; average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.04485 - 1090.81/(231.71 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

62470 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.04485 - 1090.81/(-41.44 + T/\text{K})$; temp range 225–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.66835 - 1151.96/(12.999 + T/\text{K})$; temp range 334–504 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.77490 - 1602.405/(25.282 + T/\text{K})$; temp range 326–454 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.99873 - 1619.697/(T/\text{K})$; temp range 452–503 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 38.1816 - 2.517 \times 10^3/(T/\text{K}) - 10.329 \cdot \log (T/\text{K}) - 2.3368 \times 10^{-10} \cdot (T/\text{K}) + 5.4956 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 155–504 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

766 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

751 (computed value, Yaws et al. 1991)

767 (γ^{∞} from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.60 (calculated- π const., Hansch et al. 1968)

1.61 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979, 1987)

1.61 (recommended, Sangster 1989)

1.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{AW}$ at 25°C:

1.53 (calculated-measured γ^{∞} in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $k = 2.64 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} \sim 30 \text{ d}$ at pH 7 and 25°C (Mabey & Mill 1978)

$k = 9.4 \times 10^{-4} \text{ h}^{-1}$ at pH 7 and 25°C with $t_{1/2} \sim 30 \text{ d}$ (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: $t_{1/2} \sim 30 \text{ d}$ at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

TABLE 5.1.2.4.1

Reported aqueous solubilities of bromoethane at various temperatures

$$S/(\text{wt}\%) = 1.0557 - 0.01309 \cdot (t/^\circ\text{C}) + 3.3850 \times 10^{-4} \cdot (t/^\circ\text{C})^2 - 2.950 \times 10^{-6} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 13.2481 - 8.0012 \times 10^{-2} \cdot (T/\text{K}) + 1.29448 \times 10^{-4} \cdot (T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	10670	0	10557	0	10510
10	9650	10	9557	5	10080
20	9140	20	9057	10	9710
30	8960	25	8939	15	9410
		30	8880	20	9170
		eq. 1	S/wt%	25	9000
				30	8890
				eq. 2	S/wt%
				temp range 273–303 K	

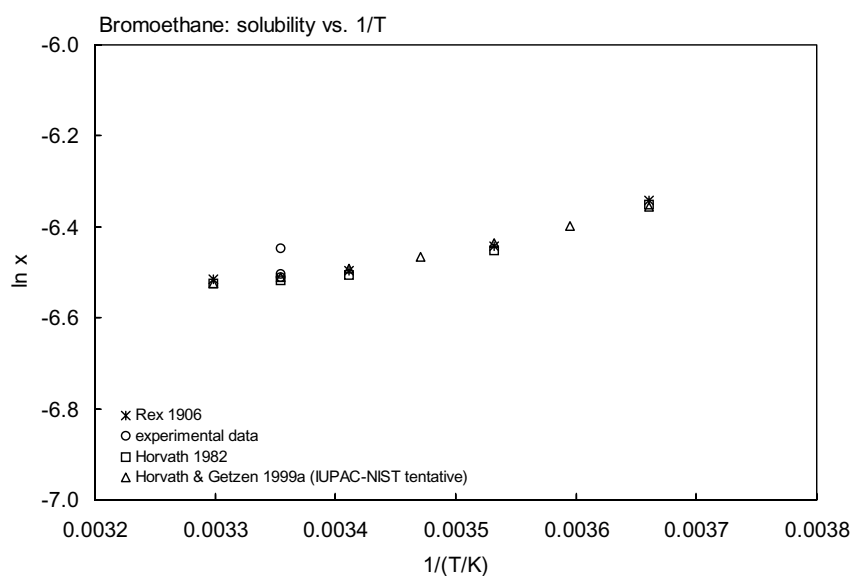
FIGURE 5.1.2.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for bromoethane.

TABLE 5.1.2.4.2

Reported vapor pressures of bromoethane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Zmaczynski 1930		Stull 1947	
		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
28.145	70095	-74.3	133.3
33.247	83515	-56.4	666.6
43.560	120803	-47.5	1333
48.771	143268	-37.8	2666
54.018	169066	-26.7	5333
59.300	198543	-19.5	7999
64.619	232113	-10.0	13332
69.94	270150	4.50	26664
75.365	312960	21.0	53329
		38.4	101325
		mp/°C	-117.8

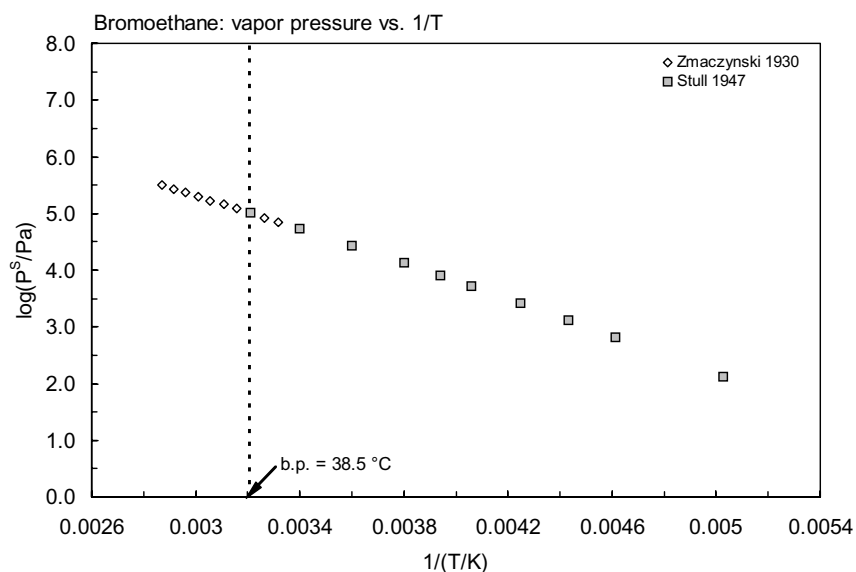
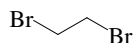


FIGURE 5.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for bromoethane.

5.1.2.5 1,2-Dibromoethane



Common Name: 1,2-Dibromoethane

Synonym: ethylene bromide, ethylene dibromide, *sym*-dibromoethane, EDB

Chemical Name: 1,2-dibromoethane

CAS Registry No: 106-93-4

Molecular Formula: $C_2H_4Br_2$, CH_2BrCH_2Br

Molecular Weight: 187.861

Melting Point ($^{\circ}C$):

9.84 (Lide 2003)

Boiling Point ($^{\circ}C$):

131.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

2.1792, 2.1688 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Horvath 1982)

2.1791, 2.1687 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

86.25 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

98.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.73, 36.35 ($25^{\circ}C$, at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.03 (calculated, Dreisbach 1959)

10.945 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

3920, 4310 ($15^{\circ}C$, $30^{\circ}C$, shake flask-interferometer, Gross & Saylor 1931)

4040* (measured range 0 – $50^{\circ}C$, van Arkel & Vles 1936)

4017 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

8600 (shake flask-volumetric method, Booth & Everson 1948)

4200 (measured by Dow Chemical, Dreisbach 1959)

3510* ($20^{\circ}C$, shake flask-GC, measured range 3 – $34^{\circ}C$, Chiou & Freed 1977)

2910 (shake flask-GC, Jones et al. 1977/78)

3520 (shake flask-GC, Chiou et al. 1979)

4320, 4321 ($20^{\circ}C$, $25^{\circ}C$, shake flask-GC, Mackay et al. 1980)

4152* (summary of literature data, Horvath 1982)

4310 ($30^{\circ}C$, Verschueren 1983)

4290 ($30^{\circ}C$, selected, Riddick et al. 1986)

3120 (shake flask-reverse phase polarography, Tokoro et al. 1988)

4120*, 4310 ($19.5^{\circ}C$, $30.7^{\circ}C$, shake flask-GC/TC, measured range 10.0 – $90.6^{\circ}C$, Stephenson 1992)

4192 ($20^{\circ}C$, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

3910* (tentative value, temp range 0 – $75^{\circ}C$. IUPAC-NIST Solubility Data Series, Hovath & Getzen 1999a)

$S/(wt\%) = 3.8651 - 2.7921 \times 10^{-2} \cdot (T/K) + 5.45647 \times 10^{-5} \cdot (T/K)^2$, temp range 273 – $348\ K$ (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1333 ($18.2^{\circ}C$, summary of literature data, temp range -27 to $131.1^{\circ}C$, Stull 1947)

1560 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 7.06245 - 1469.7/(220.0 + t/^{\circ}C)$; temp range 43 – $215^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

$\log (P/\text{mmHg}) = [-0.2185 \times 9229.4/(T/K)] + 7.93581$; temp range -27 to 304°C (Antoine eq., Weast 1972–73)
 1466, 2266 (20°C , 30°C , Verschuereen 1983)
 1626 (interpolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 5.62666 - 1156.346/(2187.446 + t/^\circ\text{C})$; temp range 52.56 – 131.41°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 6.72148 - 1280.82/(201.75 + t/^\circ\text{C})$; temp range 52 – 131°C (Antoine eq., Dean 1985, 1992)
 1540 (lit. average, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 4.32297 - 1560.3/(230.0 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P_s/\text{kPa}) = 10.03 - 2863/(T/K)$; temp range 228 – 248 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 9.009 - 2606.5/(T/K)$; temp range 251 – 281 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.501 - 2181.1/(T/K)$; temp range 283 – 317 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.18375 - 1469.7/(-53.15 + T/K)$; temp range 316 – 488 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.16941 - 3200/(117.25 + T/K)$; temp range 404 – 578 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 16.8759 - 2.4267 \times 10^3/(T/K) - 3.0891 \cdot \log (T/K) - 6.0088 \times 10^{-10} \cdot (T/K) + 3.5901 \times 10^{-7} \cdot (T/K)^2$; temp range 283 – 650 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

71.49 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 15.64, 110.7 (calculated-group contribution method, calculated-bond contribution, Hine & Mookerjee 1975)
 65.86* (EPICS-GC, measured range 10 – 30°C , Ashworth et al. 1988)
 $\ln [H/(\text{atm m}^3 \text{ mol}^{-1})] = 5.703 - 3876/(T/K)$; temp range 10 – 30°C (EPICS-GC, Ashworth et al. 1988)
 71.49, 133.12 (quoted, calculated-QSAR, Nirmalakhandan & Speece 1988)
 83.07 (20 – 25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)
 70.77 (computed value, Yaws et al. 1991)
 52.6 (20°C , equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 52.02 (20°C , exponential saturator EXPSTAT technique, Dohnal & Hovorka 1999)
 54.84 (20°C , selected from reported experimental determined values, Staudinger & Roberts 2001)
 $\log K_{AW} = 3.661 - 1556/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.96 (shake flask, Log P Database, Hansch & Leo 1987)
 1.96 (recommended, Sangster 19943)
 1.96 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

0.778 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
 0.301 (calculated- K_{OC} as per Kenaga & Goring 1978, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{OC}$:

1.556 (soil, equilibrium sorption isotherm, Chiou et al. 1979)
 1.643 (soil, quoted, Kenaga 1980; Kenaga & Goring 1980)
 1.699 (soil, calculated as per Kenaga & Goring 1978, Kenaga 1980)
 1.643 (soil, selected, Jury et al. 1990)
 1.64 (soil, organic carbon $\text{OC} \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization: estimated volatilization $t_{1/2} \sim 6.1$ h from water (Thomas 1982)

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH} = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow system, Howard & Evenson 1976)

$k_{\text{OH}}(\text{calc}) = 2.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{\text{OH}} = 2.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.01 d^{-1} , $k_{\text{O}_3} < 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 6 \times 10^{-7} \text{ d}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{O}_3}(\text{aq.}) \leq 0.014 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C , with a half-life of 28 d at pH 7 (Yao & Haag 1991).

Hydrolysis: EDB hydrolyzes to ethylene glycol and bromoethanol in water at pH 7 and 25°C with $t_{1/2} = 5\text{--}10 \text{ d}$ (Leinster et al. 1978; quoted, Verschueren 1983);

$k = 9.9 \times 10^{-6} \text{ h}^{-1}$ at pH 7 and 25°C with a calculated $t_{1/2} = 8.0 \text{ yr}$ (Jungclaus & Cohen 1986; quoted, Ellington 1989);

rate constant $k = (8.9 \pm 0.1) \times 10^{-9} \text{ s}^{-1}$ in water at 25°C and pH 7.5 with an estimated half-life of 2.5 yr (Vogel & Reinhard 1986);

$t_{1/2} = 2.2 \text{ yr}$, based on measured neutral hydrolysis rate constant at pH 7 and 25°C (Weintraub et al. 1986; quoted, Howard et al. 1991).

Biodegradation: aerobic $t_{1/2}(\text{aq.}) = 672\text{--}4320 \text{ h}$, based on unacclimated aqueous aerobic biodegradation screening test data (Bouwer & McCarty 1983; quoted, Howard et al. 1991);

anaerobic $t_{1/2}(\text{aq.}) = 48\text{--}360 \text{ h}$, based on anaerobic stream and pond water sediment die-away test data (Jafvert & Wolfe 1987; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976); photooxidation $t_{1/2} = 257\text{--}2567 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aqueous aerobic biodegradation (Howard et al. 1991); $k(\text{exptl}) \leq 0.014 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C , with $t_{1/2} \geq 28 \text{ d}$ at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 470\text{--}2880 \text{ h}$, based on data from anaerobic ground water ecosystem study (Wilson et al. 1986; quoted, Howard et al. 1991) and data from an aerobic ground water ecosystem study (Swindoll et al. 1987; quoted, Howard et al. 1991).

Sediment: calculated $t_{1/2} = 1500 \text{ d}$ at 25°C and pH 7, based on studies in pure water and in barely saturated subsurface sediment at $25\text{--}60^\circ\text{C}$ (Haag & Mill 1988).

Soil: estimated $t_{1/2} \sim 3650 \text{ d}$ of volatilization loss from soil (Jury et al. 1990);

disappearance $t_{1/2} < 2.0 \text{ d}$, estimated from the volatilization loss of mixtures (Anderson et al. 1991);

$t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.2.5.1

Reported aqueous solubilities of 1,2-dibromoethane at various temperatures

$$S(\text{wt}\%) = 0.36583 + 1.4836 \times 10^{-3} \cdot (t/^\circ\text{C}) + 3.48175 \times 10^{-6} \cdot (t/^\circ\text{C})^2 + 6.47685 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S(\text{wt}\%) = 3.8651 - 2.7921 \times 10^{-2} \cdot (T/\text{K}) + 5.45647 \times 10^{-5} \cdot (T/\text{K})^2, \quad (2)$$

1.

Gross & Saylor 1931		van Arkel & Vles 1936		Chiou & Freed 1977		Horvath 1982	
shake flask-interferometer				shake flask-GC		summary of literature data	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
15	3920	0	3340	3	2960	5	3658
30	4310	20	4020	20	3510	10	3817
		35	4490	34	4150	20	4012
		50	5290			25	4152

(Continued)

TABLE 5.1.2.5.1 (Continued)

Gross & Saylor 1931		van Arkel & Vles 1936		Chiou & Freed 1977		Horvath 1982	
shake flask-interferometer				shake flask-GC		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
						30	4310
						40	4722
						50	5297
						60	6073
						70	7089
						80	8384
						eq.1	S/wt%

2.

Stephenson 1992		Horvath & Getzen 1999a			
shake flask-GC		tentative, IUPAC-NIST			
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10.1	3950	0	3090	55	5780
19.5	4120	5	3200	60	6190
30.7	4310	10	3340	65	6630
39.6	4440	15	3500	70	7090
50	4930	20	3690	75	7580
59.9	4890	25	3910		
70.2	5420	30	4150	eq. 2	S/wt%
80.3	5720	35	4420		
90.6	6580	40	4720		
		45	5050		
		50	5400		

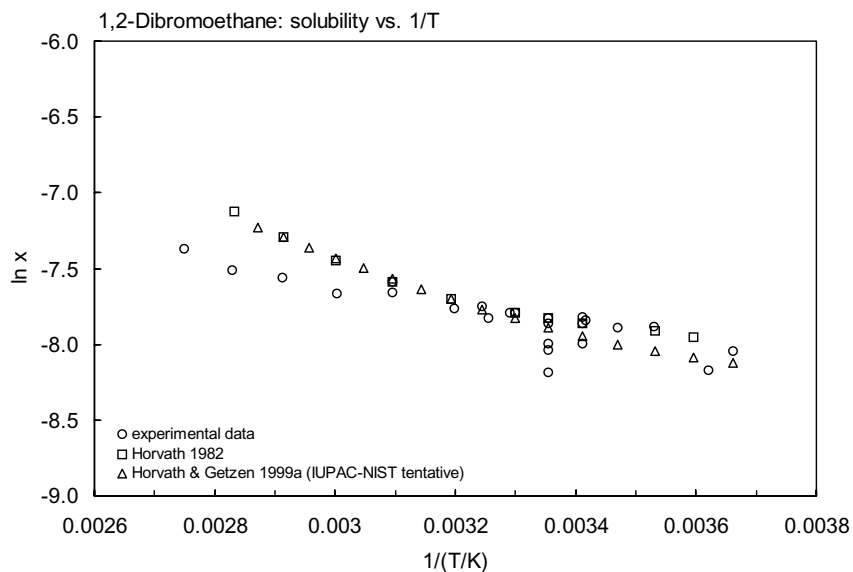
FIGURE 5.1.2.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,2-dibromomethane.

TABLE 5.1.2.5.2
Reported Henry's law constants of 1,2-dibromoethane
at various temperatures

Ashworth et al. 1988	
EPICS-GC	
t/°C	H/(Pa m ³ /mol)
10	30.4
15	48.6
20	61.8
25	65.9
30	81.1
$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/\text{K})$	
A	5.703
B	3876

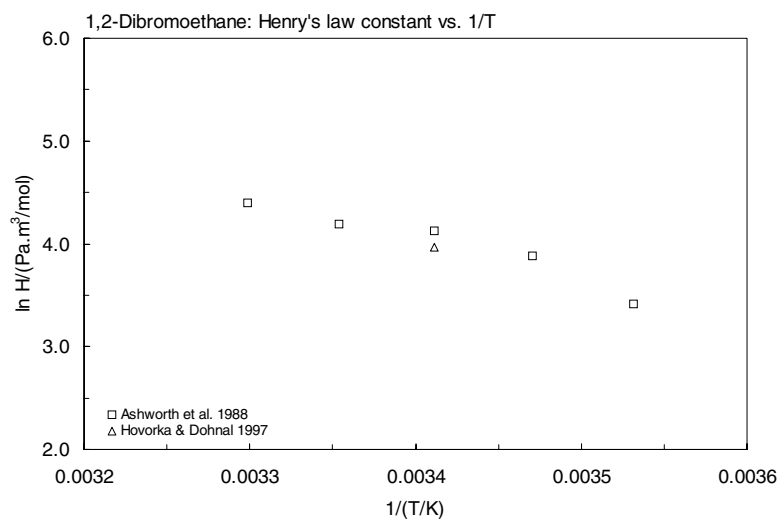
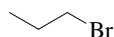


FIGURE 5.1.2.5.2 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-dibromomethane.

5.1.2.6 1-Bromopropane



Common Name: 1-Bromopropane

Synonym: bromopropane, monobromopropane, *n*-propyl bromide, propyl bromide

Chemical Name: *n*-propyl bromide, 1-bromopropane

CAS Registry No: 106-94-5

Molecular Formula: C₃H₇Br, CH₃CH₂CH₂Br

Molecular Weight: 122.992

Melting Point (°C):

−110.3 (Lide 2003)

Boiling Point (°C):

71.1 (Lide 2003)

Density (g/cm³ at 20°C):

1.3536, 1.3452 (20°C, 25°C, Dreisbach 1961)

1.3537 (Horvath 1982)

Molar Volume (cm³/mol):

90.86 (20°C, calculated-density)

97.30 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.88, 68.8 (25°C, 68.8°C, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.037 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2450* (20°C, volumetric method, measured range 0–30°C, Rex 1906)

2275 (19.5°C, shake flask, Fühner 1924)

2310 (30°C, shake flask-interferometer, Gross & Saylor 1931)

2312 (30°C, shake flask, Van Arkel & Vles 1936)

2454 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

2460 (calculated-K_{ow}, Hansch et al. 1968)

2450 (20°C, exptl., Korenman et al. 1971)

2427* (summary of literature data, Horvath 1982)

2300 (30°C, Dean 1985; Riddick et al. 1986)

2340* (tentative value, IUPAC-NIST Solubility Data Series, temp range 0–30°C Horvath & Getzen 1999)

S/(wt%) = 9.0608 − 0.05911·(T/K) + 9.8925 × 10^{−5}·(T/K)², temp range 273–303 K (Horvath & Getzen 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

14770, 22740 (20°C, 30°C, volumetric method Rex 1906)

13332* (18°C, summary of literature data, temp range −53.0 to 71°C, Stull 1947)

18440 (calculated by formula, Dreisbach 1961)

log (P/mmHg) = 6.91065 − 1194.889/(225.51 + t/°C); temp range −6 to 107°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.91065 − 1194.889/(225.51 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

18300 (interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.09224 − 1232.529/(230.19 + t/°C); temp range 0–30°C (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)

18440 (selected, Riddick et al. 1986)

log (P/kPa) = 6.03960 − 1194.33/(225.223 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.03555 - 1194.889/(-47.64 + T/\text{K})$; temp range 250–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.03823 - 1193.612/(-48.005 + T/\text{K})$; temp range 301–344 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -9.0284 - 1.8916 \times 10^3/(T/\text{K}) + 9.691 \cdot \log (T/\text{K}) - 2.7013 \times 10^{-2} \cdot (T/\text{K}) + 1.7877 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 163–544 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

964.4 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

1133, 1564 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

766.0 (calculated-QSAR, Nirmalakhandan & Speece 1988)

732 (computed value, Yaws et al. 1991)

950 (γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.10 (shake flask-GC, Fujita et al. 1964; Hansch & Anderson 1967; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)

2.10 (recommended, Sangster 1989, 1993)

2.10 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $k = 3.04 \times 10^{-7} \text{ s}^{-1}$ with estimated $t_{1/2} = 26 \text{ d}$ at pH 7 and 25°C (Mabey & Mill 1978)

$k = 1.1 \times 10^{-3} \text{ h}^{-1}$ at pH 7 and 25°C with estimated $t_{1/2} = 26 \text{ d}$. (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: estimated $t_{1/2} = 26 \text{ d}$ at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

Ground water:

Sediment:

Soil:

Biota:

TABLE 5.1.2.6.1

Reported aqueous solubilities of 1-bromopropane at various temperatures

$$S/(\text{wt}\%) = 0.2971 - 0.04225 \cdot (t/^\circ\text{C}) + 6.94998 \times 10^{-5} \cdot (t/^\circ\text{C})^2 + 5.00002 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 9.0608 - 0.05911 \cdot (T/\text{K}) + 9.8925 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	2980	0	2971	0	2980
10	2630	10	2623	5	2760
20	2450	20	2444	10	2580
30	2470	25	2427	15	2450
		30	2464	20	2370
		eq. 1	S/wt%	25	2340
				30	2360
				eq. 2	S/wt%
				temp range 273–303 K	

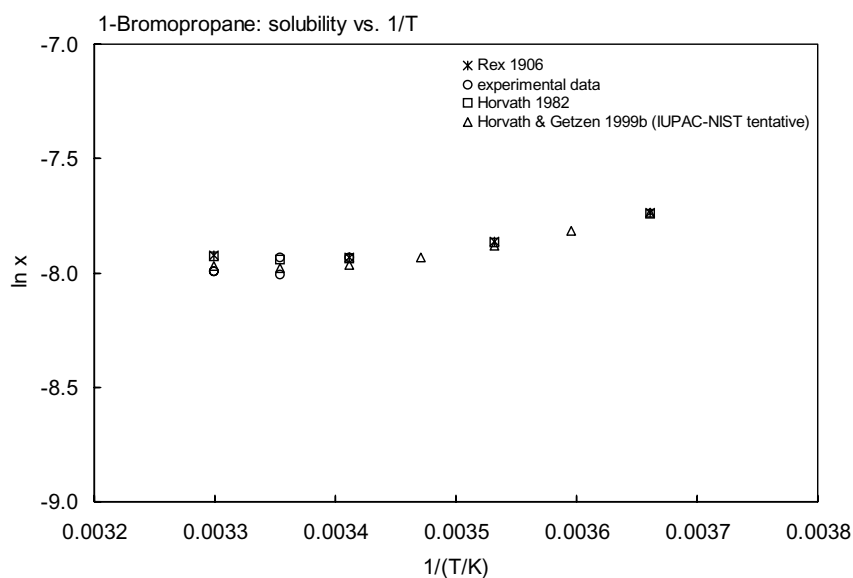
FIGURE 5.1.2.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-bromopropane.

TABLE 5.1.2.6.2

Reported vapor pressures of 1-bromopropane at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Rex 1906		Stull 1947	
		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
0	5546	-52.0	133.3
10	9091	-33.4	666.6
20	14772	-23.3	1333
30	22745	-12.4	2666
		-0.30	5333
		7.50	7999
		18.0	13332
		34.0	26664
		52.0	53329
		71.0	101325
		mp/°C	-109.0

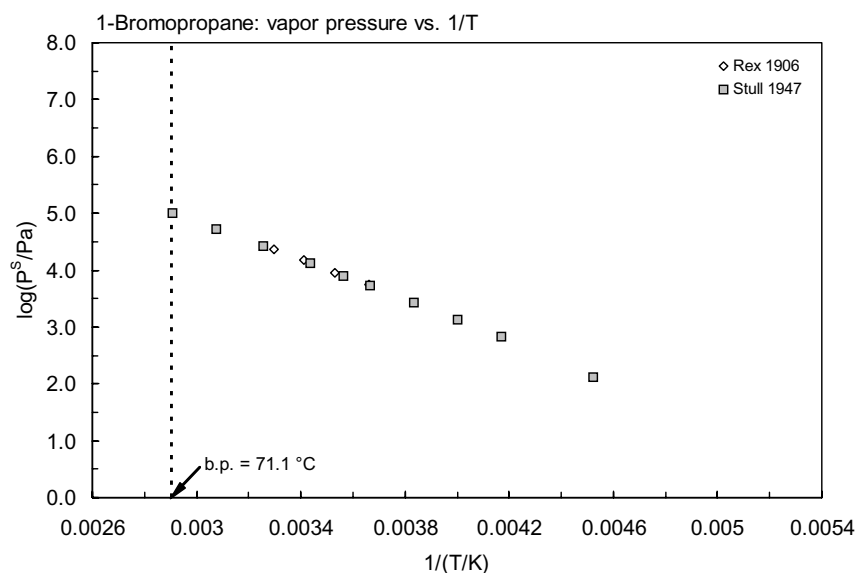


FIGURE 5.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1-bromopropane.

5.1.2.7 2-Bromopropane



Common Name: 2-Bromopropane

Synonym: isopropyl bromide

Chemical Name: 2-bromopropane, isopropyl bromide

CAS Registry No: 75-26-3

Molecular Formula: C_3H_7Br , $CH_3CHBrCH_3$

Molecular Weight: 122.992

Melting Point ($^{\circ}C$):

−89.0 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

59.50 (Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.3140, 1.3060 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961; Riddick et al. 1986)

Molar Volume (cm^3/mol):

93.6 ($20^{\circ}C$, Stephenson & Malanowski 1987)

97.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

30.16, 28.4 ($25^{\circ}C$, $58.6^{\circ}C$, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4180, 3650, 3180, 3180 (0, 10, 20, $30^{\circ}C$, volumetric method, Rex 1906)

2877 (shake flask-volumetric method, Fühner 1924)

3198 ($30^{\circ}C$, shake flask, Van Arkel & Vles 1936)

3162 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

2880, 2690 ($20^{\circ}C$, Korenman et al. 1971)

3000 (selected exptl., Horvath 1982)

2900 ($18^{\circ}C$, Dean 1985)

2860 ($18^{\circ}C$, selected, Riddick et al. 1986)

4160, 3640, 3170, 3170 (0, 10, 20, $30^{\circ}C$, tentative values of IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

23380, 35220 ($20^{\circ}C$, $30^{\circ}C$, volumetric method Rex 1906)

26664 ($23.8^{\circ}C$, summary of literature data, temp range -61.8 to $60^{\circ}C$, Stull 1947)

31500 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 6.61405 - 1072.9/(228.0 + t/^{\circ}C)$; temp range -19 to $95^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 7591.7/(T/K)] + 7.887729$; temp range -61.8 to $60^{\circ}C$ (Antoine eq., Weast 1972–73)

28780 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.09819 - 1200.652/(233.815 + t/^{\circ}C)$; temp range 0 – $30^{\circ}C$ (Antoine eq. from reported exptl. data of Rex 1906, Boublik et al. 1984)

31500 (selected, Riddick et al. 1986)

$\log(P/kPa) = 5.92741 - 1106.82/(222.851 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

31940 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.28473 - 858.03/(-71.18 + T/K)$; temp range 236 – 328 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.91155 - 1098.573/(-51.268 + T/K)$; temp range 299 – 332 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 31.3032 - 2.4924 \times 10^3/(T/K) - 8.4645 \cdot \log (T/K) + 1.6459 \times 10^{-10} \cdot (T/K) + 3.7859 \times 10^{-6} \cdot (T/K)^2;$$

temp range 184–532 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1107	(calculated- $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)
2479, 1564	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
1082	(calculated-QSAR, Nirmalakhandan & Speece 1988)
978	(computed value, Yaws et al. 1991)
1192	(γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.90	(calculated- π const., Hansch et al. 1968)
2.14	(recommended, Hansch et al. 1995)
1.80	(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $k = 3.86 \times 10^{-6} \text{ s}^{-1}$ with estimated $t_{1/2} \sim 2.0 \text{ d}$ at pH 7 and 25°C (Mabey & Mill 1978)

$k = 1.4 \times 10^{-2} \text{ h}^{-1}$ at pH 7 and 25°C with estimated $t_{1/2} \sim 2.0 \text{ d}$ (Mabey & Mill 1978; quoted, Schwarzenbach et al. 1985; Vogel & Reinhard 1986);

rate constants at 25°C : $k = (379 \pm 41) \times 10^{-8} \text{ s}^{-1}$ in distilled water at pH 3–11 for equal or more than 72% conversion (Mill et al. 1980; quoted, Haag & Mill 1988),

$k = (383 \pm 33) \times 10^{-8} \text{ s}^{-1}$ in distilled water for 89% conversion, $k = (372 \pm 64) \times 10^{-8} \text{ s}^{-1}$ in sediment-extracted water for 87% conversion, and $k = (420 \pm 80) \times 10^{-8} \text{ s}^{-1}$ in sediment pores at pH 7.3 for 88% conversion (Haag & Mill 1988).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: estimated $t_{1/2} \sim 2.0 \text{ d}$ at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

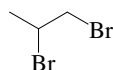
Ground water:

Sediment: $t_{1/2} = 2.1 \text{ d}$, based on neutral and base-catalyzed hydrolysis studies at 25°C in pure water and in barely saturated subsurface sediment at $25\text{--}60^\circ\text{C}$ (Haag & Mill 1988).

Soil:

Biota:

5.1.2.8 1,2-Dibromopropane



Common Name: 1,2-Dibromopropane

Synonym: propylene bromide, propylene dibromide

Chemical Name: 1,2-dibromopropane

CAS Registry No: 78-75-1

Molecular Formula: $C_3H_6Br_2$, $CH_3CHBrCH_2Br$

Molecular Weight: 201.888

Melting Point ($^{\circ}C$):

−55.49 (Lide 2003)

Boiling Point ($^{\circ}C$):

141.0 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.93268, 1.92344 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959)

1.9324, 1.9241 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

1.9324 (Horvath 1982; Weast 1982–83)

Molar Volume (cm^3/mol):

104.5 ($20^{\circ}C$, calculated-density)

120.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

42.43, 35.52 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.937 (calculated, Dreisbach 1959; quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1430 (measured by Dow Chemical, Dreisbach 1955–1961)

1463 (Hine & Mookerjee 1975)

1428 (recommended, Horvath 1982)

2000 (Dean 1985)

2986 (calculated-fragment const., Wakita et al. 1986)

1919 (predicted-MCI χ and polarizability, Nirmalakhandan & Speece 1988)

1420 (calculated-AI, Okouchi et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2000 ($37.3^{\circ}C$, Kahlbaum & Arndt 1898)

1036 (Antoine eq. regression, temp range -7.0 to $141.6^{\circ}C$, Stull 1947)

1071 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.89105 - 1419.6/(212.0 + t/^{\circ}C)$; temp range 50 – $210^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

688 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.34875 - 1572.7/(212.0 + t/^{\circ}C)$; temp range 56 – $183^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 9801.9/(T/K)] + 8.073203$; temp range -7.0 to $141.6^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = 7.30398 - 1644.4/(232.0 + t/^{\circ}C)$; temp range 0 – $50^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.89105 - 1419.6/(212.0 + t/^{\circ}C)$; temp range 50 – $250^{\circ}C$ (Antoine eq., Dean 1985, 1992)

1072 (quoted from Dreisbach 1959, 1961, Riddick et al. 1986)

$\log(P/kPa) = 6.01595 - 1419.6/(212.0 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.47365 - 1572.7/(-61.15 + T/K)$; temp range 329 – $456 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.00898 - 1409.6/(-62.856 + T/\text{K})$; temp range 312–403 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

94.2	(calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
21.1, 164	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
226.1	(calculated-QSAR, Nirmalakhandan & Speece 1988)
150	(computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.54	(calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)
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Bioconcentration Factor, $\log \text{BCF}$:

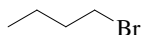
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Hydrolysis: rate constant $k = (2.5 \pm 0.5) \times 10^{-8} \text{ s}^{-1}$ in water at 25°C and pH 7 with $t_{1/2} \sim 320 \text{ d}$ (Vogel & Reinhard 1986).

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

5.1.2.9 1-Bromobutane (*n*-Butyl bromide)

Common Name: 1-Bromobutane

Synonym: *n*-butyl bromide, monobromobutane

Chemical Name: 1-bromobutane, *n*-butyl bromide, monobromobutane

CAS Registry No: 109-65-9

Molecular Formula: C_4H_9Br , $CH_3CH_2CH_2CH_2Br$

Molecular Weight: 137.02

Melting Point ($^{\circ}C$):

-112.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

101.6 (Dreisbach 1961; Horvath 1982; Dean 1985; Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2758, 1.2687 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961; Horvath 1982; Riddick et al. 1986)

Molar Volume (cm^3/mol):

107.9 ($20^{\circ}C$, calculated-density)

119.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

38.83, 31.85 ($25^{\circ}C$, normal bp, Dreisbach 1961)

36.60, 31.85 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.694 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

580 ($16^{\circ}C$, volumetric method, Fühner 1924)

608 ($30^{\circ}C$, shake flask-interferometer, Gross & Saylor 1931)

598 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

254 (shake flask-volumetric method, Booth & Everson 1948)

509 (exptl., Korenman et al. 1971)

600 (selected exptl., Horvath 1982)

869 (generator column-GC, Tewari et al. 1982)

601 (calculated-UNIFAC activity coeff., Arbuckle 1986)

608 ($30^{\circ}C$, quoted, Riddick et al. 1986)

680, 868, 871, 608 (16 , 25 , 25 , $30^{\circ}C$, reported values, IUPAC-NIST Series, Horvath & Getzen 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

10972 ($20^{\circ}C$, manometry, measured range 20 – $70^{\circ}C$, Smyth & Engel 1929)

5333 ($24.8^{\circ}C$, summary of literature data, measured range -33.0 to $101.6^{\circ}C$, Stull 1947)

5502 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 6.92254 - 1298.608/(219.70 + t/^{\circ}C)$; temp range 19 – $141^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 6.92254 - 1298.608/(219.70 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log(P/mmHg) = [-0.2185 \times 8789.1/(T/K)] + 8.028836$; temp range -33.0 to $101.6^{\circ}C$ (Antoine eq., Weast 1972–73)

5502 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.04744 - 1298.608/(219.70 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

5502 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.04744 - 1298.608/(-53.45 + T/K)$; temp range 273 – 400 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.1388 - 1349.142/(-48.003 + T/K)$; temp range 338–373 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 74.7061 - 4.0663 \times 10^3/(T/K) - 25.61 \cdot \log (T/K) + 1.3166 \times 10^{-2} \cdot (T/K) + 1.421 \times 10^{-13} \cdot (T/K)^2$; temp range 161–577 K (vapor pressure eq., Yaws 1994)

5506 (static method-manometer, measured range 278.15–323.15 K, Garriga et al. 2002)

$\ln (P/\text{kPa}) = 14.12331 - 3088.751/[(T/K) - 49.418]$; temp range 278.15–323.15 K (static method, Garriga et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25° C):

1242 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

1600, 2313 (calculated-group contribution method, calculated-bond contribution Hine & Mookerjee 1975)

964.4 (calculated-QSAR, Nirmalakhandan & Speece 1988)

1223 (computed value, Yaws et al. 1991)

1215 (γ^∞ from gas stripping-GC, Li et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.75 (generator column-GC, DeVoe et al. 1981; Wasik et al. 1981; Tewari et al. 1982)

2.75 (generator column-HPLC, DeVoe et al. 1981)

2.79 (estimated-activity coefficients, Wasik et al. 1981)

2.64 (estimated-activity coefficients, Schantz & Martire 1987)

2.75 (recommended, Sangster 1989)

2.75 (recommended, Hansch et al. 1995)

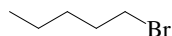
Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h for the reaction with OH radical in air (USEPA 1974; quoted, Darnall et al. 1976).

5.1.2.10 1-Bromopentane (*n*-Amyl bromide)

Common Name: 1-Bromopentane

Synonym: *n*-amyl bromide, monobromopentane, pentyl bromide

Chemical Name: *n*-amyl bromide, 1-bromopentane, monobromopentane, pentyl bromide

CAS Registry No: 110-53-2

Molecular Formula: C₅H₁₁Br, CH₃CH₂CH₂CH₂CH₂Br

Molecular Weight: 151.045

Melting Point (°C):

−88.0 (Lide 2003)

Boiling Point (°C):

129.8 (Lide 2003)

Density (g/cm³ at 20°C):

1.2182, 1.2119 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)

Molar Volume (cm³/mol):

124.0 (20°C, calculated- density; Stephenson & Malanowski 1987)

141.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.78, 34.49 (25°C, at normal bp, Dreisbach 1961)

41.43, 34.49 (25°, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.46 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

127 (generator column-GC, Tewari et al. 1982)

141 (calculated-UNIFAC activity coeff., Arbuckle 1986)

127 (selected, Riddick et al. 1986)

127 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

1754 (calculated by formula, Dreisbach 1961)

log (P/mmHg) = 6.95580 − 1401.634/(214.38 + t/°C); temp range 41–171°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.95580 − 1401.634/(214.38 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

1680 (quoted, Riddick et al. 1986)

log (P/kPa) = 6.08070 − 11401.634/(214.38 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

1680 (interpolated-Antoine eq., Malanowski 1987)

log (P_l/kPa) = 6.0807 − 1401.634/(−58.77 + T/K); temp range 293–443 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):

2005 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow}:

3.37 (generator column-GC, DeVoe et al. 1981; Tewari et al. 1982)

3.37 (generator column-HPLC, DeVoe et al. 1981)

3.49 (generator column-GC, Wasik et al. 1981)

3.32 (estimated-measured activity coefficients, Schantz & Martire 1987)

3.37 (recommended, Sangster 1989)

3.37 (calculated-UNIFAC activity coeff., Dallos et al. 1993)

3.37 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

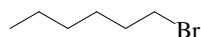
Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h for the reaction with OH radicals in air (USEPA 1974; quoted, Darnall et al. 1976).

5.1.2.11 1-Bromohexane



Common Name: 1-Bromohexane

Synonym: *n*-hexyl bromide

Chemical Name: 1-bromohexane

CAS Registry No: 111-25-1

Molecular Formula: $C_6H_{13}Br$; $CH_3(CH_2)_4CH_2Br$

Molecular Weight: 165.071

Melting Point ($^{\circ}C$):

−83.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

155.3 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

1.1744, 1.1667 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

1.1744 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

140.6 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

163.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

46.77, 37.07 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

25.75 (generator column-GC/FID, Tewari et al. 1982)

25.8 (tentative value, IUPAC-NIST Solubility Data Series, Hovrath & Getzen 1999b)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

520 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.0023 - 1503.52/(209.5 + t/^{\circ}C)$; temp range 63 – $202^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.0023 - 1503.52/(209.5 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log(P_L/kPa) = 6.1272 - 1503.52/(T/K - 63.65)$; temp range 333 – $456\ K$ (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.80 (generator column-GC, Tewari et al. 1982)

4.58 (HPLC-RT correlation, Burkhard et al. 1985)

3.80; 3.804 (generator column-GC; calculated-activity coeff. γ , Schantz & Martire 1987)

3.80 (recommended, Sangster 1989, 1993; Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

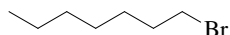
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

5.1.2.12 1-Bromoheptane



Common Name: 1-Bromoheptane

Synonym: heptyl bromide

Chemical Name: 1-bromoheptane

CAS Registry No: 629-04-9

Molecular Formula: $C_7H_{15}Br$

Molecular Weight: 179.098

Melting Point ($^{\circ}C$):

-56.1 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

178.9 (Dreisbach 1961; Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.140, 1.1347 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

1.140 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

157.1 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

186.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

51.83, 39.59 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.68 (generator column-GC/GID, Tewari et al. 1982; Miller et al. 1985)

6.68 (tentative value, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

163 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.0582 - 1603.71/(205.0 + t/^{\circ}C)$; temp range 82 – $228^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.0582 - 1603.71/(205.0 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log(P_L/kPa) = 6.1831 - 1603.71/(T/K - 68.15)$; temp range 333–483 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 43.3327 - 4.0389 \times 10^3/(T/K) - 12.105 \cdot \log(T/K) - 1.5959 \times 10^{-10} \cdot (T/K) + 3.0522 \times 10^{-6} \cdot (T/K)^2$; temp range 217–651 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.36 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

4.36; 4.44 (generator column-GC; calculated-activity coeff., Schantz & Mairtire 1987)

4.36 (recommended, Sangster 1989; 1994; Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

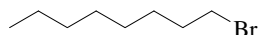
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

5.1.2.13 1-Bromooctane



Common Name: 1-Bromooctane

Synonym: octyl bromide

Chemical Name: 1-bromooctane

CAS Registry No: 111-83-1

Molecular Formula: $C_8H_{17}Br$, $CH_3(CH_2)_6CH_2Br$

Molecular Weight: 193.125

Melting Point ($^{\circ}C$):

-55 (Dreisbach 1961; Weast 1982-83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

200.8 (Dreisbach 1961; Weast 1982-83; Lide 2003)

Density (g/cm^3):

1.1122, 1.1072 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

1.1122 ($20^{\circ}C$, Weast 1982-83)

Molar Volume (cm^3/mol):

174.3 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

208.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.92, 42.04 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section)

1.67 (generator column-GC/FID, Tewari et al. 1982; Miller et al. 1985)

1.67 (tentative value, IUPAC-NIST Solubility Data Series, Hovrath & Getzen 1999b)

1.72* ($24.9^{\circ}C$, generator column-GC, measured range $1.1-40.1^{\circ}C$, Sarraute et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

50.66 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.1179 - 1701.61/(200.8 + t/^{\circ}C)$; temp range $101-253^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.1179 - 1701.61/(200.8 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log(P_L/kPa) = 6.2428 - 1701.61/(T/K - 72.35)$; temp range $373-475 K$ (Antoine eq., liquid, Stephenson & Malanowski 1987)

50.53* ($24.9^{\circ}C$, calculated-Antoine eq. of Li & Rossini 1961, temp range $1.1-40.1^{\circ}C$, Sarraute et al. 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$. Additional data at other temperatures designated * are compiled at the end of this section):

5699* (calculated-P/C, temp range $1.1-40.1^{\circ}C$, Sarraute et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.89 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

4.89; 5.09 (generator column-GC; correlated-activity coeff., Schantz & Martire 1987)

4.89 (recommended, Sangster 1989, 1994; Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

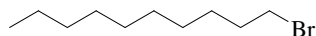
Half-Lives in the Environment:

TABLE 5.1.2.13.1

Reported aqueous solubilities, vapor pressures and Henry's law constants of 1-bromooctane at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Aqueous solubility		Vapor pressure		Henry's law constant	
Sarraute et al. 2004		Sarraute et al. 2004		Sarraute et al. 2004	
generator column-GC		extrapolated -Antoine eq.#		calculated-P/C	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
1.10	2.66	1.10	6.567	1.10	478.8
5.0	2.22	5.0	9.431	5.0	809.4
5.2	2.414	5.2	9.606	5.2	777.4
9.9	1.76	9.9	14.69	9.9	1600
9.9	1.77	9.9	14.68	9.9	1600
14.9	1.82	14.9	22.60	14.9	2395
24.9	1.715	24.9	50.53	24.9	5699
29.9	2.18	29.9	73.61	29.9	6500
34.0	2.78	34.0	105.5	34.0	7350
40.0	3.65	40.0	150.1	40.0	7941
40.1	3.48	40.1	150.6	40.1	8360
Antoine eq.					
#see ref. Li & Rossini 1961					
eq. 2		P/mmHg			
A		7.1231			
B		1369.20			
C		204.4			
pressure range 10–1500 torr mmHg					

5.1.2.14 1-Bromodecane



Common Name: 1-Bromodecane

Synonym: decyl bromide

Chemical Name: 1-bromodecane

CAS Registry No: 112-29-8

Molecular Formula: $C_{10}H_{21}Br$, $CH_3(CH_2)_8CH_2Br$

Molecular Weight: 221.178

Melting Point ($^{\circ}C$):

-29.2 (Dreisbach 1961; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

240.6 (Dreisbach 1961; Weast 1982–83; Riddick et al. 1986; Lide 2003)

Density (g/cm^3):

1.0702, 1.0656 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961; Riddick et al. 1986)

1.0702 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

206.7 ($10^{\circ}C$, Stephenson & Malanowski 1987)

252.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

67.12, 46.66 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.33 (calculated-Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = 7.2336 - 1888.67/(193.3 + t/^{\circ}C)$; temp range 135 – $297^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.2336 - 1888.67/(193.3 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

5.0 (quoted value from Dreisbach 1961, Riddick et al. 1986)

$\log(P/kPa) = 6.3585 - 1888.67/(193.3 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.3585 - 1888.67/(T/K - 79.85)$; temp range 383 – $570 K$ (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.43 (HPLC-RT correlation, McDuffie 1981)

6.35, 5.84 (HPLC-RT correlation; calculated-CLOGP, Burkhard et al. 1985)

6.43 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

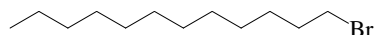
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

5.1.2.15 1-Bromododecane



Common Name: 1-Bromododecane

Synonym: lauryl bromide

Chemical Name: 1-bromododecane

CAS Registry No: 143-15-7

Molecular Formula: $C_{12}H_{25}Br$, $CH_3(CH_2)_{10}CH_2Br$

Molecular Weight: 249.231

Melting Point ($^{\circ}C$):

-9.5 (Dreisbach 1961; Weast 1982-83; Lide 2003)

Boiling Point ($^{\circ}C$):

276 (Dreisbach 1961; Weast 1982-83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

1.0399, 1.0355 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

1.0399 ($20^{\circ}C$, Weast 1982-83)

Molar Volume (cm^3/mol):

240.1 ($20^{\circ}C$, Stephenson & Malanowski 1987)

297.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.38, 50.91 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 7.3390 - 2061.93/(186.6 + t/^{\circ}C)$; temp range 165-237 $^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = 7.3390 - 2061.93/(186.6 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini. 1961)

$\log(P/kPa) = 6.4639 - 2061.93/(T/K - 86.55)$; temp range 411-610 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.98; 6.90 (HPLC-RT correlation; calculated-CLOPG, Burkhard et al. 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

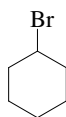
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

5.1.2.16 Bromocyclohexane



Common Name: Bromocyclohexane

Synonym: cyclohexyl bromide

Chemical Name: bromocyclohexane

CAS Registry No: 108-85-0

Molecular Formula: $C_6H_{11}Br$

Molecular Weight: 163.055

Melting Point ($^{\circ}C$):

-56.5 (Weast 1982-83; Lide 2003)

Boiling Point ($^{\circ}C$):

166.2 (Weast 1982-83; Lide 2003)

Density (g/cm^3):

1.33585, 1.32976 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.3359 ($20^{\circ}C$, Weast 1982-83)

Molar Volume (cm^3/mol):

122.06, 122.6 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

141.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

37.59, 44.80 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.70 (Dreisbach 1955)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

421 (calculated by formula, Dreisbach 1955)

$\log (P/mmHg) = 6.97980 - 1572.19/(217.38 + t/^{\circ}C)$; temp range $68-260^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log P/mmHg = 6.97980 - 1572.19/(t/^{\circ}C + 217.38)$; temp range $68-200^{\circ}C$ (Antoine eq., Dean 1992)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.20 (shake flask-GC, Canton & Wagman 1983)

3.20 (recommended, Sangster 1993)

3.20 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

5.1.2.17 Vinyl bromide



Common Name: Vinyl bromide

Synonym: bromoethene, bromoethylene, ethylene bromide

Chemical Name: bromoethene

CAS Registry No: 593-60-2

Molecular Formula: C_2H_3Br , $CH_2 = CHBr$

Molecular Weight: 106.949

Melting Point ($^{\circ}C$):

-139.54 (Dreisbach 1959; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

15.80 (Dreisbach 1959; Dean 1985; Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4933, 1.4738($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1959; Riddick et al. 1986)

1.4930 (Dean 1985)

Molar Volume (cm^3/mol):

71.6 ($20^{\circ}C$, calculated-density)

67.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

22.60, 23.45 ($25^{\circ}C$, bp, Dreisbach 1959; Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.121 (Dreisbach 1959; Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4310 ($30^{\circ}C$, shake flask-interferometry, Saylor & Gross 1931)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

101325 ($15.8^{\circ}C$, summary of literature data, temp range -95.4 – $15.8^{\circ}C$, Stull 1947)

137700 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/mmHg) = 6.66715 - 953.4/(236.0 + t/^{\circ}C)$; temp range -60 to $60^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1959)

145350 (extrapolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 6076.9/(T/K)] + 7.490979$; temp range -95.4 to $15.8^{\circ}C$ (Antoine eq., Weast 1972–73)

144330, 139840 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.03256 - 1494.17/(281.722 + t/^{\circ}C)$; temp range -66 – $11.9^{\circ}C$ (Antoine eq. derived from exptl data of Mehl 1934, Boublik et al. 1984)

$\log(P/kPa) = 6.08611 - 1083.017/(249.845 + t/^{\circ}C)$; temp range -87.5 – $16.0^{\circ}C$ (Antoine eq. derived from exptl data of Guyer et al. 1937, Boublik et al. 1984)

137700 (selected lit. value, Riddick et al. 1986)

$\log(P/kPa) = 5.79205 - 953.4/(236.0 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

140480 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.03266 - 1014.0/(-37.15 + T/K)$; temp range 224–319 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -10.9281 - 1.1619 \times 10^3/(T/K) + 9.3115 \cdot \log(T/K) - 2.2655 \times 10^{-2} \cdot (T/K) - 4.531 \times 10^{-5} \cdot (T/K)^2$; temp range 135–473 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.57 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Hansch et al. 1995)
- 1.57 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 6.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25.4°C (Perry et al. 1977)

$k_{\text{OH}}(\text{calc}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 6.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320 \text{ h}$, based on aqueous screening test data for vinyl chloride (Heffgott et al. 1977; Freitag et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2880\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 9.4\text{--}94 \text{ h}$, based on measured rate constant for reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}69000 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991) and an estimated half-life for anaerobic biodegradation of vinyl chloride from a ground water field study of chlorinated ethenes (Silka & Wallen 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

5.1.3 IODOALKANES

5.1.3.1 Iodomethane (Methyl iodide)



Common Name: Methyl iodide

Synonym: iodomethane, moniodomethane

Chemical Name: methyl iodide

CAS Registry No: 74-88-4

Molecular Formula: CH₃I

Molecular Weight: 141.949

Melting Point (°C):

-66.4 (Lide 2003)

Boiling Point (°C):

42.43 (Lide 2003)

Density (g/cm³ at 20°C):

2.2790, 2.265 (20°C, 25°C, Dreisbach 1961)

2.2792, 2.265 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

62.28 (20°C, calculated-density)

62.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.97, 27.338 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

14190* (20°C, volumetric method, measured range 0–30°C, Rex 1906)

13630 (20°C, Merckel 1937)

14200 (Seidell 1940; Seidell 1941)

log [C/(mol/L)] = -110.278 + 37.621·log (T/K) + 4823/(T/K); temp range 278.16–322.91 K (Glew & Moelwyn-Hughes 1953)

13900* (recommended, temp range 0–40°C, Horvath 1982)

14000 (20°C, Verschueren 1983; Riddick et al. 1986)

14000 (Dean 1985)

Vapor Pressure (Pa at 25°C, or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

44180, 64440(20°C, 30°C, Rex 1906)

75860* (34.4°C, temp range 0.10–34.4°C, Thompson & Linnett 1936)

53329* (25.3°C, summary of literature data, temp range -55.0 to 25.3°C, Stull 1947)

log (P/mmHg) = 22.974 - 5.346·log (T/K) - 2132/(T/K); temp range 278.16–322.91 K (Glew & Moelwyn-Hughes 1953)

54120 (calculated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.87991 - 1093.235/(230.94 + t/°C); temp range -29 to 76°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.87991 - 1093.235/(230.94 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

49704* (22.879°C, temp range -13.819 to 41.427°C, Boublik & Aim 1972; quoted, Boublik et al. 1984)

47750 (interpolated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 6616.5/(T/K)] + 7.403018$; temp range -55.0 to 254.8°C (Antoine eq., Weast 1972–73)

53980 (calculated-Antoine eq., Kudchadker et al. 1979)

$\log (P/\text{mmHg}) = 6.97241 - 1138.29/(t/^\circ\text{C} + 235.774)$; temp range -14 to 42°C (Antoine eq., Kudchadker et al. 1979)

54120 (lit. average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.09731 - 1138.29/(235.774 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

53960 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.10541 - 1142.67/(-36.87 + T/K)$; temp range 228 – 337 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = A6.17197 - 1240.17/(-17.887 + T/K)$; temp range 315 – 502 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -20.3718 - 1.2536 \times 10^3/(T/K) + 13.645 \cdot \log (T/K) - 2.6955 \times 10^{-2} \cdot (T/K) + 1.6389 \times 10^{-5} \cdot (T/K)^2$; temp range 207 – 528 K (vapor pressure eq., Yaws 1994)

54009 (selected summary of literature data, temp range 206.71 – 363.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

541*, 536 (exptl.-concn ratio, measured range 0 – 49°C , calculated-P/C, Glew & Moelwyn-Hughes 1953)

$\log \{H/(\text{mmHg} \cdot \text{L/mol})\} = 133.252 - 42.967 \cdot \log (T/K) - 6955.2/(T/K)$; temp range 273.16 – 322.91 K (Glew & Moelwyn-Hughes 1953)

653* (29.43°C , concn ratio, measured range 29.43 – 40.34°C , Swain & Thornton 1962)

554.9 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

$\ln K_{AW} = 10.34 - 3541/(T/K)$; measured range 5 – 33°C (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)

287 (computed value, Yaws et al. 1991)

159, 442 (0 , 20°C , distilled water, headspace-GC, Elliott & Rowland 1993)

429 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)

414 (20°C , selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{AW} = 4.059 - 1416/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.69 (19°C , shake flask, Collander 1951)

1.51 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)

1.51 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C :

2.16 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 535$ – 5348 h, based on a measured rate constant for the vapor phase reaction with hydroxyl radical in air (Garraway & Donovan 1979; quoted, Howard et al. 1991).

Hydrolysis: $k = 7.28 \times 10^{-8} \text{ s}^{-1}$ at pH 7 (extrapolated to 25°C) with $t_{1/2} = 110$ d (Mabey & Mill 1978).

Biodegradation: aqueous aerobic $t_{1/2} = 1168$ – 672 h, based on estimated aerobic half-life (Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ – 2688 h, based on estimated aerobic half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); $t_{1/2} = 535\text{--}5348$ h, based on a measured rate constant for the vapor phase reaction with hydroxyl radical in air (Garraway & Donovan 1979; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 336\text{--}1344$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.3.1.1

Reported aqueous solubilities of iodomethane (methyl iodide) at various temperatures

$$S/(\text{wt}\%) = 1.53863 - 0.012169 \cdot (t/^\circ\text{C}) + 1.2714 \times 10^{-4} \cdot (t/^\circ\text{C})^2 + 4.834 \times 10^{-6} \cdot (t/^\circ\text{C})^3 \quad (1)$$

Rex 1906		Horvath 1982	
volumetric method		summary of literature data	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	15650	0	15386
10	14460	10	14345
20	14190	20	13848
30	14290	25	13848
		30	14185
		40	15646
		eq. 1	$S/\text{wt}\%$

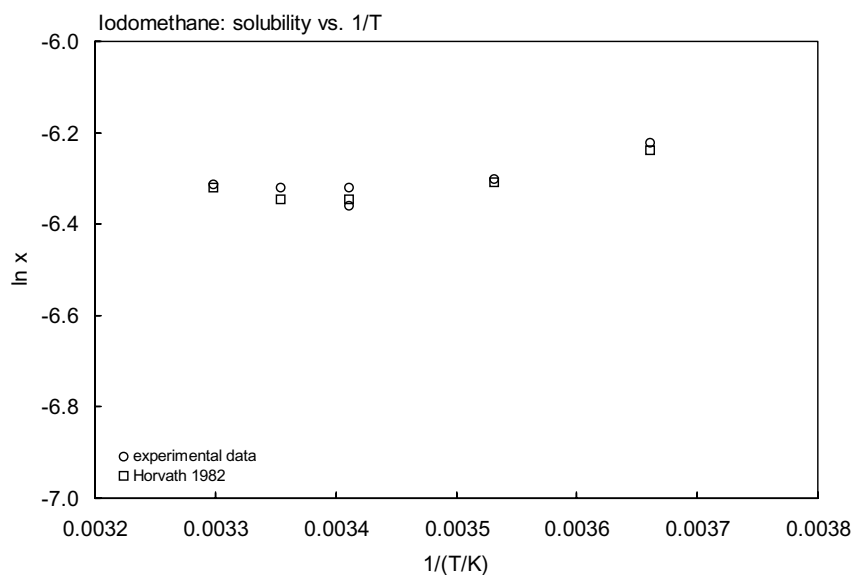


FIGURE 5.1.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for iodomethane.

TABLE 5.1.3.1.2

Reported vapor pressures of iodomethane (methyl iodide) at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Thompson & Linnett 1936		Stull 1947		Boublik & Aim 1972	
		summary of literature data		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0.10	18932			-13.819	9306
4.30	22798	-55.5	666.6	-8.883	12046
11.70	31331	-45.8	1333	-5.101	14549
34.4	75860	-35.0	2666	-0.780	17921
		-24.2	5333	2.954	21314
		-16.9	7999	7.146	25780
		-7.0	13332	10.542	29923
		8.0	26664	14.567	35493
		25.3	53329	18.341	41470
		42.4	101325	22.879	49704
				28.342	61295
		mp/°C	-64.4	34.600	77125
				41.427	97913
				eq. 2	P/kPa
				A	6.11297
				B	1146.368
				C	236.677
				bp	42.431

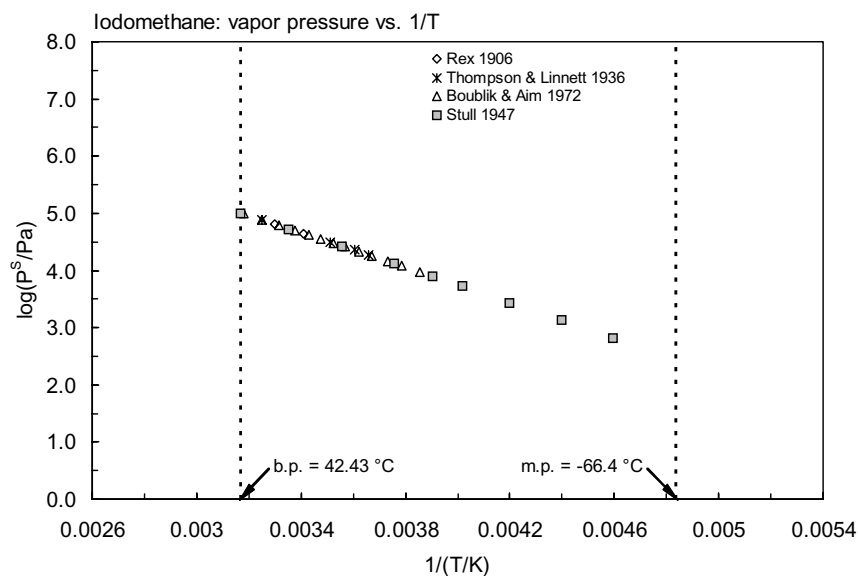


FIGURE 5.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for iodomethane.

TABLE 5.1.3.1.3

Reported Henry's law constants of iodomethane (methyl iodide) at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1) \qquad \log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \qquad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln H = A - B/(T/K) \quad (4)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

$$\log H = A - B \cdot \log (T/K) - C/(T/K) \quad (6)$$

Glew & Moelwyn-Hughes 1953		Swain & Thornton 1962		Elliot & Rowland 1993	
concentration ratio		concentration ratio		headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
0	169.9	29.45	653	0	159
5.03	224.8	29.44	651	20	442
10.2	288.0	40.35	923		
15.12	364.0	40.34	913		
19.94	450.6				
24.92	541.2				
34.92	630.6				
39.86	738.6				
44.87	850.6				
49.75	1072				
25.0	536				
eq 6	P/(mmHg·L/mol)				
A	71.005				
B	21.656				
C	4043.9				

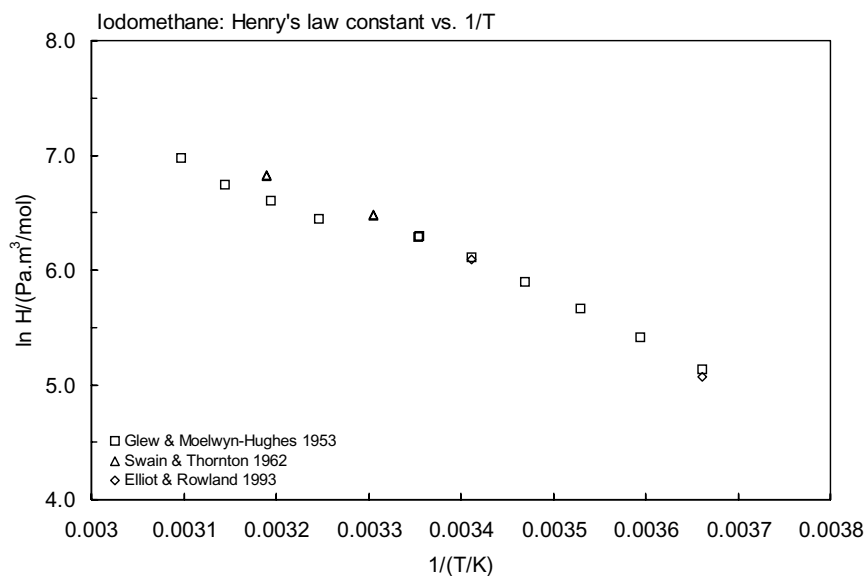


FIGURE 5.1.3.1.3 Logarithm of Henry's law constant versus reciprocal temperature for iodomethane.

5.1.3.2 Iodoethane (Ethyl iodide)



Common Name: Ethyl iodide

Synonym: iodoethane

Chemical Name: ethyl iodide, iodoethane,

CAS Registry No: 75-03-6

Molecular Formula: C_2H_5I , CH_3CH_2I

Molecular Weight: 155.965

Melting Point ($^{\circ}C$):

-111.1 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

72.30 (Rex 1906; Dreisbach 1961; Horvath 1982; Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.9358, 1.9245 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

1.9357, 1.9244 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

80.6 ($20^{\circ}C$, calculated from density)

85.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.93, 29.77 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

4030* ($20^{\circ}C$, volumetric method, measured range $0-30^{\circ}C$, Rex 1906;)

3910 ($22.5^{\circ}C$, volumetric method, Fühner 1924)

4040 ($30^{\circ}C$, shake flask-interferometry, Gross & Saylor 1931)

4040 ($30^{\circ}C$, shake flask, Van Arkel & Vles 1936)

3915 ($20^{\circ}C$, Merckel 1937)

3918 (Seidell 1940, 1941; quoted, Deno & Berkheimer 1960; Hansch et al. 1968; Hine & Mookerjee 1975)

3915 ($22.5^{\circ}C$, Saracco & Spaccamela Marchetti 1958)

3920 ($20^{\circ}C$, exptl., Korenman et al. 1971)

4041* (summary of literature data temp range $0-30^{\circ}C$, Horvath 1982)

3880 ($30^{\circ}C$, selected, Riddick et al. 1986)

4000* (tentative value, temp range $0-30^{\circ}C$, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

$S/(wt\%) = 8.5757 - 5.5568 \times 10^{-2} \cdot (T/K) + 9.43918 \times 10^{-5} \cdot (T/K)^2$, temp range 273–303 K (eq. derived from literature solubility data, Horvath & Getzen 1999a)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

14280, 22150 ($20^{\circ}C$, $30^{\circ}C$, Rex 1906)

21678* ($30^{\circ}C$, manometry, measured range $30-60^{\circ}C$, Smyth & Engel 1929)

14612* ($20^{\circ}C$, temp range -19.36 to $20.4^{\circ}C$, Milazzo 1944)

13332* ($18^{\circ}C$, summary of literature data, temp range -54.4 to $72.4^{\circ}C$, Stull 1947)

18160 (calculated-Antoine eq., Dreisbach 1961)

$\log (P/mmHg) = 6.83198 - 1175.709/(225.26 + t/^{\circ}C)$; temp range -6 to $109^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.83198 - 1175.709/(225.26 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log (P/mmHg) = [-0.2185 \times 6843.1/(T/K)] + 7.635277$; temp range -74.3 to $229.5^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log (P/\text{kPa}) = 7.12695 - 1823.148/(285.30 + t/^{\circ}\text{C})$; temp range -19.36 to 20.4°C (Antoine eq. derived from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.06765 - 1222.410/(228.368 + t/^{\circ}\text{C})$, temp range 30 – 60°C (Antoine eq. derived from reported experimental data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.959 - 1232.0/(229.0 + t/^{\circ}\text{C})$; temp range 30 – 60°C (Antoine eq., Dean 1985, 1992)

$\log (P/\text{kPa}) = 5.95688 - 1175.709/(225.26 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986) 18430 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.95686 - 1175.709/(-47.89 + T/\text{K})$; temp range 249 – 369 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 31.4422 - 2.5719 \times 10^3/(T/\text{K}) - 8.4867 \cdot \log (T/\text{K}) - 9.0736 \times 10^{-11} \cdot (T/\text{K}) + 3.571 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 162 – 561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

732 (calculated- $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

840 (calculated-QSAR, Nirmalakhandan & Speece 1988)

545 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.00 (shake flask-GC, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)

2.00 (recommended, Sangster 1989, 1993)

2.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C :

2.59 (calculated-measured infinite dilution activity coeff. and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Hydrolysis: rate constant $k = 1.62 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 49$ d at 25°C and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4$ – 24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: $t_{1/2} = 49$ d at 25°C and pH 7 (Mabey & Mill 1978)

Ground water:

Sediment:

Soil:

Biota:

TABLE 5.1.3.2.1**Reported aqueous solubilities of 1-iodoethane at various temperatures**

$$S/(\text{wt}\%) = 0.4391 - 3.24498 \times 10^{-3} \cdot (t/^{\circ}\text{C}) + 4.49991 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 1.15001 \times 10^{-6} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 8.5757 - 5.5568 \times 10^{-2} \cdot (T/\text{K}) + 9.43918 \times 10^{-4} \cdot (T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999a	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	4410	0	4391	0	4400
10	4140	10	4123	5	4220
20	4030	20	4014	10	4090
30	4150	25	4041	15	4010
		30	4133	20	3980
		eq. 1	S/wt%	25	4000
				30	4050
				eq. 2	S/wt%
				temp range 273–303 K	

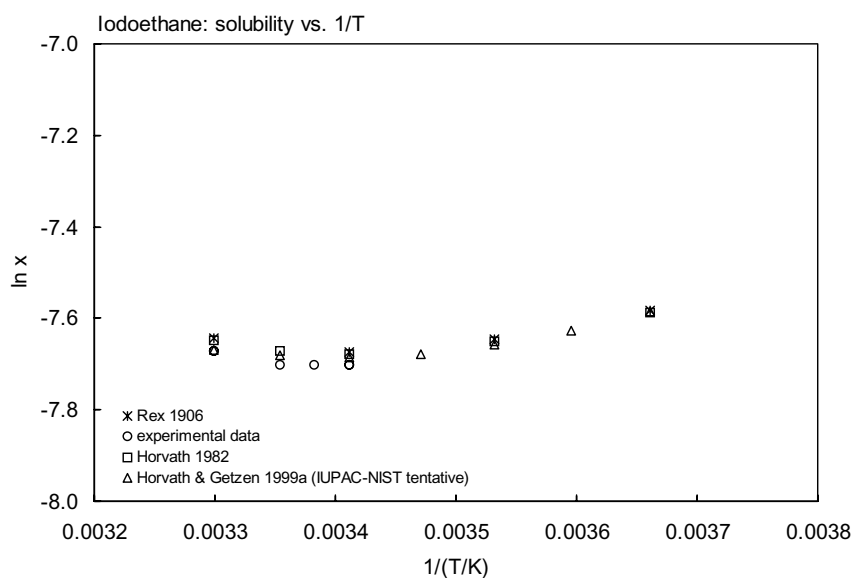
**FIGURE 5.1.3.2.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for iodoethane.

TABLE 5.1.3.2.2

Reported vapor pressures of iodoethane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & \end{aligned}$$

Smyth & Engel 1929		Milazzo 1944		Stull 1947	
Manometry				summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30.0	21678	-19.36	1867	-54.4	133.3
40.0	32637	0.040	5533	-34.3	666.6
50.0	47329	9.34	8666	-24.3	1333
60.0	67448	10.4	9066	-13.1	2666
		20.4	14612	-0.90	5333
				7.2	7999
				18.0	13332
				34.1	26664
				52.3	53329
				72.4	101325
				mp/°C	-105

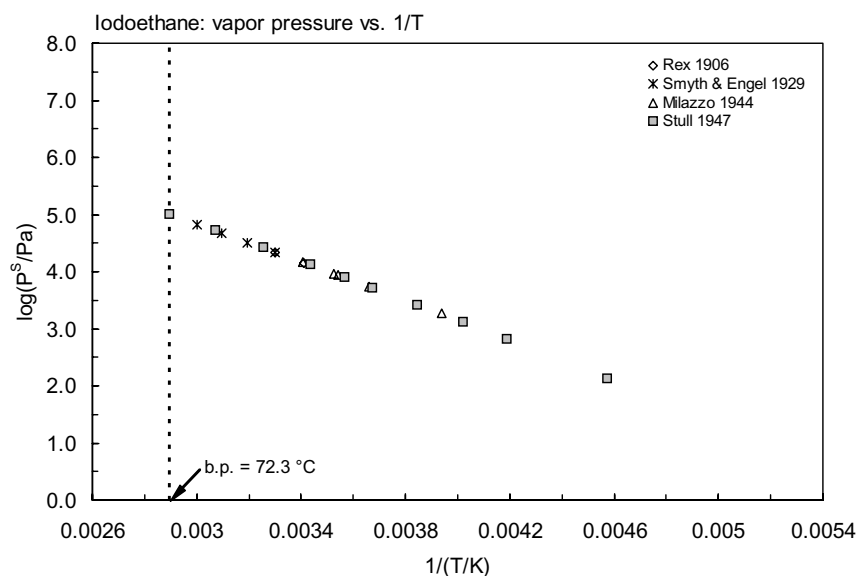
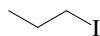


FIGURE 5.1.3.2.2 Logarithm of vapor pressure versus reciprocal temperature for iodoethane.

5.1.3.3 1-Iodopropane



Common Name: 1-Iodopropane

Synonym: monoiodopropane, *n*-propyl iodide, propyl iodide

Chemical Name: 1-iodopropane, monoiodopropane, *n*-propyl iodide, propyl iodide

CAS Registry No: 107-08-4

Molecular Formula: C₃H₇I, CH₃CH₂CH₂I

Molecular Weight: 169.992

Melting Point (°C):

−101.3 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):

102.5 (Lide 2003)

Density (g/cm³ at 20°C):

1.7489, 1.7394 (20°C, 25°C, Dreisbach 1961; Riddick et al. 1986)

Molar Volume (cm³/mol):

97.2 (20°C, calculated-density)

107.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.98, 31.70 (25°C, bp, Dreisbach 1961)

36.25 (25°C, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1070* (20°C, volumetric method, measured range 0–30°C, Rex 1906)

867 (20°C, volumetric method, Fühner 1924)

1040 (30°C, shake flask-interferometer, Gross & Saylor 1931)

1037 (30°C, shake flask, Van Arkel & Vles 1936)

1073 (Seidell 1940; quoted, Deno & Berkheimer 1960; Hine & Mookerjee 1975)

872 (Seidell 1941)

1110 (calculated-K_{OW}, Hansch et al. 1968)

1070, 1060 (23.5°C, elution chromatography, Schwarz 1980)

1051* (summary of literature data, temp range 0–30°C, Horvath 1982)

1000 (Dean 1985)

1040 (30°C, quoted, Riddick et al. 1986)

1010* (tentative value, temp range 0–30°C, IUPAC-NIST Series, Horvath & Getzen 1999b)

S/(wt%) = 3.4659 − 0.023046·(T/K) + 3.94424 × 10^{−5}·(T/K)², temp range 273–303 K (equation derived from literature data, Horvath & Getzen 1999b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

4679, 7305 (20°C, 30°C, volumetric method Rex, 1906)

5333 (23.6°C, summary of literature, data temp range −36.0 to 102.5°C, Stull 1947)

5745 (calculated-Antoine eq., Dreisbach 1961)

log (P/mmHg) = 6.81603 − 1267.062/(219.53 + t/°C); temp range 18–143°C (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = 6.81603 − 1267.062/(219.53 + t/°C); pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

log (P/mmHg) = [−0.2185 × 8467.1/(T/K)] + 7.824521; temp range −36.0 to 102.5°C (Antoine eq., Weast 1972–73)

5745 (quoted lit. average, Riddick et al. 1986)

log (P/kPa) = 5.94053 − 1267.062/(219.53 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

5745 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.6036 - 1160.5/(-59.55 + T/\text{K})$; temp range 171–271 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.94093 - 1267.062/(-52.62 + T/\text{K})$; temp range 271–402 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 1.2733 - 2.0214 \times 10^3/(T/\text{K}) + 4.1138 \cdot \log (T/\text{K}) - 1.2477 \times 10^{-2} \cdot (T/\text{K}) + 7.678 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 172–593 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

921 (calculated as $1/K_{\text{AW}}, C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

1033, 1082 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1057 (calculated-QSAR, Nirmalakhandan & Speece 1988)

844 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.50 (calculated- π const., Hansch et al. 1968)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 5.1.3.3.1

Reported aqueous solubilities of 1-iodopropane at various temperatures

$$S/(\text{wt}\%) = 0.1139 - 4.86669 \times 10^{-4} \cdot (t/^\circ\text{C}) + 1.25003 \times 10^{-5} \cdot (t/^\circ\text{C})^2 - 2.8334 \times 10^{-7} \cdot (t/^\circ\text{C})^3 \quad (1)$$

$$S/(\text{wt}\%) = 3.4659 - 0.023046 \cdot (T/\text{K}) + 3.94424 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

Rex 1906		Horvath 1982		Horvath & Getzen 1999b	
volumetric method		summary of literature data		tentative, IUPAC-NIST	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	1140	0	1139	0	1140
10	1030	10	1100	5	1070
20	1070	20	1069	10	1030
30	1030	25	1051	15	1000
		30	1029	20	1000
				25	1010
		eq. 1	$S/\text{wt}\%$	30	1040
				eq. 2	$S/\text{wt}\%$
				temp range 273–303 K	

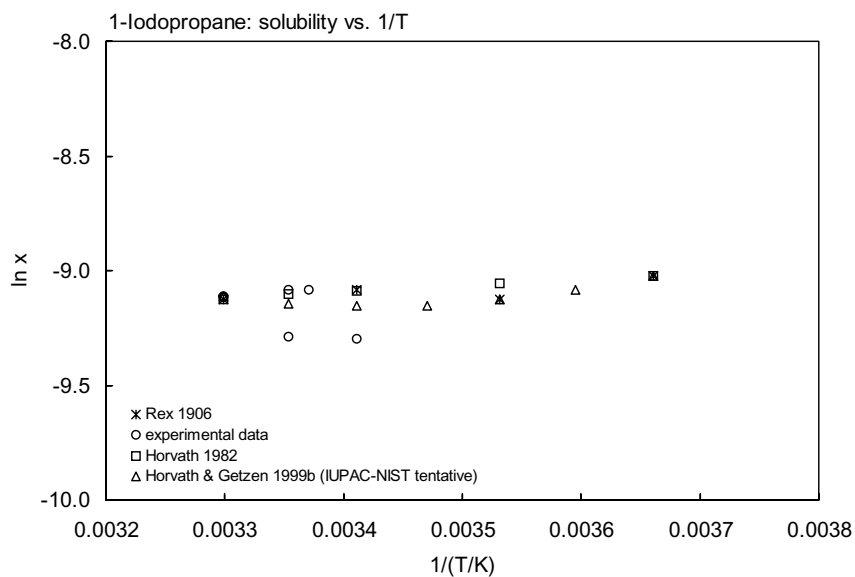


FIGURE 5.1.3.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-iodopropane.

5.1.3.4 2-Iodopropane



Common Name: 2-Iodopropane

Synonym: isopropyl iodide

Chemical Name: 2-iodopropane, isopropyl iodide

CAS Registry No: 75-30-9

Molecular Formula: C_3H_7I , CH_3CHICH_3

Molecular Weight: 169.992

Melting Point ($^{\circ}C$):

−90.0 (Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

89.50 (Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.7042, 1.6946 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

99.8, 100.3 ($20^{\circ}C$, $25^{\circ}C$, calculated-density)

107.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

34.06 ($25^{\circ}C$, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1670, 1430, 1400, 1340 (0, 10, 20, $30^{\circ}C$, volumetric method, Rex 1906)

1343 ($30^{\circ}C$, shake flask, Van Arkel & Vles 1936)

1667, 1428, 1398, 1387, 1338 (0, 10, 20, 25, $30^{\circ}C$, summary of literature data, Horvath 1982)

$S/(wt\%) = 0.1667 - 4.23167 \times 10^{-3} \cdot t/^{\circ}C + 0.000224 \cdot (t/^{\circ}C)^2 - 3.98334 \times 10^{-6} \cdot (t/^{\circ}C)^3$ (Horvath 1982)

1400 ($20^{\circ}C$, selected, Riddick et al. 1986)

1670, 1430, 1400, 1340 (0, 10, 20, $30^{\circ}C$, reported exptl data of Rex 1906, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999b)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

7518, 11780 ($20^{\circ}C$, $30^{\circ}C$, Rex 1906)

7999 ($21.6^{\circ}C$, summary of literature data, temp range -43.3 to $89.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 8243.4/(T/K)] + 7.873828$; temp range -43.3 to $89.5^{\circ}C$ (Antoine eq., Weast 1972–73)

5700 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.87492 - 1765.15/(T/K)$; temp range not specified (Antoine eq., Riddick et al. 1986)

9360 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.2763 - 1414.85/(-31.45 + T/K)$; temp range 261–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.2724 - 989.55/(-69.18 + T/K)$; temp range 173–262 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 33.2023 - 2.7569 \times 10^3/(T/K) - 9.0585 \cdot \log(T/K) - 1.2099 \times 10^{-10} \cdot (T/K) + 3.5044 \times 10^{-6} \cdot (T/K)^2$; temp range 183–578 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

1133 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

2479, 1982 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1840 (calculated-QSAR, Nirmalakhandan & Speece 1988)

903 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Hydrolysis: rate constant $k = 2.77 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 2.9 \text{ d}$ at 25°C and pH 7 (Mabey & Mill 1978)

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water: $t_{1/2} = 2.9 \text{ d}$ at 25°C and pH 7 based on hydrolysis rate constant (Mabey & Mill 1978)

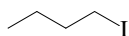
Ground water:

Sediment:

Soil:

Biota:

5.1.3.5 1-Iodobutane



Common Name: 1-Iodobutane

Synonym: *n*-butyl iodide, moniodobutane

Chemical Name: *n*-butyl iodide, 1-iodobutane, moniodobutane

CAS Registry No: 542-69-8

Molecular Formula: C_4H_9I , $CH_3CH_2CH_2CH_2I$

Molecular Weight: 184.018

Melting Point ($^{\circ}C$):

−103.0 (Dreisbach 1961; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

130.53 (Dreisbach 1961; Riddick et al. 1986)

130.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.6154, 1.6072 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961; Riddick et al. 1986)

Molar Volume (cm^3/mol):

113.9, 114.5 ($20^{\circ}C$, $25^{\circ}C$, calculated- density, Riddick et al. 1986)

129.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.63, 33.40 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

210 ($17.5^{\circ}C$, volumetric method, Fühner 1924)

202 ($20^{\circ}C$, Merckel 1937)

211 (Seidell 1940; quoted, Deno & Berkheimer 1960)

202 (Seidell 1941)

313 (Kakovsky 1957)

182 (selected exptl., Horvath 1982)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1848 (calculated-Antoine eq., Dreisbach 1961)

$\log (P/mmHg) = 6.82262 - 1358.860/(214.2 + t/^{\circ}C)$; temp range 40 – $174^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.82262 - 1358.860/(214.20 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq., from correlation of selected lit. data, Li & Rossini 1961)

$\log (P/kPa) = 5.94752 - 1358.860/(214.20 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

1848 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.94752 - 1358.86/(-58.95 + T/K)$; temp range 292–431 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1600 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

1426, 600 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

1331 (calculated-QSAR, Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.00 (calculated- π const., Hansch et al. 1968)

2.51 (calculated-fragment const. with correction factors in multiCASE program, Damborsky et al. 2001)

Bioconcentration Factor, log BCF:

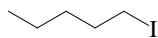
Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976).

5.1.3.6 1-Iodopentane



Common Name: 1-Iodopentane

Synonym: pentyl iodide

Chemical Name: 1-iodopentane

CAS Registry No: 628-17-1

Molecular Formula: $C_5H_{11}I$, $CH_3(CH_2)_3CH_2I$

Molecular Weight: 198.045

Melting Point ($^{\circ}C$):

-85.6 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

157 (Dreisbach 1961; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

1.5061, 1.5088 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

1.5161 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

130.6 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

151.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

43.33, 35.81 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

585 (calculated-Antoine eq., Dreisbach 1961)

$\log (P/mmHg) = 6.85172 - 1454.028/(209.17 + t/^{\circ}C)$; temp range 61 – $204^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = 6.85172 - 1454.028/(209.17 + t/^{\circ}C)$; pressure range of 10 to 1500 mmHg (Antoine eq. from correlation of selected lit. data, Li & Rossini 1961)

$\log P_L/kPa = 5.97662 - 1454.028/(-63.98 + T/K)$; temp range 312–413 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

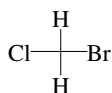
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

5.1.4 MIXED HALOGENATED HYDROCARBONS

5.1.4.1 Bromochloromethane



Common Name: Bromochloromethane

Synonym: chlorobromomethane, methylene bromochloride

Chemical Name: bromochloromethane, chlorobromomethane

CAS Registry No: 74-97-5

Molecular Formula: CH_2BrCl

Molecular Weight: 129.384

Melting Point ($^{\circ}\text{C}$):

-87.9 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

68.0 (Lide 2003)

Density (g/cm^3 at 20°C):

1.9344 (Dreisbach 1959; Weast 1982–83; Riddick et al. 1986)

1.9229 (25°C , Dreisbach 1959)

Molar Volume (cm^3/mol):

66.89 (20°C , calculated-density)

73.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

15000 (O'Connell 1963)

9000 (Kirk-Othmer 1964, Irmann 1965, Dean 1985)

15000 (Jolls 1966)

14778 (at saturated pressure, recommended, Horvath 1982)

16690 (generator column-GC, Tewari et al. 1982)

38900 (calculated-UNIFAC activity coeff., Arbuckle 1986)

17000 (selected, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

18808 (24.06°C , ebulliometric method, measured range 15.72 – 68°C , McDonald et al. 1959)

$\log(P/\text{mmHg}) = 6.38587 - 895.556/(186.703 + t/^{\circ}\text{C})$; temp range 15.72 – 68.0°C (Antoine eq. from ebulliometric measurements, McDonald et al. 1959)

19620 (calculated-Antoine eq., Dreisbach 1959)

$\log(P/\text{mmHg}) = 6.86624 - 1132.3/(215.0 + t/^{\circ}\text{C})$; temp range -6 to 297°C (Antoine eq. for liquid state, Dreisbach 1959)

19520 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/\text{mmHg}) = 6.49606 - 942.267/(192.587 + t/^{\circ}\text{C})$; temp range 15.7 – 68°C (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1973)

19520 (calculated-Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 6.41307 - 903.382/(187.594 + t/^{\circ}\text{C})$; temp range 16 – 68°C (Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{kPa}) = 6.60056 - 932.609/(191.376 + t/^{\circ}\text{C})$; temp range 15.7 – 68°C (Antoine eq. from reported exptl. data of McDonald & Shrader 1959, Boublik et al. 1984)

19530 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.51146 - 891.345/(-86.965 + T/\text{K})$; temp range 226 – 341 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 2.7704 - 2.0139 \times 10^3/(T/K) + 3.7817 \cdot \log (T/K) - 1.3241 \times 10^{-2} \cdot (T/K) + 8.1979 \times 10^{-6} \cdot (T/K)^2$;
temp range 185–557 K (vapor pressure eq., Yaws 1994)
19257 (selected summary of literature data, temp range 185.21–368.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.41 (generator column-GC, Tewari et al. 1982)
1.41 (recommended, Sangster 1993)
1.41 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

rate constant for the reaction with OH: $k = (2.5 \pm 0.3) \times 10^{-6} \text{ M}^{-1} \text{ s}^{-1}$ was measured in 66.7% dioxane-water at 35.7°C (Hine et al. 1956; quoted, Roberts et al. 1992)

$k_{\text{OH}} = 1.11 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetime $\tau = 0.43 \text{ yr}$ at 298 K, measured range 277–377 K (flash photolysis resonance fluorescence and discharge flow electron paramagnetic resonance, Orkin et al. 1997)

Hydrolysis: rate constant $k = 1.2 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 44 \text{ yr}$ at pH 7 and 25°C (Mabey & Mill 1978)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

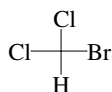
Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976)

Atmospheric lifetime $\tau = 0.21 \text{ yr}$ reduced from 0.43 yr due to reaction with OH with ocean removal (Orkin et al. 1997)

Surface water: hydrolysis rate constant $k = 1.2 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 44 \text{ yr}$ at pH 7 and 25°C (Mabey & Mill 1978)

5.1.4.2 Bromodichloromethane



Common Name: Bromodichloromethane

Synonym: dichlorobromomethane

Chemical Name: bromodichloromethane, dichlorobromomethane

CAS Registry No: 75-27-4

Molecular Formula: CHBrCl_2

Molecular Weight: 163.829

Melting Point ($^{\circ}\text{C}$):

-57 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

90.0 (Weast 1977; Lide 2003)

Density (g/cm^3 at 20°C):

1.9710 (25°C , Verschueren 1983)

Molar Volume (cm^3/mol):

83.1 (20°C , calculated-density)

94.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

4700 (22°C , Mabey et al. 1981)

2968 (30°C , headspace-GC, McNally & Grob 1984)

8880, 8668, 8506 ($20, 30, 40^{\circ}\text{C}$, infinite dilution activity coeff. γ -GC, Tse et al. 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

6665 (20°C , Dreisbach 1952;)

8555, 13440, 20444 ($20, 30, 40^{\circ}\text{C}$, DIPPR compilation, Tse et al. 1992)

Henry's Law Constant (Pa m^3/mol at 25°C and reported temperature dependence equations):

244.2 (20°C , calculated-P/C, Mabey et al. 1982)

162 (20°C , batch air stripping-GC, Nicholson et al. 1984)

162, 152, 152 (20°C , batch stripping-GC, natural potable water samples, Nicholson et al. 1984)

$\ln [H/(\text{atm m}^3/\text{mol})] = 11.30 - 5210/(T/K)$; temp range 10 – 30°C (air stripping-GC measurements, Nicholson et al. 1984)

214.8 (gas stripping-GC, Warner et al. 1987)

243.1 (20 – 25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

243 (calculated-P/C, Mackay & Shiu 1990)

162, 263, 405 ($20, 30, 40^{\circ}\text{C}$, infinite dilution activity coeff. γ -GC, Tse et al. 1992)

55.2, 106, 192 ($0, 10, 20^{\circ}\text{C}$, seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

$\ln K_{\text{AW}} = 13.43 - 4678/(T/K)$; seawater of salinity of 30.4‰, temp range: 0 – 10°C (Moore et al. 1995)

185 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 6.143 - 2130/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

347 (37°C , equilibrium headspace-GC, Batterman et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.88 (calculated as per Tute 1971, Callahan et al. 1979; Mills et al. 1982)

2.10 (Hansch & Leo 1979)

2.10 (calculated, Mabey et al. 1982)

2.00 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$

2.98; 2.97 (equilibrium headspace-GC; calculated- K_{OW}/K_{AW} , Batterman et al. 2002)

Bioconcentration Factor, $\log BCF$:

1.544 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

0.72–1.37 (estimated as per Lyman et al. 1982, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.785 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.724–2.40 (estimated from S & K_{OW} , Swann et al. 1983; quoted, Howard 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: typical $t_{1/2}$ ~35 h for a range of 33 min to 12 d was estimated from experimentally determined gas transfer rates (Kaczmar et al. 1984; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

calculated rate constants at 25°C: $k < 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 0.2 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982).

Hydrolysis: first-order rate constant $k = 1.6 \times 10^{-10} \text{ s}^{-1}$ at pH 7 and 25°C with a maximum $t_{1/2} = 137 \text{ yr}$ (Mabey & Mill 1978; quoted, Mabey et al. 1982; Howard 1990).

Biodegradation:

Biotransformation: estimated rate constant $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

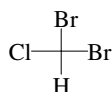
Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24 \text{ h}$ from air for the reaction with OH radical (Darnall et al. 1976);

$t_{1/2} = 3.92 \text{ months}$, based on an estimated rate constant $k = 8.522 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with hydroxyl radical (GEMS 1987; quoted, Howard 1990).

Surface water: hydrolysis rate constant $k = 1.6 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 137 \text{ yr}$ at pH 7 and 25°C (Mabey & Mill 1978)

5.1.4.3 Dibromochloromethane



Common Name: Dibromochloromethane

Synonym: chlorodibromomethane

Chemical Name: dibromochloromethane, chlorodibromomethane

CAS Registry No: 124-48-1

Molecular Formula: CHBr_2Cl

Molecular Weight: 208.280

Melting Point ($^{\circ}\text{C}$):

−22.0 (Dean 1985)

−20 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

119–120 (Weast 1977; Weast 1982–83)

120 (Lide 2003)

Density (g/cm^3 at 20°C):

2.451 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

84.98 (20°C , calculated-density)

97.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

4000 (calculated- K_{OW} , Mabey et al. 1982)

5814, 6000, 6102 (20, 30, 40°C , infinite dilution activity coeff. γ -GC, Tse et al. 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

10131 (20°C , extrapolated-Antoine eq., Mabey et al. 1982)

2000 (20°C , selected, Mills et al. 1982)

6667 (20°C , Warner et al. 1987)

2324, 3877, 6232 (20, 30, 40°C , DIPPR compilation, Tse et al. 1992)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

100 (20°C , calculated-P/C, Mabey et al. 1982)

88.2; 88.1, 85.1 (20°C , batch air stripping-GC; quoted lit. values, Nicholson et al. 1984)

86.1, 81.06, 78.02 (20°C , batch stripping-GC, natural potable water samples, Nicholson et al. 1984)

$\ln [H/(\text{atm m}^3/\text{mol})] = 10.70 - 5210/(T/K)$; temp range 10 – 30°C (air stripping-GC measurements, Nicholson et al. 1984)

80.4 (gas stripping-GC, Warner et al. 1987)

120* (EPICS-GC/FID, measured range 10 – 30°C , Ashworth et al. 1988)

$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 14.62 - 6373/(T/K)$; temp range 10 – 30°C , (EPICS measurements, Ashworth et al. 1988)

100 (20 – 25°C and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

81.06, 142, 223 (20, 30, 40°C , infinite dilution activity coeff. γ -GC, Tse et al. 1992)

28.2, 56.3, 103 (0, 10, 20°C , seawater of salinity of 30.4‰, gas stripping-GC, Moore et al. 1995)

$\ln K_{\text{AW}} = 13.62 - 4914/(T/K)$; seawater of salinity of 30.4‰, temp range: 0 – 10°C (Moore et al. 1995)

85.3 (20°C , selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 6.296 - 2273/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

218 (37°C , equilibrium headspace-GC, Batterman et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.09 (calculated as per Tute 1971, Callahan et al. 1979)
- 2.24 (Hansch & Leo 1979)
- 2.24 (calculated, Mabey et al. 1982)
- 2.16 (recommended, Sangster 1993)
- 2.04 (infinite dilution activity coeff.-GC, Tse & Sandler 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 3.59 (calculated-measured infinite dilution activity coeff. and vapor pressure P, Abraham et al. 2001)
- 3.33; 3.31 (equilibrium headspace-GC; calculated- K_{OW}/K_{AW} , Batterman et al. 2002)

Bioconcentration Factor, $\log BCF$:Sorption Partition Coefficient, $\log K_{OC}$:Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: calculated $t_{1/2} = 43$ min to 16.6 d (using Langbein & Durum 1967 published O_2 re-aeration values) and $t_{1/2} = 45.9$ h both from rivers and streams (Kaczmar et al. 1984).

Photolysis:

Oxidation: calculated rate constants at 25°C: $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 0.5 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radicals (Mabey et al. 1982);

photooxidation $t_{1/2} = 1025\text{--}10252$ h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: rate constant $k = 8.0 \times 10^{-11} \text{ s}^{-1}$ with hydrolytic $t_{1/2} = 274$ yr at pH 7 and 25°C (Mabey & Mill 1978; quoted, Callahan et al. 1979; Howard et al. 1991);

$k = 2.88 \times 10^{-8} \text{ h}^{-1}$ at pH 7 and 25°C (analogy to chloroform as per Mabey & Mill 1978, Mabey et al. 1982).

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672\text{--}4320$ h, based on unacclimated anaerobic screening test data (Bouwer & McCarty 1983; Bouwer et al. 1981; quoted, Howard et al. 1991).

Biotransformation: estimated rate constant $k = 1.0 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); $t_{1/2} = 1025\text{--}10252$ h, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 274$ yr at pH 7 and 25°C based on hydrolysis rate constant (Mabey & Mill 1978)

$t_{1/2} = 672\text{--}4320$ h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 336\text{--}4320$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Biota:

TABLE 5.1.4.3.1
Reported Henry's law constants of dibromochloromethane
at various temperatures

Ashworth et al. 1988	
EPICS-GC	
t/°C	H/(Pa m ³ /mol)
10	38.50
15	45.60
20	104.4
25	119.6
30	154.0
ln [H/(atm·m ³ /mol)] = A – B/(T/K)	
A	14.62
B	6373

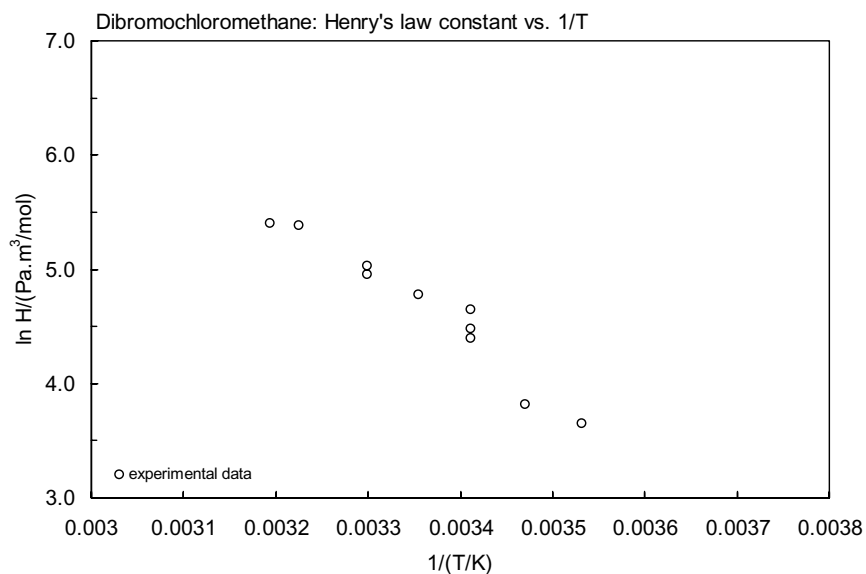


FIGURE 5.1.4.3.1 Logarithm of Henry's law constant versus reciprocal temperature for dibromochloromethane.

5.1.4.4 Chlorodifluoromethane (HCFC-22)



Common Name: Chlorodifluoromethane

Synonym: difluorochloromethane, Freon 22, CFC-22, CF-22

Chemical Name: chlorodifluoromethane

CAS Registry No: 75-45-6

Molecular Formula: CHClF_2

Molecular Weight: 86.469

Melting Point ($^{\circ}\text{C}$):

−157.42 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

−40.7 (Lide 2003)

Density (g/cm^3 at 20°C):

1.2090 (21°C , Dean 1985)

1.1940 (25°C , Kirk-Othmer 1985)

1.2136, 1.1942 (20°C , 25°C , Riddick et al. 1986)

Molar Volume (cm^3/mol):

71.2 (20°C , calculated-density)

60.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

20.238 (bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.123 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F:

Water Solubility (g/m^3 or mg/L at 25°C . Additional data at other temperatures designated * are compiled at the end of this section):

2800, 2900 (quoted values, Irmann 1965)

3000 (DuPont 1966, 1969; quoted, Horvath 1982; Riddick et al. 1986)

2930 (selected, Hine & Mookerjee 1975)

3000 (Weast 1976; quoted, Horvath 1982)

2899* (summary of literature data, temp range 0 – 60°C , Horvath 1982)

3000 (Dean 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

101325* (-40.8°C , summary of literature data, temp range -122.8 to -40.8°C , Stull 1947)

1083100 (calculated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 5212.9/(T/\text{K})] + 7.730042$; temp range -122.8 to 85.3°C (Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = 6.93892 - 808.919/(t/^{\circ}\text{C} + 240.161)$; temp range -79 to -37°C (Antoine eq., Kudchadker et al. 1979)

1027400 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.0741 - 815.920/(241.369 + t/^{\circ}\text{C})$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

35120, 570500 (-61.26°C , 4.5°C , Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.06382 - 808.919/(240.161 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

1043900 (Interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.33292 - 919.834/(-19.718 + T/\text{K})$; temp range 170 – 233 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.19138 - 863.436/(-26.04 + T/\text{K})$; temp range 230–275 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.35713 - 950.38/(-13.474 + T/\text{K})$; temp range 275–327 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.13064 - 1490.048/(64.627 + T/\text{K})$; temp range 324–366 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 40.3847 - 2.0731 \times 10^3/(T/\text{K}) - 12.317 \cdot \log (T/\text{K}) - 2.5116 \times 10^{-10} \cdot (T/\text{K}) + 1.0498 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 116–369 K (vapor pressure eq., Yaws 1994)

132020 (238.15 K, selected summary of literature data, temp range 15.74–238.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

$\log (H/\text{atm}) = 8.18 - 1469.55/(T/\text{K})$ (least-square regression of data from lit., Kavanaugh & Trussell 1980)

2980 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

2478.8 (calculated-QSAR, Nirmalakhandan & Speece 1988)

3058 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.08 (shake flask, Log P Database, Hansch & Leo 1987)

1.08 (recommended, Sangster 1993)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^* = (4.75 \pm 0.48) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 297–434 K, with estimated lifetime of ~1.5 yr (flash photolysis-resonance fluorescence, Atkinson et al. 1975)

$k_{OH} = (3.4 \pm 0.7) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH}^* = (4.25 \pm 0.28) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 253–427 K, with calculated lifetime of 16–25 yr in troposphere (discharge flow-resonance fluorescence, Chang & Kaufman 1977)

$k_{OH} = 4.8 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K with lifetime of 43 yr in troposphere, measured range 250–350 K (FP-RF, Watson et al. 1977; quoted, Altshuller 1980)

$k_{OH} = (2.76 \pm 0.35) \times 10^9 \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (relative rate, Paraskevopoulos et al. 1981)

$k_{OH}(\text{calc}) = 6.8 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{OH}(\text{obs.}) = 4.68 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH}^* = 4.68 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 4.7 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated tropospheric lifetime of 4.3 yr, Bunce et al. 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} = 2.4\text{--}24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); lifetime of 44 yr in troposphere (Altshuller 1980);

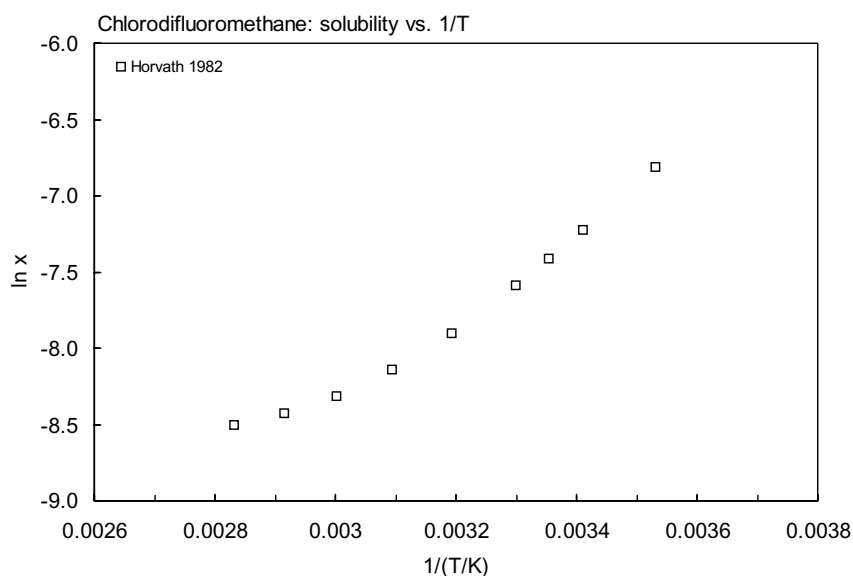
estimated tropospheric lifetime of 4.3 yr as global average for the reaction with hydroxyl radical in air (Bunce et al. 1991);

estimated tropospheric lifetime of 7.5 yr and 15.8 yr by rigorous calculation (Nimitz & Skaggs 1992).

TABLE 5.1.4.4.1**Reported aqueous solubilities and vapor pressures of chlorodifluoromethane (HCFC-22) at various temperatures**

$$S/(\text{wt}\%) = 0.8171 - 3.5818 \times 10^{-2} \cdot (t/^{\circ}\text{C}) + 8.0081 \times 10^{-4} \cdot (t/^{\circ}\text{C})^2 - 1.0075 \times 10^{-5} \cdot (t/^{\circ}\text{C})^3 + 6.9823 \times 10^{-8} \cdot (t/^{\circ}\text{C})^4 \quad (1)$$

Aqueous solubility		Vapor pressure	
Horvath 1982		Stull 1947	
summary of literature data		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	P/Pa
10	5296	-122.8	133.3
20	3510	-110.2	666.6
25	2899	-103.7	1333
30	2428	-96.5	2666
40	1783	-88.6	5333
50	1402	-83.4	7999
60	1180	-76.4	13332
70	1052	-65.8	26664
80	972.8	-53.6	53329
		-40.8	101325
eq. 1	S/(wt%)	mp/°C	-160.0

**FIGURE 5.1.4.4.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for chlorodifluoromethane.

5.1.4.5 Dichlorodifluoromethane (CFC-12)



Common Name: Dichlorodifluoromethane

Synonym: difluorodichloromethane, Freon 12, CFC-12

Chemical Name: dichlorodifluoromethane

CAS Registry No: 75-71-8

Molecular Formula: CF_2Cl_2

Molecular Weight: 120.914

Melting Point ($^{\circ}\text{C}$):

-158.0 (Weast 1982-83; Dean 1985; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

-29.8 (Weast 1982-83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at 20°C):

1.3110 (25°C , Kirk-Othmer 1985)

1.3292, 1.3113 (20°C , 25°C , Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.2 (Stephenson & Malanowski 1987)

81.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

20.112 (bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.14 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F:

Water Solubility (g/m^3 or mg/L at 25°C):

280 (DuPont 1966; quoted, Horvath 1982; Riddick et al. 1986)

276 (Gmelins 1974)

280 (shake flask-GC, Pearson & McConnell 1975)

300 (recommended, Horvath 1982)

280 (Verschuereen 1983; Dean 1985; Kirk-Othmer 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

745000, 1031000 (20°C , 30°C , static method, Gilkey et al. 1931)

101325 (-29.8°C , summary of literature data, temp range -118.5 to -29.8°C , Stull 1947)

214220 (calculated-Antoine eq., Weast 1975)

$\log(P/\text{mmHg}) = 6.82101 - 839.622/(t/^{\circ}\text{C} + 242.861)$; temp range -101 to $+6^{\circ}\text{C}$ (Antoine eq., Kudchadker et al. 1979)

566500, 769940 (20°C , 30°C , Verschuereen 1983)

566600 (20°C , quoted, Riddick et al. 1986)

$\log(P/\text{kPa}) = 5.94591 - 839.622/(242.861 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

651040 (interpolated-Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log(P_1/\text{kPa}) = 5.94677 - 839.6/(-30.311 + T/\text{K})$; temp range 173-244 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_1/\text{kPa}) = 6.0058 - 860.828/(-28.11 + T/\text{K})$; temp range 173-240 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_1/\text{kPa}) = 5.92289 - 826.707/(-32.274 + T/\text{K})$; temp range 236-285 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_1/\text{kPa}) = 6.30541 - 1035.857/(-1.496 + T/\text{K})$; temp range 282-345 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.51271 - 2016.711/(132.578 + T/\text{K})$; temp range 341–385 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 52.5701 - 2.2537 \times 10^3/(T/\text{K}) - 18.265 \cdot \log (T/\text{K}) + 1.298 \times 10^{-2} \cdot (T/\text{K}) + 2.0286 \times 10^{-13} \cdot (T/\text{K})^2$;
temp range 115–385 K (vapor pressure eq., Yaws 1994)

123390 (248.15 K, selected and summary of literature data, temp range 115.16–249.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

151960 (calculated-P/C, Mackay & Wolkoff 1973; quoted, Roberts & Dändliker 1983)

43080 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

22800 (estimated, Roberts 1984)

28704 (19.93°C, equilibrium cell-GC, measured range 0–40°C, Warner & Weiss 1985)

$\log K_{AW} = 5.811 - 1399/(T/\text{K})$; temp range: 10–30°C (EPICS-GC measurements, Munz & Roberts 1987)

304000 (20–25°C and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)

39557 (computed value, Yaws et al. 1991)

26566 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

26810 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{AW} = 5.739 - 1380/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.16 (shake flask-GC, Hansch et al. 1975)

2.21 (calculated-fragment const., Rekker & de Kort 1979)

2.16 (recommended, Sangster 1993)

2.16 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

2.05 (soil, selected, Jury et al. 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: half-life of about few minutes (Mills et al. 1982); loss half-lives in marine mesocosm were estimated to be 20 d in spring at 8–16°C and $t_{1/2} = 13$ d in winter at 3–7°C (Wakeham et al. 1983).

Photolysis: photolytic dissociation of atmospheric CFCl_3 and CF_2Cl_2 gives chlorine atoms which destroys the ozone layer, these halomethanes may remain at altitudes of 20–40 km for 40–150 yr and will reach saturation values of 10–30 times the present levels (Molina & Rowland 1974).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}^* < 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297.3 K, measured range 297–423.8 K (flash photolysis-RF, Atkinson et al. 1975)

$k_{OH} < 0.4 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{OH} < 0.012 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Cox et al. 1976)

photooxidation $t_{1/2} = 2118\text{--}21180$ h in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k_{OH} < 4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1985)

$k_{OH} < 4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with estimated tropospheric lifetime of > 50 yr for a global average concentration of OH radical (Bunce et al. 1991).

$k_{OH} < 1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on acclimated aerobic screening test data for trichlorofluoromethane (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}16128$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} > 10$ d from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); residence time of about 50 yr in N. troposphere, estimated by one-compartment nonsteady state model (Singh et al. 1978) and

residence time of 60–70 yr by two-compartment nonsteady state model (Singh et al. 1979);

estimated residence time in troposphere about 1 year (Lyman 1982);

$t_{1/2} = 2118\text{--}21180$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);

estimated global average tropospheric lifetime $\tau > 50$ yr for the reaction with hydroxyl radical in air (Bunce et al. 1991).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

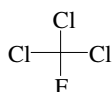
Sediment:

Soil: estimated $t_{1/2} \sim 10000$ d for volatilization loss from soil (Jury et al. 1990);

$t_{1/2} = 672\text{--}4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

5.1.4.6 Trichlorofluoromethane (CFC-11)



Common Name: Trichlorofluoromethane

Synonym: Arcton 11, fluorotrichloromethane, fluorocarbon-11, Freon-11, Frigen 11, R 11, CFC-11

Chemical Name: trichlorofluoromethane, fluorotrichloromethane

CAS Registry No: 75-69-4

Molecular Formula: CFCl_3

Molecular Weight: 137.368

Melting Point ($^{\circ}\text{C}$):

−110.44 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

23.7 (Lide 2003)

Density (g/cm^3 at 20°C):

1.4879, 1.4760 (20°C , 25°C , Riddick et al. 1986)

Molar Volume (cm^3/mol):

93.1 (Stephenson & Malanowski 1987)

97.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

25.02, 25.06 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.895 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

1400 (21°C , Irmann 1965; Chiou & Freed 1977)

1100 (20°C , DuPont 1966; quoted, Riddick et al. 1986)

1100 (20°C , Pearson & McConnell 1975)

1100 (Verschueren 1977, 1983)

1080 (recommended, Horvath 1982)

1080 (30°C , Horvath 1982)

1400 (Dean 1985)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

88550* (19.895°C , measured range -36.673 to 19.895°C , Osborne et al. 1941)

$\log(P/\text{mmHg}) = 18.54101 - 1841.72/(T/\text{K}) - 3.8423 \cdot \log(T/\text{K})$; temp range 236.487–296.822 K (static method-manometry, Osborne et al. 1941)

101325* (23.7°C , summary of literature data, temp range -84.3 to 23.7°C , Stull 1947)

95670 (calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 6424.1/(T/\text{K})] + 7.563786$; temp range -84.3 to 13.1°C (Antoine eq., Weast 1972–73)

88500 (20°C , Pearson & McConnell 1975)

106390 (Antoine eq., Reid et al. 1977)

106349 (20°C , calculated-Antoine eq., Kudchadker et al. 1979)

$\log(P/\text{mmHg}) = 6.89396 - 1074.04/(t/^{\circ}\text{C} + 237.276)$; temp range -37 to 20°C (Antoine eq., Kudchadker et al. 1979)

91580 (20°C , Verschueren 1983)

$\log(P/\text{kPa}) = 6.01333 - 1044.954/(237.102 + t/^{\circ}\text{C})$; temp range -36.67 to 19.89°C (Antoine eq. derived from exptl data of Osborne et al. 1941, Boublik et al. 1984)

107010 (Daubert & Danner 1985)

102200 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.01886 - 1047.04/(237.276 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

106340 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.99210 - 1032.23/(-37.85 + T/\text{K})$; temp range 213–249 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.99652 - 1034.048/(-37.672 + T/\text{K})$; temp range 213–301 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.03083 - 1053.874/(-34.955 + T/\text{K})$; temp range 295–363 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.36472 - 1285.088/(-0.653 + T/\text{K})$; temp range 357–429 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.75501 - 2744.806/(196.225 + T/\text{K})$; temp range 424–486 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 44.0884 - 2.5022 \times 10^3/(T/\text{K}) - 14.193 \cdot \log (T/\text{K}) + 7.8086 \times 10^{-3} \cdot (T/\text{K}) + 1.3769 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 162–471 K (vapor pressure eq., Yaws 1994)

10640 (selected summary of literature data, temp range 162.05–313.15 K, Xiang 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

81200 (20°C , Pearson & McConnell 1975)

11650 (calculated-P/C, Neely 1976)

11050 (20°C , calculated-P/C, Mackay & Shiu 1981)

11044 (20°C , calculated-P/C, Mabey et al. 1982)

11754 (estimated-P/C, Lyman 1985)

$\ln K_{\text{AW}} = 9.25 - 2372/(T/\text{K})$; measured range $5\text{--}33^{\circ}\text{C}$ (distilled water, multiply equilibrium-GC, Hunter-Smith 1983)

$\ln K_{\text{AW}} = 10.50 - 2652/(T/\text{K})$; measured range $5\text{--}33^{\circ}\text{C}$ (seawater, multiply equilibrium-GC, Hunter-Smith 1983)

7925 (19.93°C , equilibrium cell-GC, measured range $0\text{--}40^{\circ}\text{C}$, Warner & Weiss 1985)

9827 (interpolated data of Warner & Weiss 1985; Howard 1990)

5907 (gas stripping-GC, Warner et al. 1987)

10234* (EPICS-GC/FID, measured range $10\text{--}30^{\circ}\text{C}$, Ashworth et al. 1988)

$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 9.480 - 3513/(T/\text{K})$; temp range $10\text{--}30^{\circ}\text{C}$ (EPICS measurements, Ashworth et al. 1988)

11144 ($20\text{--}25^{\circ}\text{C}$ and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

12341 (computed value, Yaws et al. 1991)

8019 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)

7824 (20°C , selected from reported experimental determined values, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 5.023 - 1324/(T/\text{K})$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.53 (shake flask-GC, Hansch et al. 1975; Hansch & Leo 1979)

2.53 (recommended, Sangster 1993)

2.53 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

1.92 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

1.95 (calculated, Klöpffer et al. 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.20 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

2.31, 2.42, 2.16, 2.21 (estimated- K_{OW} , Karickhoff 1985)

2.13, 2.26 (estimated-S, Karickhoff 1985)

2.20 (best estimate, Karickhoff 1985)

2.13 (average from estimates of K_{OW} and S, Karickhoff 1985; quoted, Neely & Blau 1985)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 3.4$ h from Henry's law constant for a river 1.0 m deep with a 3 m/s wind and 1 m/s current (Lyman et al. 1982; Cadena et al. 1984; quoted, Howard 1990);
 $t_{1/2} \sim$ few minutes (Mills et al. 1982).

Photolysis: photolytic dissociation of atmospheric CFCl_3 and CF_2Cl_2 gives chlorine atoms which destroys the ozone layer, these halomethanes may remain at altitudes of 20–40 km for 40–150 yr and will reach saturation values of 10–30 times the present levels (Molina & Rowland 1974).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}^* < 0.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296.8 K, measured range 297–424 K (flash photolysis-resonance fluorescence, Atkinson et al. 1975)

$k_{\text{OH}} < 0.05 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (discharge flow-LMR, Howard & Evenson 1976a)

$k_{\text{OH}} < 0.005 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Cox et al. 1976)

$k_{\text{OH}} < 1.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis: estimated exptl. rate constant $k = 9.5 \times 10^{-7} \text{ d}^{-1}$, based on carbon tetrachloride (Neely 1985).

Biodegradation: aqueous aerobic $t_{1/2} = 4032$ –8640 h, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 16128$ –34560 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} > 10$ d from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976);
 estimated residence time about 1000 yr in troposphere for the reaction with OH radical (CEQ 1975);
 estimated residence time in N. troposphere about 15–20 yr by one-compartment nonsteady state model and
 40–45 yr in troposphere by two-compartment nonsteady state model (Singh et al. 1979);
 estimated residence time in troposphere about 1–6 yr (Lyman 1982);
 $t_{1/2} = 14.7$ –147 yr, based on an measured rate data for the vapor phase reaction with hydroxyl radical in air
 (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 4032$ –8640 h, based on acclimated aerobic screening test data (Tabak et al. 1981; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 8640$ –17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 4320$ –8640 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.4.6.1

Reported vapor pressures and Henry's law constants of trichlorofluoromethane (CFC-11) at various temperatures and the coefficients for the vapor pressure equations

Vapor pressure				Henry's law constant	
Osborne et al. 1941		Stull 1947		Ashworth et al. 1988	
static method		summary of literature data		EPICS-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
-36.673	6313	-84.3	133.3	10	5431
-21.825	14416	-67.6	666.6	15	6890
-6.887	29811	-59.0	1333	20	8147
-2.352	44611	-49.7	2666	25	10234
-10.362	61790	-39.0	5333	30	12362
15.108	74147	-32.3	7999	ln [H/(atm·m ³ /mol)] = A - B/(T/K)	
19.895	88550	-23.0	13332		
23.662	101325	-9.10	26664		
		6.80	53329		
		23.7	101325	A	9.480
				B	3513
		mp/°C	-		

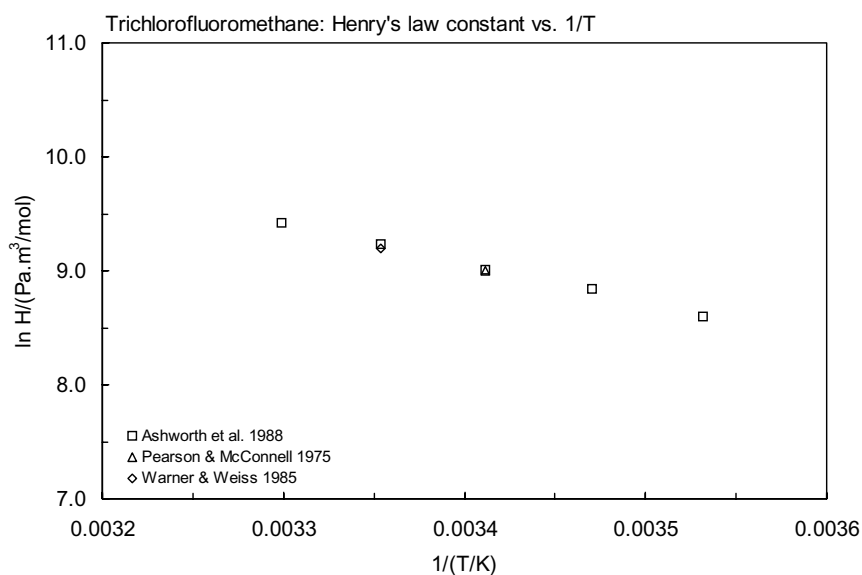
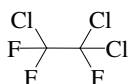


FIGURE 5.1.4.6.1 Logarithm of Henry's law constant versus reciprocal temperature for trichlorofluoromethane.

5.1.4.7 1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)



Common Name: 1,1,2-Trichloro-1,2,2-trifluoroethane

Synonym: CFC-113, Freon 113, 1,2,2-trifluoro-1,1,2-trichloroethane

Chemical Name: 1,1,2-trichloro-1,2,2-trifluoroethane, Arklone

CAS Registry No: 76-13-1

Molecular Formula: $C_2Cl_3F_3$, $CClF_2CCl_2F$

Molecular Weight: 187.375

Melting Point ($^{\circ}C$):

−36.22 (Lide 2003)

Boiling Point ($^{\circ}C$):

47.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5635 ($25^{\circ}C$, Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

119.8 ($20^{\circ}C$, calculated-density)

129.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$. Additional data at other temperatures designated * are compiled at the end of this section):

170 (DuPont 1966; quoted, Riddick et al. 1986)

170 (shake flask-GC, Rauws et al. 1973)

170 ($20^{\circ}C$, Jones et al. 1977/1978)

166.4* (summary of literature data, Horvath 1982)

170 (Dean 1985)

170 (recommended, IUPAC-NIST Solubility Data Series, Horvath & Getzen 1999a)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

53329* ($30.2^{\circ}C$, summary of literature data, temp range -68.0 to $47.4^{\circ}C$, Stull 1947)

48476* (static method-isoteniscope, measured range 273.35 – 318.10 K, Hiraoka & Hildebrand 1963)

39040 (calculated-Antoine eq., Weast 1972–73)

48320 (calculated-Antoine eq., Boublik et al. 1984)

48480 (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.6783 - 1499.2/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/kPa) = 5.91657 - 1094.37/(-39.61 + T/K)$; temp range 273 – 319 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.01641 - 1115.812/(-42.515 + T/K)$; temp range 238 – 364 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.53093 - 1500.489/(12.469 + T/K)$; temp range 360 – 473 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.95163 - 1082.588/(-46.427 + T/K)$; temp range 297 – 317 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/mmHg) = 33.7911 - 2.5323 \times 10^3/(T/K) - 9.3175 \cdot \log (T/K) + 1.455 \times 10^{-8} \cdot (T/K) + 2.914 \times 10^{-6} \cdot (T/K)^2$; temp range 238 – 481 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 32320* (EPICS-GC/FID, measured range $10\text{--}30^\circ\text{C}$, Ashworth et al. 1988)
 $\ln [H/(\text{atm m}^3/\text{mol})] = 9.649 - 3243/(T/K)$; temp range $10\text{--}30^\circ\text{C}$ (EPICS measurements, Ashworth et al. 1988)
 53300 (calculated-P/C, Howard 1990)
 49132 (computed value, Yaws et al. 1991)
 24616 (20°C , selected from reported experimental determined values, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 5.375 - 1281/(T/K)$ (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.16 (HPLC- k' correlation, McDuffie 1981; quoted, Howard 1990, Sangster 1993))
 3.16 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.531, 1.041 (calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.28, 2.41 (soil, calculated- K_{OW} , calculated-S, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 4$ h was estimated for a model river 1 m deep flowing 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: both aqueous and atmospheric photolysis half-lives are infinite (Howard et al. 1991).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} < 0.3 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-laser magnetic resonance, Howard & Enenson 1976b)

photooxidation $t_{1/2} = 40\text{--}1000$ yr in troposphere, based on measured rates with singlet oxygen (Davidson et al. 1978; Pitts Jr. et al. 1974; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 4320\text{--}8640$ h, based on a relative resistance of completely halogenated aliphatics to biodegrade; aqueous anaerobic $t_{1/2} = 17280\text{--}34560$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

degradation rates in microcosms at 20°C : $k = 7.6 \times 10^{-3} \text{ d}^{-1}$ by control buffer with $t_{1/2} = 90$ d, $k = 9.1 \times 10^{-3} \text{ d}^{-1}$ by redox buffer with $t_{1/2} = 75$ d, $k = 1.2 \times 10^{-2} \text{ d}^{-1}$ by 1 mg/L redox-hematin with $t_{1/2} = 57$ d, $k = 1.6 \times 10^{-2} \text{ d}^{-1}$ by 2 mg/L redox-hematin with $t_{1/2} = 43$ d, $k = 9.9 \times 10^{-2} \text{ d}^{-1}$ by purged leachate with $t_{1/2} = 7$ d, and $k = 0.14 \text{ d}^{-1}$ by leachate with $t_{1/2} = 5$ d (Lesage et al. 1992).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} > 10$ d from air for the reaction with OH radicals (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 40\text{--}1000$ yr in troposphere, based on measured rates with singlet oxygen (Davidson et al. 1978; Pitts Jr. et al. 1974; quoted, Howard et al. 1991);

$t_{1/2} = 20$ yr in troposphere (Dilling 1982; quoted, Howard 1990).

Surface water: $t_{1/2} = 4320\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1440\text{--}17280$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 4320\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 5.1.4.7.1
Reported aqueous solubilities, vapor pressures and Henry’s law constants of 1,1,2-trichloro-1,2,2-trifluoroethane (CFC-113) at various temperatures

$$S/(\text{wt}\%) = 1.0648 \times 10^{-2} + 3.51135 \times 10^{-4} \cdot (t/^{\circ}\text{C}) - 6.1331 \times 10^{-6} \cdot (t/^{\circ}\text{C})^2 + 6.70235 \times 10^{-8} \cdot (t/^{\circ}\text{C})^3$$
(1)

$$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/\text{K})$$
(2)

Aqueous solubility		Vapor pressure				Henry's law constant	
Horvath 1982		Stull 1947		Hiraoka & Hildebrand 1963		Ashworth et al. 1988	
summary of literature data		summary of literature data		static method isoteniscope		EPICS-GC	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
0	106.5	−68.0	133.3	0.20	17252	10	15604
10	136.1	−49.4	666.6	5.0	21278	15	21785
20	157.5	−40.3	1333	10.3	26731	20	24825
25	166.4	−30.0	2666	10.45	26891	25	32323
30	174.7	−18.5	5333	15.1	32597	30	32525
40	191.7	−11.2	7999	20.0	39970		
50	212.5	−1.70	13332	25.05	48476	eq. 2	H/(atm m ³ /mol)
60	241.1	13.5	26664	30.1	58528	A	9.649
70	281.6	30.2	53329	35.1	69887	B	3243
80	338.0	47.4	101325	40.1	82286		
				44.95	96898		
eq.1	S/wt%	mp/°C	−35				

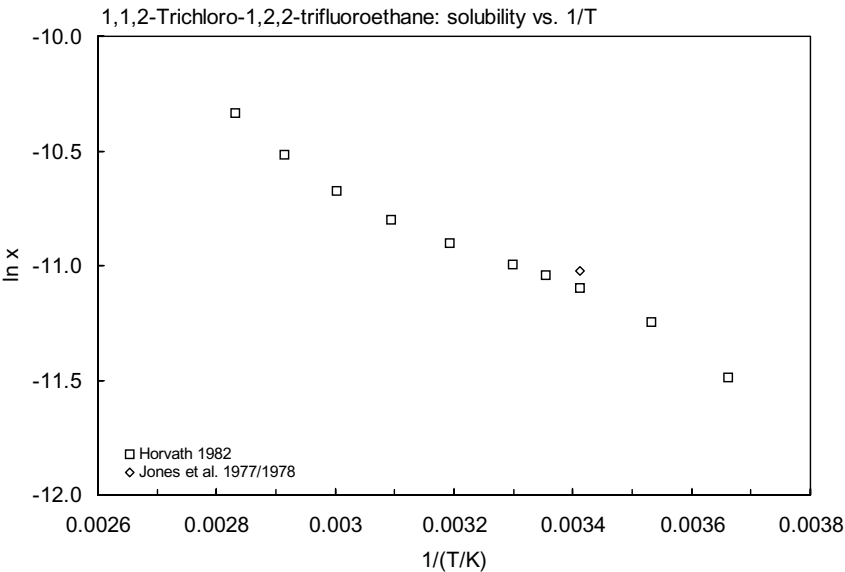


FIGURE 5.1.4.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

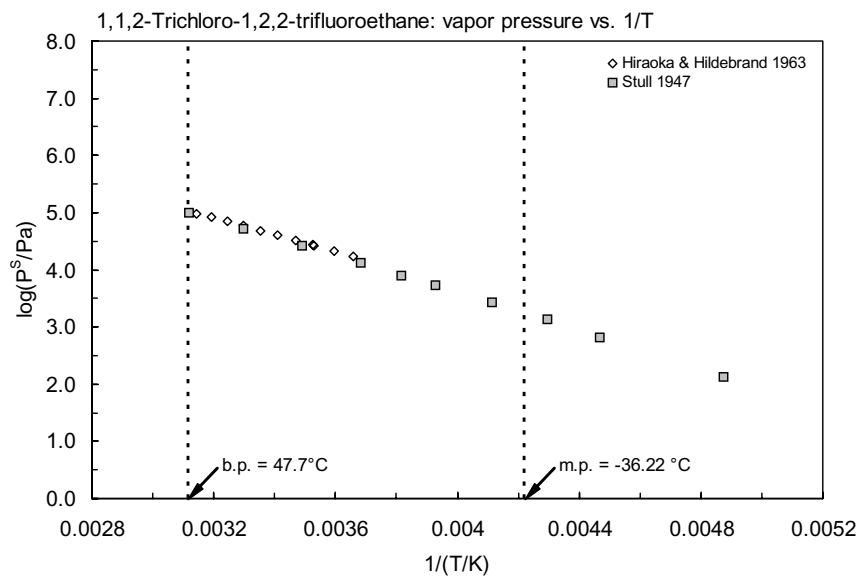


FIGURE 5.1.4.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

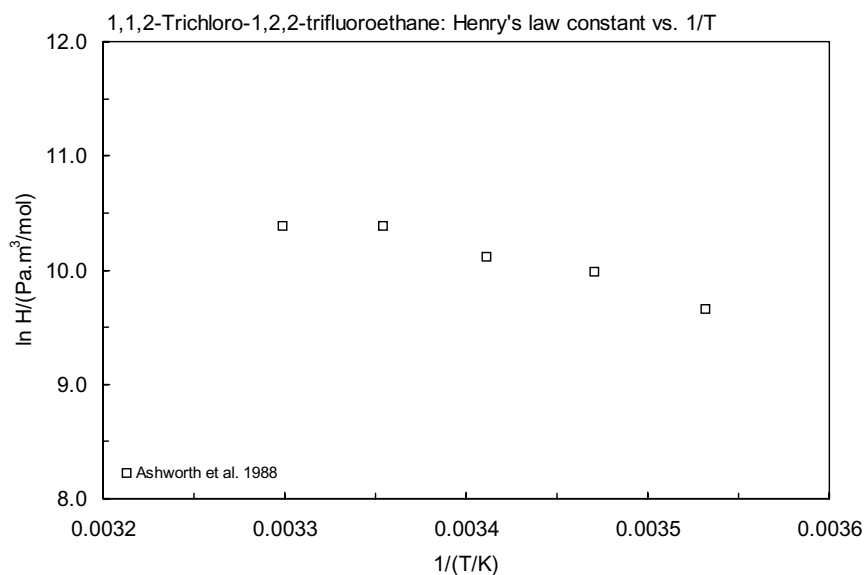
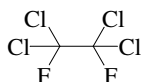


FIGURE 5.1.4.7.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,1,2-trichloro-1,2,2-trifluoroethane.

5.1.4.8 1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112)



Common Name: 1,1,2,2-Tetrachloro-1,2-difluoroethane

Synonym: Freon-112, CFC-112

Chemical Name: 1,2-difluorotetrachloroethane

CAS Registry No: 76-12-0

Molecular Formula: $C_2F_2Cl_4$, Cl_2FCCl_2

Molecular Weight: 203.830

Melting Point ($^{\circ}C$):

26.55 (Riddick et al. 1986)

24.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

92.80 (Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.6447 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

145.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of vaporization, ΔH_v (kJ/mol):

35 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

3.666 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

120 (DuPont 1966; quoted, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

6106 ($20^{\circ}C$, measured range 10 – $91.5^{\circ}C$, Hovorka & Geiger 1933)

7609 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 9.94341 - 4259.092/(444.991 + t/^{\circ}C)$, temp range 10 – $91.5^{\circ}C$ (Antoine eq. derived from exptl. data of Hovorka & Geiger 1933, Boublik et al. 1984)

8770 (selected, Riddick et al. 1986)

$\log(P/kPa) = 7.2972 - 1929.27/(T/K)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_s/kPa) = 6.50788 - 1526.24/(-28.93 + T/K)$; temp range 235 – 293 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.67780 - 1567.8/(-29.58 + T/K)$; temp range 301 – 365 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.97313 - 1239.993/(-53.468 + T/K)$; temp range 312 – 362 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -38.1282 - 1.2604 \times 10^3/(T/K) + 23.347 \cdot \log(T/K) - 3.4436 \times 10^{-2} \cdot (T/K) + 1.7407 \times 10^{-5} \cdot (T/K)^2$; temp range 299 – 551 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

9869 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

248, 1426 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

161419 (computed value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.82 (shake flask, Log P Database, Hansch & Leo 1987)

3.73 (Howard 1990)

2.82 (recommended, Sangster 1993)

Bioconcentration Factor, log BCF:

1.62 (estimated-S, Lyman et al. 1982)

Sorption Partition Coefficient, log K_{oc} :

2.50 (soil, estimated-linear regression with S, Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} \sim 4.0$ h from a model river 1 m deep flowing 1 m/s with a wind velocity of 3 m/s, based on estimated Henry's law constant (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Photolysis: will not undergo direct photolysis in the troposphere (quoted, Howard 1990).

Oxidation: inert to react with photochemically produced radicals and ozone molecules (Dilling 1982; Atkinson 1985,1987; quoted, Howard 1990).

Hydrolysis: not an environmentally significant fate process (DuPont 1980; quoted, Howard 1990).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: by analogy to other Freon compounds, Freon-112 is predicted to have a stratospheric lifetime on the order of several decades (Chou et al. 1978; quoted, Howard 1990).

Surface water: will volatilize very rapidly (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Ground water: will volatilize very rapidly (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Sediment: will volatilize very rapidly from soil surfaces (estimated-P/C, Lyman et al. 1982; quoted, Howard 1990).

Soil:

Biota:

5.1.5 FLUOROALKANES AND FLUOROALKENES

A large number of stable and volatile fluorinated and chlorinated alkanes and alkenes have been synthesized and used, primarily as refrigerants. These “freons” have been implicated as the cause of observed reductions in stratospheric ozone levels, thus permitting greater penetration of ultraviolet radiation to the Earth’s surface. Their high vapor pressures and relatively low solubilities in water result in high Henry’s law constants or air-water partition coefficients. Fate calculations show that when released into the environment virtually the total mass of these substances will partition to the atmospheric compartment. Levels in water, soil, sediments and biota are likely to be very low and of little concern. Accordingly, there is little merit in compiling detailed data on these substances in a format comparable to that, for example, the chlorobenzenes or PCBs.

In the interest of conserving space in this handbook, a compact tabular presentation format has been adopted. [Table 5.1.5.1](#) lists the chemical name, and its freon number (if applicable), molecular formula, molar weight and melting and boiling points. These data are available for virtually all substances in this group. Also shown in this table is the availability, expressed as a tick mark, of data on vapor pressure, solubility in water, octanol-water partition coefficient (K_{OW}) and the second order reaction rate constant with hydroxyl radicals. This rate constant is the critical determinant of persistence in the atmosphere. [Tables 5.1.5.2](#) to [Table 5.1.5.5](#) list the compounds and give the available property data with citations.

TABLE 5.1.5.1
Summary of physical constants for fluoroalkanes and fluoroalkenes

Compound	Freon no.	CAS no.	Molecular formula	Molecular weight g/mol	mp°C	bp°C	LeBas molar volume, V _M cm ³ /mol	Properties**			
								S	P	K _{OW}	k _{OH}
Fluoroalkanes											
Fluoromethane	HFC-41	593-53-3	CH ₃ F	34.05	−141.8	−79.1	34.6	✓	✓	✓	✓
Difluoromethane	HFC-32	75-10-5	CH ₂ F ₂	52.02	−136	−51.6	39.6	✓	✓	✓	✓
Trifluoromethane	HFC-23	75-46-7	CHF ₃	70.01	−155.2	−82.16	44.6	✓	✓	✓	✓
Tetrafluoromethane	FC-14	75-73-0	CF ₄	88.005	−183.60	−128.0	49.6	✓	✓	✓	✓
Chlorofluoromethane	HCFC-31	593-70-4	CH ₂ ClF	68.48	−133	−9.1	55.5	✓	✓		✓
Dichlorofluoromethane	HCFC-21	75-43-4	CHCl ₂ F	102.92	−135	8.92	76.4	✓	✓	✓	✓
Chlorodifluoromethane	HCFC-22*	75-45-6	CHClF ₂	86.47	−160	−40.7	60.5	✓	✓	✓	✓
Chlorotrifluoromethane	CFC-13	75-72-9	CF ₃ Cl	104.46	−181	−82	65.5	✓	✓	✓	✓
Dichlorodifluoromethane	CFC-12*	75-71-8	CCl ₂ F ₂	120.91	−155	−29.8	81.4	✓	✓	✓	✓
Trichlorofluoromethane	CFC-11*	75-69-4	CFCl ₃	137.37	−111	23.82	97.3	✓	✓	✓	✓
Fluoroethane	HFC-161	353-36-6	CH ₃ CH ₂ F	48.06	−143	−37.7	56.8	✓	✓		✓
1,1-Difluoroethane	HFC-152a	75-37-6	CH ₃ CHF ₂	66.05	−117	−24.7	61.8	✓	✓	✓	✓
1,2-Difluoroethane	HFC-152	624-72-6	CH ₂ FCH ₂ F	66.05		26	61.8	✓			✓
1,1,1-Trifluoroethane	HFC-143a	420-46-2	CF ₃ CH ₃	84.04	−111.3	−47.4	66.8	✓	✓		✓
1,1,2-Trifluoroethane	HFC-143b	430-66-0	CH ₂ FCHF ₂	84.04	−84	3.7	66.8	✓			✓
1,1,2,2-Tetrafluoroethane	HFC-134	359-35-3	CHF ₂ CHF ₂	102.03	−89	−19.9	71.8	✓	✓		✓
1,1,1,2-Tetrafluoroethane	HFC-134a	811-97-2	CH ₂ FCF ₃	102.03	−103.3	−26.08	71.8	✓	✓	✓	✓
Pentafluoroethane	HFC-125	354-33-6	CF ₃ CHF ₂	120.02	−103	−48.5	76.8	✓	✓		✓
Hexafluoroethane	FC-116	76-16-4	CF ₃ CF ₃	138.01	−100.6	−79	81.8	✓	✓	✓	
1-Chloro-2-fluoroethane	HCFC-151	762-50-5	CH ₂ FCH ₂ Cl	82.5	<−50	52.8	77.7	✓			
1-Chloro-1,1-difluoroethane	HCFC 142b	75-68-3	CH ₃ CClF ₂	100.5	−130.8	−9.5	82.7	✓	✓	✓	✓
1-Chloro-1,1,2-trifluoroethane	HCFC-133a	421-04-5	CH ₂ ClCF ₃	118.49		12	87.7				✓
1-Chloro-1,2,2,2-tetrafluoroethane	HCFC-124	2837-89-0	CHClF ₂ CF ₃	136.5		−11.0	92.7	✓	✓	✓	✓
1-Chloropentafluoroethane	CFC-115	76-15-3	CClF ₂ CF ₃	154.47	−99.4	−39.1	97.7	✓	✓	✓	
1,1-Dichloro-1-fluoroethane	HCFC-141b	1717-00-6	CCl ₂ FCH ₃	116.95	−103.5	32.0	98.6	✓	✓	✓	✓
1,2-Dichloro-1,1-difluoroethane	HCFC-132b	1649-08-7	CClF ₂ CH ₂ Cl	134.97	−101.2	46.8	103.6				✓
1,1-Dichlorotrifluoroethane	HCFC-123	306-83-2	CHCl ₂ CF ₃	152.93	−107	27.6	108.6	✓	✓		✓
1,2-Dichloro-1,1,2,2-tetrafluoroethane	CFC-114	76-14-2	CClF ₂ CClF ₂	170.92	−93.9	3.8	113.6	✓	✓	✓	
1,1-Dichloro-1,2,2,2-tetrafluoroethane	CFC-114a	374-07-2	CCl ₂ FCF ₃	170.92	−56.6	3.4	113.6	✓		✓	
1,1,1-Trichloro-2,2,2-trifluoroethane	CFC-113a	354-58-5	CCl ₃ CF ₃	187.38	14.2	47.57	129.5		✓		
1,1,2-Trichloro-1,2,2-trifluoroethane	CFC-113*	76-13-1	CCl ₂ FCClF ₂	187.38	−36.4	47.7	129.5	✓	✓	✓	

1,1-Difluorotetrachloroethane			CClF ₂ CCl ₃	203.83	38	91	145.4			✓	
1,1,2,2-tetrachloro-1,2-difluoroethane	CFC-112*	76-12-0	CCl ₂ FCCL ₂ F	203.83	25	93	145.4	✓	✓	✓	
2-Fluoropropane	HFC-281ea	420-26-8	CH ₃ CHFCH ₃	62.09	-133.4	-10	79.0	✓	✓		
1,1,2,2,3-Pentafluoropropane	HFC-245ca	679-86-7	CH ₂ FCF ₂ CHF ₂	134.05			99.0		✓		✓
1,1,1,3,3-Pentafluoropropane	HFC-245fa	460-73-1	CF ₃ CH ₂ CHF ₂	134.05			99.0		✓		
1,1,1,2,2-Pentafluoropropane	HFC-245cb	1814-88-6	C ₃ H ₃ F ₅	134.05		-17.4	99.0		✓		✓
1,1,1,2,3,3-Hexafluoropropane	HFC-236ea	431-63-0	CHF ₂ CHFCF ₃	152.04		6.1	104.0		✓		✓
1,1,1,3,3,3-Hexafluoropropane	HFC-236fa	690-39-1	CF ₃ CH ₂ CF ₃	152.04	-93.6	-1.0	104.0		✓		✓
1,1,1,2,3,3,3-Heptafluoropropane	HFC-227ea	431-89-0	CF ₃ CHFCF ₃	170.03	-131	-16.4	109.0		✓		✓
Octafluoropropane	FC-218	76-19-7	CF ₃ CF ₂ CF ₃	188.02	-183	-38	114.0	✓	✓		
Trichlorotrifluoropropane									✓		
1-Chloro-2,2,2-trifluoropropane			CH ₂ ClCH ₂ CF ₃	132.51	-106.2	45.1	109.9	✓	✓		
Perfluorobutane	FC-3110	355-25-9	C ₄ F ₁₀	238.03	-129.1	-1.9	146.2		✓		
Perfluorocyclobutane	FC-118	115-25-3	C ₄ F ₈	200.03	-40.19	-5.9	120.3	✓	✓		
Perfluoropentane	FC-87	678-26-2	C ₅ F ₁₂	288	-10	29.2	178.4		✓		
Perfluorocyclopentane		376-77-2							✓		
Perfluoro-2-methylcyclopentane									✓		
Perfluoro-3-methylcyclopentane									✓		
Perfluorocyclohexane		355-68-0	C ₆ F ₁₂	300.05	48	52	178.2		✓		
Perfluorohexane	FC-72	355-42-0	C ₆ F ₁₄	338.04	-88.2	56.6	210.6		✓		
Fluoroalkenes											
Fluoroethene	HFC-1141	75-02-5	CHF=CH ₂	46.05	-160	-72.2	49.4	✓			
1,1-Difluoroethene	HFC-1132a	75-38-7	CF ₂ =CH ₂	64.04	-144	-82	54.4	✓			✓
Tetrafluoroethene	FC-1114	116-14-3	CF ₂ =CF ₂	100.02	-131.15	-75.9	64.4	✓	✓		
Chlorotrifluoroethene	CFC-1113	79-38-9	CClF=CF ₂	116.47	-158.2	-26.2	80.3		✓		
1,2-Dichloro-1,2-difluoroethene	CFC-1112	311-81-9	CClF=CClF	132.92	-119.6	21.1	96.2		✓		
1,1-Dichloro-2,2-difluoroethene	CFC-1112a	79-35-6	CCl ₂ =CF ₂	132.925	-115	19	96.2		✓		
3-Fluoropropene		818-92-8	CH ₂ FCH=CH ₂	60.07		-3.0	71.6	✓			
Hexafluoropropene	FC-1216	116-15-4	C ₃ F ₆	150.002	-156.5	-29.6		✓	✓		

* See [Section 5.1.4. Mixed halogenated hydrocarbons](#).

** S = water solubility; P = vapor pressure; K_{OW} = octanol-water partition coefficient; k_{OH} = second order reaction rate constant with hydroxyl radicals.

TABLE 5.1.5.2
Aqueous solubilities for fluoroalkanes and fluoroalkenes

Compound	Temp.°C	Solubility	Unit	Range, wt %	Mole fraction x	Temp./pressure range	Reference
Fluoroalkanes							
Fluoromethane	25	0.2001	wt %	0.4227–0.08005	0.001061	0–80°C, 1 atm partial pressure	1
	25	2390	ppm (wt)				2
Difluoromethane	25	4390	ppm (wt)				2
Trifluoromethane	25 at 1 atm	0.09	g/100 mL	0.09–0.02		25–75°C, pressure 1–20.41 atm	1
	25	0.4087	wt %		0.001056	1 atm partial pressure	1
	25	900	ppm (wt)				2
Tetrafluoromethane	25	0.0733	g/100 mL			from Hine & Mookerjee (1975)	3
	25	0.001877	wt %	0.003892–0.001300	3.84×10 ⁻⁶	0–50°C, 1 atm partial pressure	1
	25 at 1 atm	0.00160	g/100 mL	0.00160–0.0005		25–75°C, 1–10.2 atm	1
	25	16.0	ppm (wt)				2
Chlorofluoromethane	25	0.4592	10 ³ L _{2,1} , Ostwald coefficient			288–303 K, 1atm partial pressure	4
	25	1.0522	wt %	1.6840–0.3285	0.002790	10–50°C, 1 atm partial pressure	1
	25	10500	ppm (wt)			1 atm partial pressure	2
Dichlorofluoromethane	25 at 1 atm	1.880	g/100 mL	1.88–0.418		25–75°C, 0.068–3.40 atm	1
	25	0.95	wt %			DuPont	5
	25	18800	ppm (wt)				2
Chlorodifluoromethane	25	0.2899	wt %	0.5296–0.09728	6.055×10 ⁻⁴	10–50°C, 1 atm partial pressure	1
	25 at 1 atm	0.277	g/100 mL	0.792–0.089		5–76.7°C, 1–33.34 atm	1
	25	0.30	wt %				5
	25	27.7	ppm (wt)				2
Chlorotrifluoromethane	25 at 1 atm	0.2899	g/100 mL			from Horvath (1982)	3
	25 at 1 atm	0.009	g/100 mL	0.009–0.004		25–75°C, 1–23.81 atm	1
	25	0.009	wt %				5
	25	90	ppm (wt)				
Dichlorodifluoromethane	25	2.253	10 ³ L _{2,1} , Ostwald coefficient			288–303 K, 1 atm partial pressure	4
	25 at 1 atm	0.030	g/100 mL	0.030–0.008		25–76.7°C, 1–6.80 atm	1
	25	0.028	wt %				5
	25 at 1 atm	0.028	g/100 mL			quoted Riddick (1986)	6
	25	300	ppm (wt)				2
Trichlorofluoromethane	25	7.110	10 ³ L _{2,1} , Ostwald coefficient			288–303 K, 1 atm partial pressure	4
	30 at 1 atm	0.1080	g/100 mL	0.108–0.031		30–75°C, 1–3.4 atm	1
	25	0.11	wt %			DuPont	5
	25	1080	ppm (wt)				1

	25	0.108	g/100 mL			from Horvath (1982)	9
Fluoroethane	25	0.2158	wt %	0.4022–0.2158	8.10×10^{-4}	14–25°C, 1 atm partial pressure	1
	25	2160	ppm (wt)			1 atm partial pressure	
1,1-Difluoroethane	21	0.32	wt %	0.54–0.25	8.748×10^{-4}	0–27.5°C, 1 atm partial pressure	1
	25	2500	ppm (wt)			1 atm partial pressure	2
	25 at 1 atm	0.280	g/100 mL			from Horvath (1982)	3
1,2-Difluoroethane	25	0.0157	wt %	0.012–0.02660	1.342×10^{-5}	25–80°C, saturation pressure	1
1,1,2-Trifluoroethane	25	0.01664	wt %	0.01065–0.03380	1.60×10^{-5}	0–80°C, saturated pressure	1
	30	0.011	g/100 mL	0.011–0.026		30–75°C, 0.34–2.04 atm	1
1,1,1,2-Tetrafluoroethane	37	0.0550	wt %		9.71×10^{-5}	37°C, 1 atm partial pressure	1
1,1,2,2-Tetrafluoroethane	25	0.2962	wt %	0.3299–0.4199	3.187×10^{-4}	1 atm	1
Pentafluoroethane	25	0.04995	wt %	0.05411–0.07783	4.45×10^{-5}	0–80°C, saturated pressure	1
	25	58.0	ppm (wt)				2
	25	0.0039	g/100 mL			estimated from K_{OW}	6
Hexafluoroethane	22.3	0.0050	wt %		3.805×10^{-6}	22.3°C, 0.0050 atm	1
	25	7.90	ppm (wt)				2
	25.314				9.975×10^{-7}	287–328 K, 96.6–120.5 kPa	7
1-Chloro-2-fluoroethane	25	2.4390	wt %		0.005429	saturated pressure	1
1-Chloro-1,1-difluoro-	21 at 1 atm	0.140	wt %	0.214–0.140	2.512×10^{-4}	13–21°C, 1 atm partial pressure	1
1-Chloro-1,2,2,2-tetrafluoro-	25	0.0404	g/100 mL			estimated from K_{OW}	6
1-Chloropentafluoro-	25 at 1 atm	0.0058	g/100 mL	0.0058–0.0013		25–75°C, 1–6.80 atm	1
	25	0.006	wt %				5
1,1-Dichloro-1-fluoro	25	0.066	wt %				
1,1-Dichlorotrifluoroethane	25	0.0046	wt %				8
	25	0.01857	g/100 mL			estimated from K_{OW}	6
1,2-Dichloro-1,1,2,2-tetra-	25	0.0120	wt %	0.0120–0.02662	1.061×10^{-5}	25–80°C, saturated pressure	1
	25	0.1792	wt %	0.1792–0.03487	1.586×10^{-6}	25–80°C, 1 atm partial pressure	1
	30 at 1 atm	0.009	g/100 mL	0.009–0.020		30–75°C, 0.068–0.612 atm	1
	25	0.013	wt %				5
	25	137	ppm (wt)				2
	25	0.013	g/100 mL			from Riddick (1986)	9
1,1-Dichloro-1,2,2,2-tetra-	25	0.1100	wt %	0.1197–0.1848	11.82×10^{-6}	0–80°C, saturation pressure	1
	21	0.0060	g/100 mL			from Horvath (1982)	3
1,1,2-Trichloro-1,2,2-tri-	25	0.01664	wt %	0.01065–0.003380	1.60×10^{-5}	0–80°C, saturated pressure	8
	30 at 0.34 atm	0.011	g/100 mL			30–75°C, 0.34–2.04 atm	1
	25	0.017	wt %				5
	25	170	ppm (wt)				2
	25	0.017	g/100 mL			from Riddick (1986)	9

(Continued)

TABLE 5.1.5.2 (Continued)

Compound	Temp.°C	Solubility	Unit	Range, wt %	Mole fraction x	Temp./pressure range	Reference
1,2-Difluorotetrachloro-	25	0.012	wt %				5
	25	0.012	g/100 mL			from Riddick (1986)	9
2-Fluoropropane	15	0.3663	wt %		0.001066	1 atm partial pressure	1
	15	3660	ppm (wt)			1 atm partial pressure	2
Octafluoropropane	15	0.001495	wt %		1.432×10^{-6}	15°C, saturated pressure	1
Perfluorocyclobutane	21	0.014	wt %		1.259×10^{-5}	21°C, 1 atm partial pressure	1
	26 at 1 atm	0.005	g/100 mL			0–37.8°C, 1–2.72 atm	1
	26	50.0	ppm (wt)				2
Fluoroalkenes							
1-Fluoroethene	80 at 34 atm	0.9312	wt %		0.003664	34 atm	1
	80 at 68 atm	1.5166	wt %		0.005988	68 atm	1
1,1-Difluoroethene	25	0.01649	wt %		4.638×10^{-5}	1 atm partial pressure	1
	25	165	ppm (wt)			1 atm partial pressure	2
Tetrafluoroethene	25	0.01585	wt %	0.04062–0.008782	2.856×10^{-5}	0–70°C, 1 atm partial pressure	1
	23 at 4.4 atm	0.001	wt %	0.001–1.274	1.78×10^{-6}	23°C, total pressure 4.4–13.45 atm	1
	25	158	ppm (wt)				2
3-Fluoropropene	13	0.007167	wt %		2.149×10^{-5}	1 atm partial pressure	1
Hexafluoropropene	25	0.01691	wt %	0.04164–0.007132	2.327×10^{-5}	0–70°C, 1 atm partial pressure	1

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TABLE 5.1.5.3
Vapor pressures for fluoroalkanes and fluoroalkenes

Compound	Temp. °C or K	P° kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
Fluoroalkanes						
Fluoromethane				−103 – −76°C	20–116	Moles and Batuecas 1919 [#]
			static	−133.1 – −78.5°C	1.33–101	Grosse et al. 1940
			literature summary	−147.3 – −78.2°C	0.1333–101.325	Stull 1947
	15.28°C	3045.3	manometer	−109–15°C	13–3045	Michels and Wassenaar 1948
Difluoromethane	298.15 K	3824.9	literature summary	131–317 K	0.43–5880	Xiang 2002
	298.16 K	1689	static	191–352 K	16.36–5828	Malbrunot et al. 1968
			comparative ebulliometry	208–237 K	49–214	Weber and Goodwin 1993
	298.174 K	1690.81	Burnett	268–348 K	690–5409	Defibaugh et al. 1994
			apparatus/densimeter			
			isochoric	320–351 K	2919–5783.6	Sato et al. 1994
			ebulliometry (metal)	236–266 K	200–650	Weber and Silva 1994
	299.985 K	1774	manometer/densimeter	220–325 K	95–3278	Widiatmo et al. 1994
	297.15 K	1645.1	Burnett apparatus	233–351 K	177–5767.9	Fu et al. 1995
	298.15 K	1689.7	literature summary	137–351 K	5.69×10 ^{−2} – 5780	Xiang 2002
Trifluoromethane	308.15 K	2191	VLE			Horstmann et al. 2004
			calorimetry static	145–192 K	2.72–102.51	Valentine et al. 1962
Tetrafluoromethane	298.15 K	4714.9	literature summary	118–299 K	5.71×10 ^{−2} – 4800	Xiang 2002
			literature summary	−184.6 – −127.7°C	0.1333–101.325	Stull 1947
			calorimetry static	115–146 K	7–106	Smith and Pace 1969
						Bonifácio et al. 2001
Chlorofluoromethane			literature summary	90–228 K	1.04×10 ^{−1} –3740	Xiang 2002
	298.15 K	343.82	literature summary	138–427 K	2.28×10 ^{−3} –5700	Xiang 2002
Dichlorofluoromethane			isoteniscopic	−29.65–174.6°C	17.31–4894	Benning and McHarness 1940
			literature summary	−91.3–8.90°C	0.1333–101.325	Stull 1947
	298.15 K	181.67	literature summary	138–452 K	2.94×10 ^{−4} – 5183	Xiang 2002
Chlorodifluoromethane	22.6°C	951	manometer	22.6–96.4°C	951–4912	Booth and Swinehart 1935
	25.15°C	1050.74	isoteniscopic	−61.26–92.6°C	35.12–4652.84	Benning and McHarness 1940
			literature summary	−122.8 – −40.8°C	0.1333–101.325	Stull 1947
	50°C	1955	VLE			Leu and Robinson 1992
	65°C	2710	VLE			Leu and Robinson 1992
	70°C	3003	VLE			Leu and Robinson 1992
	75°C	3843	VLE			Leu and Robinson 1992

(Continued)

TABLE 5.1.5.3 (Continued)

Compound	Temp. °C or K	P° kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
Chlorotrifluoromethane	289.10 K	811.7	isochoric	245–328 K	180–2195	Giuliani et al. 1995a
	298.15 K	1044.2	literature summary	115–369 K	4.26×10 ⁻⁴ –4988	Xiang 2002
			literature summary	–149.5 – –81.2°C	0.1333–101.325	Stull 1947
Dichlorodifluoromethane	298.15 K	3578.3	literature summary	92–302 K	4.40×10 ⁻⁴ –3890	Xiang 2002
			literature summary	–118.5 – –29.8°C	0.1333–101.325	Stull 1947
Trichlorofluoromethane	25.338°C	656		25–111°C	656–4062	Michels et al. 1966
	298.15 K	650.91	literature summary	115–385 K	2.33×10 ⁻⁴ –4100	Xiang 2002
	24.02°C	102.24	isoteniscopic	–29.65–195.65°C	1.05–4273.89	Benning and McHarness 1940
	293.055 K	88.55	calorimetry static	236–293 K	6.31–88.55	Osborne et al. 1941
	23.7°C	101.325	literature summary	–84.3–23.7°C	0.1333–101.325	Stull 1947
Fluoroethane	298.15 K	106.4	literature summary	162–471 K	6.26×10 ⁻³ –4408	Xiang 2002
	25.65°C	932	manometer	25.65–102.16°C	932–5028	Booth and Swinehart 1935
			static	–103.6 – –37.1°C	1.33–101	Grosse et al. 1940
	295.82 K	865.9	static	228–322 K	70–1699	Vidaauri 1975
1,1-Difluoroethane	20°C	833.3		16–78°C	738–3197	Beyerlein et al. 1998
	290.76 K	22	mercury manometer	234–291 K	0.858–22	Li and Pitzer 1956
	298.15 K	596	isochoric	239–368 K	59–3334	Zhao et al. 1992
			ebulliometry	220–273 K	23–264	Silva and Weber 1993
1,1,1-Trifluoroethane	295.452 K	550.01	ebulliometry	281–335 K	352–1550	Defibaugh and Morrison 1996
	298.15 K	597	strain gauge	243–333 K	73–1499	Takagi et al. 2004
			mercury manometer	174–226 K	3.49–101.01	Russell et al. 1944
	299.995 K	1331	manometer/densimeter	278–340 K	769–3337	Widiatmo et al. 1994
	298.22 K	1265.1	isochoric	244–345 K	226–3717	Giuliani et al. 1995b
	300 K	1327.0	Burnett apparatus	295–342 K	1164–3474	Zhang et al. 1995a
	279.484 K	751.294	ebulliometry	236–279 K	160–751	Weber and Defibaugh 1996b
	298.165 K	1262.0	PVT apparatus	279–343 K	744–3556	Weber and Defibaugh 1996b
	293.149 K	1104.8		263–346 K	447–3763	Fujiwara et al. 1998
	283.11 K	834.8	VLE			Bobbo et al. 2000b
1,1,2,2-Tetrafluoroethane	298.16 K	1260.7	VLE			Bobbo et al. 2000b
	313.21 K	1832.5	VLE			Bobbo et al. 2000b
	300 K	1325.3	isochoric	300–345 K	1325–3748	Widiatmo et al. 2001
	298.16 K	1262.62	Burnett apparatus	251–343 K	292–3554	Duan et al. 2004
	299.994 K	546		200–390 K	15–4465	Maezawa et al. 1991b
	299.976 K	699		280–350 K	38–2459	Maezawa et al. 1990

	297.15 K	645.53		279–363 K	363–3236	Zhu et al. 1992
	298.21 K	666.7	isochoric	250–347 K	116–2316	Giuliani et al. 1995a
	298.13 K	666	acoustic interferometer	243–333 K	83–1673	Takagi 1996a
	293.66 K	580	VLE			Bobbo et al. 1998
	303.68 K	780.9	VLE			Bobbo et al. 1998
	283.62 K	420.7	VLE			Bobbo et al. 1998
	293.14 K	571.5		263–373 K	200–3973	Fujiwara et al. 1998
	293.15 K	571.3	VLE			Bobbo et al. 2001
	303.15 K	769.4	VLE			Bobbo et al. 2001
	313.15 K	1014.6	VLE			Bobbo et al. 2001
Pentafluoroethane			isochoric	195–339 K	20–100 bars	Wilson et al. 1992
			ebulliometry (glass)	219–247 K	74–262	Weber and Silva 1994
	284.714 K	951.5741	ebulliometry (metal)	240–285 K	200–952	Weber and Silva 1994
	299.985 K	1444	manometer/densimeter	220–335 K	79–3303	Widiatmo et al. 1994
	300 K	1446.6	Burnett apparatus	290–339 K	1107–3606	Ye et al. 1995
	298.21 K	1380	acoustic interferometer	242–333 K	221–3171	Takagi 1996b
	299.998 K	1447.57	isochoric	220–338 K	79–3529	Duarte-Garza et al. 1997b
	303.19 K	1568.5	VLE			Bobbo et al. 1999
	323.26 K	2539.3	VLE			Bobbo et al. 1999
	308.15 K	1778.8	VLE			Horstmann et al. 2004
Hexafluoroethane			calorimetry static	180–195 K	42–103	Pace and Aston 1948
	291.2 K	2902.1		177–291 K	35–2902	Kao and Miller 2000
1-Chloro-1,1-difluoroethane				320–400 K	632–3388	Maezawa et al. 1991a
	284.688 K	218.216	ebulliometry	225–285 K	15–218	Silva and Weber 1993
1-Chloro-1,2,2,2-tetrafluoroethane	286.098 K	258.829	ebulliometry (glass)	222–286 K	14–259	Weber and Silva 1994
1-Chloropentafluoroethane			calorimetry static	178–234 K	3–101	Aston et al. 1955
				178–346 K	3–2696	Mears et al. 1966
1,1-Dichloro-1-fluoroethane	300 K	84.20	Burnett apparatus	250–450 K	9–2791	Duarte-Garza et al. 1997a
	299.968 K	86		200–400 K	4–1177	Maezawa et al. 1991b
	299.795 K	83.43	comparative ebulliometry	271–313 K	25–129	Weber 1992
1,1-Dichlorotrifluoroethane	289.988 K	67		280–350 K	46–440	Maezawa et al. 1990
	308.26 K	131	isochoric	308–457 K	131–3658	Piao et al. 1991
	293.143 K	76.6	isochoric	243–448 K	7–3172	Oguchi et al. 1992
	299.950 K	97.45	comparative ebulliometry	272–308 K	30–130	Weber 1992
1,2-Dichloro-1,1,2,2-tetrafluoroethane			literature summary	–95.4–3.50°C	0.133–101.325	Stull 1947
1,1,1-Trichloro-2,2,2-trifluoroethane	298.2 K	48.143	isoteniscopic	287–309 K	31–72	Hiraoka and Hildebrand 1963
1,1,2-Trichloro-1,2,2-trifluoroethane	20.19°C	36.64	isoteniscopic	–8.4–210.62°C	10.08–3266.72	Benning and McHarness 1940
	30.2°C	53.329	literature summary	–68.0–47.6°C	0.133–101.325	Stull 1947

(Continued)

TABLE 5.1.5.3 (Continued)

Compound	Temp. °C or K	P ^s kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
1,1,2,2-Tetrachloro-1,2-difluoroethane	298.2 K	48.476	isoteniscopic	273–318 K	17–97	Hiraoka and Hildebrand 1963
	20°C	6.106		10–92°C	4–101	Hovorka and Geiger 1933
	19.8°C	5.333	literature summary	–37.5–92.0°C	0.1333–101.325	Stull 1947
2-Fluoropropane	30°C	407	VLE			Parrish and Sitton 1982
	50°C	700	VLE			Parrish and Sitton 1982
1,1,2,2,3-Pentafluoropropane	298.98 K	100.7	isochoric	258–353 K	16–573	Di Nicola and Passerini 2002
1,1,1,3,3-Pentafluoropropane	298.17 K	151.9	isochoric	293–426 K	127–3595	Sotani & Kubota 1999
	298.21 K	149.04	Burnett apparatus	255–393 K	21–1951	Wang and Duan 2004
	293.15 K	122.8	VLE			Bobbo et al. 2001
	303.15 K	178.4	VLE			Bobbo et al. 2001
	313.15 K	250.8	VLE			Bobbo et al. 2001
	293.15 K	123.1	VLE			Bobbo et al. 2001
	303.15 K	178.1	VLE			Bobbo et al. 2001
	313.15 K	250.6	VLE			Bobbo et al. 2001
	297.97 K	147.1	isochoric	266–352 K	35–762	Di Nicola 2001
	30°C	535.05	mercury piston gauge	–5.34–106.96°C	33.33–3137.4	Shank 1967
	292.955 K	397.36	comparative ebulliometry	248–326 K	74–995	Weber and Defibaugh 1996a
	300 K	219.6	Burnett apparatus	300–410 K	220–3264	Zhang et al. 1995b
1,1,1,2,3,3-Hexafluoropropane	283.12 K	118.6	VLE			Bobbo et al. 2000c
	298.16 K	205.8	VLE			Bobbo et al. 2000c
	313.21 K	340.4	VLE			Bobbo et al. 2000c
	283.12 K	118.4	VLE			Bobbo et al. 2000c
	298.17 K	207.0	VLE			Bobbo et al. 2000c
	313.22 K	338.5	VLE			Bobbo et al. 2000c
	298.41 K	208.1	isochoric	255–363 K	35–1266	Di Nicola and Giuliani 2000
	299.15 K	281.15	Burnett apparatus	253–396 K	44–3064	Duan et al. 2004
	283.62 K	162.6	VLE			Bobbo et al. 1998
	303.68 K	325.8	VLE			Bobbo et al. 1998
1,1,1,3,3,3-Hexafluoropropane	303.2 K	322.2	VLE			Bobbo et al. 1999
	323.26 K	584.2	VLE			Bobbo et al. 1999
	323.26 K	585.7	VLE			Bobbo et al. 1999
	298.27 K	272.5	isochoric	248–360 K	34–1472	Di Nicola et al. 1999
	283.13 K	160.0	VLE			Bobbo et al. 2000a
	303.19 K	322.3	VLE			Bobbo et al. 2000a

	323.26 K	586.3	VLE			Bobbo et al. 2000a
	283.11 K	160.9	VLE			Bobbo et al. 2000b
	298.16 K	272.5	VLE			Bobbo et al. 2000b
	313.21 K	439.3	VLE			Bobbo et al. 2000b
	283.12 K	159.1	VLE			Bobbo et al. 2000c
1,1,1,2,3,3,3-Heptafluoropropane				238–373 K	41–2831	Salvi-Narkhede et al. 1992
	299.06 K	467.35	Burnett apparatus	243–375 K	54–2936	Shi et al. 1999
				273–373 K	192–2818	Gruzdev et al. 2002
	298.152 K	441.234		233–375 K	32–2937	Hu et al. 2002
	295.27 K	416.1	isochoric	235–365 K	36–2402	Di Nicola 2003
	297.22 K	441.61	Burnett apparatus	253–373 K	87–2825	Wang and Duan 2004
Octafluoropropane	29.17°C	9.69 atm		–60.15 – 67.65°C	0.306–24.13 atm	Brown 1963
				182–237 K	3.29–106.47	Crowder et al. 1967
	50°C	1652	VLE			Leu and Robinson 1992
	65°C	2304	VLE			Leu and Robinson 1992
	70°C	2554	VLE			Leu and Robinson 1992
Trichlorotrifluoropropane				48 – 90°C	19–88	Varuschenko & Druzhinina 1972#
1-Chloro-2,2,2-trifluoropropane				29 – 68°C	19–88	Varuschenko & Druzhinina 1972#
Perfluorobutane	20°C	232.033	isoteniscopic recirculating still	–28–90°C	35–1388	Fowler et al. 1947
				233–260 K	16–64	Simons and Mausteller 1952
	31.73°C	330.3		–40–110°C	17–2178	Brown and Mears 1958
Perfluorocyclobutane	17.70°C	249		–36–18°C	26–249	Whipple 1952
				–32–0°C	30–131	Furukava et al. 1954#
	22.53°C	288.76		–40–115°C	19–2778	Martin 1962
	293.21 K	265.2		234–387 K	20–2697	Kao and Miller 2000
Perfluoropentane	24.10°C	83.23	equilibrium still	10–65°C	46.34–318.84	Barber and Cady 1956
	297.59 K	84.71		221–303 K	1–104	Crowder et al. 1967
Perfluorocyclopentane	22.57°C	101.53	equilibrium still	17–56°C	82–307	Barber and Cady 1956
	296.83 K	105.72		230–297 K	2.60–105.72	Crowder et al. 1967
Perfluoro-2-methylcyclopentane	23.82°C	27.464	equilibrium still	4–68°C	11–143	Stiles and Cady 1952
	298.86 K	30.15		254–451 K	2.71–1763.46	Crowder et al. 1967
Perfluoro-3-methylcyclopentane	300.78 K	32.13		255–450 K	2.99–1674.8	Crowder et al. 1967
Perfluorocyclohexane				63–121°C	152–709	Rowlinson and Thacker 1957#
	300.74 K	33.75		253–451 K	2.11–2006.54	Crowder et al. 1967
Perfluorohexane	24.9°C	29.051	equilibrium still	11–69°C	15–149	Stiles and Cady 1952
	30.06°C	36.461	equilibrium still	30–57°C	36–102	Dunlap et al. 1958

(Continued)

TABLE 5.1.5.3 (Continued)

Compound	Temp. °C or K	P ^s kPa	Method*	Temp. Range** °C or K	Pressure Range kPa	Reference
	291.52 K	21.85		256–447 K	3.28–1701.14	Crowder et al. 1967
Fluoroalkenes						
Tetrafluoroethene				–131 – –65°C	1–177	Furukava et al. 1953 [#]
Chlorotrifluoroethene			manometer	195–250 K	6–123	Booth et al. 1933
	21.9°C	577.55	manometer	21.9–107°C	577.55–3951.68	Booth and Swinehart 1935
			literature summary	–116 – –27.9°C	0.1333–101.325	Stull 1947
			calorimetry static	–67 – –11°C	13–205	Oliver et al. 1951
1,2-Dichloro-1,2-difluoroethene	295 K	105.8	manometer	240–295 K	8–106	Booth et al. 1933
	20.9°C	101.325	literature summary	–82.0–20.9°C	0.1333–101.325	Stull 1947
1,1-Dichloro-2,2-difluoroethene	295 K	105.8	manometer	240–295 K	8–106	Booth et al. 1933
Hexafluoropropene	19.75°C	652.7		–41–20°C	62–653	Whipple 1952

* VLE – vapor-liquid equilibrium.

** For temperature dependence equation, see [reference](#).

[#] Boublik et al. 1984.

TABLE 5.1.5.4

Henry's law constants and octanol-water partition coefficients for fluoroalkanes and fluoroalkenes

Compound	Henry's law constant Pa•m ³ /mol	Temp. °C	Method/temp. range	Reference	K _{OW}	Reference
Fluoroalkanes						
Fluoromethane	1418	25	calculated	Yaws et al. 1991	0.51	Sangster 1993
	1948	20		Glew & Moelwyn-Hughes 1953	0.51	Hansch et al. 1995
	1717	25	calculated C _A /C _W	Hine & Mookerjee 1975		
	1742	20T		Staudinger & Roberts 2001		
Difluoromethane	1160	25		Yaws et al. 1991	0.20	Sangster 1993, Hansch et al. 1995
Trifluoromethane	5907	25	gas stripping-GC	Warner et al. 1987	0.64	Hansch & Leo 1985
	9211	25		Hine & Mookerjee 1975	0.64	Sangster 1993
	7794	25		Yaws et al. 1991	0.64	Hansch et al. 1995
	9626	25	calculated-P/C	Howard 1993	0.64	Howard 1993, Hansch et al. 1995
Tetrafluoromethane	539961	25		Yaws et al. 1991	1.18	Sangster 1993, Hansch et al. 1995
Chlorofluoromethane	654.4	25		Yaws et al. 1991		
Dichlorofluoromethane	529.1	25		Yaws et al. 1991	1.55	Hansch et al. 1995
Chlorodifluoromethane	3058	25		Yaws et al. 1991	1.08	Hansch et al. 1995
	2979	25		Howard 1993	1.08	Howard 1993
Chlorotrifluoromethane	113889	25		Yaws et al. 1991	1.65	Hansch et al. 1995
Dichlorodifluoromethane	28704	19.93	0–40°C	Warner & Weiss 1985	2.16	Hansch et al. 1996
	39557	25		Yaws et al. 1991	2.16	Howard 1997
	27976	25		Howard 1997		
	26810	20T		Staudinger & Roberts 2001		
Trichlorofluoromethane	7925	19.93	0–40°C	Warner & Weiss 1985	2.53	Hansch et al. 1995
	10234	25T		Ashworth et al. 1988	2.53	Howard 1990
	9827	25		Howard 1990		
	12341	25		Yaws et al. 1991		
	7824	20T		Staudinger & Roberts 2001		
Fluoroethane	2253	25		Yaws et al. 1991		
1,1-Difluoroethane	2672	25		Yaws et al. 1991	0.75	Hansch et al. 1995
	2203	25		Hine & Mookerjee 1975	0.75	Sangster 1993
	2061			Howard 1993	0.75	Howard 1993

(Continued)

TABLE 5.1.5.4 (Continued)

Compound	Henry's law constant Pa•m ³ /mol	Temp. °C	Method/temp. range	Reference	K _{OW}	Reference
1,1,2-Trifluoroethane	1876	25	EPICS-GC	Zheng et al. 1997		
	32323	25T		Ashworth et al.1988		
	24616	20T		Staudinger & Roberts 2001		
1,1,1,2-Tetrafluoroethane	5629	25	calc-bond contribution	Zheng et al. 1997	1.06	Franklin 1993
Hexafluoroethane	1715432	25		Yaws et al. 1991	2.00	Sangster 1993
1-Chloro-1,1-difluoroethane	1652940	25T		Bonifacio et al. 2001	2.00	Hansch et al. 1995
	24217	25		Howard 1990	1.60	Howard 1990
1-Chloro-1,2,2,2-tetrafluoro-	54716	25		Howard 1997	1.867	estimated, Howard 1997
1-Chloropentafluoroethane	261418	25		Yaws et al. 1991	2.30	Howard 1997
	309041	25		Howard 1997		
1,1-Dichloro-1-fluoroethane	2442	25		Howard 1997	2.04	Howard 1997
1,2-Dichlorotetrafluoroethane	122502	25		Yaws et al. 1991	2.82	Sangster 1993, Hansch et al. 1995
					2.85	Sangster 1993, Hansch et al. 1995
1,1,2-Trichloro-1,2,2-trifluoro-	49132	25	calculated-P/C	Yaws et al. 1991	3.16	McDuffie 1981, Sangster 1993
	53297			Howard 1990	3.16	Howard 1990, Hansch 1995
1,1-Difluorotetrachloroethane	171239		calculated-P/C	Howard 1993	2.85	estimated, Howard 1993
1,2-Difluoro-1,1,2,2-tetrafluoro-	283710			Howard 1990	2.82	Howard 1990, Sangster 1993, Hansch et al. 1995
1,1,2,2-Tetrachloro-1,2-difluoro-	9869		calculated-C _A /C _W	Hine & Mookerjee 1975	3.73	Howard 1990
1-Fluoropropane	1627	14		Yaws et al. 1991		
2-Fluoropropane	1713	15		Yaws et al. 1991		
Perfluorocyclobutane	391925	25		Yaws et al. 1991		
Fluoroalkenes						
1,1-Difluoroethene	39344	25		Yaws et al. 1991	1.24	Hansch et al. 1995
Tetrafluoroethene	61981	25		Yaws et al. 1991		
Chlorotrifluoroethene	63328	25		Yaws et al. 1991		
Hexafluoropropene	349397	25		Wilhelm et al. 1977		

TABLE 5.1.5.5
Atmospheric fate rates for fluoroalkanes

Compound	Atmospheric fate rate (photooxidation in air)			Lifetime, τ	Reference
	T/K	$k_{OH}^*/(\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1})$	Temp. range**		
Fluoroalkanes					
Fluoromethane	296	16×10^{-15}	294–480 K	2–4.1 yr	Howard & Evenson 1976a
	298	1.68×10^{-14}			Atkinson 1989
Difluoromethane	296	7.8×10^{-15}	293–425 K	7.1–7.7 yr	Cooper et al. 1992
	298	7.2×10^{-15}			Howard & Evenson 1976a
	298	1.09×10^{-14}	250–492 K	4–7.3 yr	Clyne et al. 1978
	298	1.13×10^{-14}	222–381 K		Atkinson 1989
Trifluoromethane	296	0.2×10^{-15}	387–1445	17.2 yr	Talukdar et al. 1991
	298	2.4×10^{-16}			Cooper et al. 1992
Tetrafluoromethane	298	$< 4 \times 10^{-16}$			Howard & Evenson 1976a
Chlorofluoromethane	296	37×10^{-15}	245–486 K		Atkinson 1989
	298	4.41×10^{-14}			Howard & Evenson 1976a
Dichlorofluoromethane	296	26×10^{-15}	293–425 K		Atkinson 1989
	298	3.9×10^{-14}			Howard & Evenson 1976a
	298	3.03×10^{-14}			Clyne et al. 1978
Chlorodifluoromethane	296	3.4×10^{-15}	241–483 K		Atkinson 1989
	298	4.1×10^{-15}			Howard & Evenson 1976a
	298	4.68×10^{-15}			Clyne et al. 1978
Chlorotrifluoromethane	296	$< 0.7 \times 10^{-15}$	293–425 K		Atkinson 1989
	298	$< 7 \times 10^{-16}$			Brown et al. 1990
	298	$< 1.0 \times 10^{-15}$			Howard & Evenson 1976a
Dichlorodifluoromethane	296	$< 0.4 \times 10^{-15}$	250–482 K	>330 yr	Atkinson et al. 1975
	293	$< 10^{-16}$			Howard & Evenson 1976a
	298	$< 1.0 \times 10^{-17}$			Cox et al. 1976
					Atkinson 1989
					Brown et al. 1990
Trichlorofluoromethane	296	$< 1.0 \times 10^{-15}$		1000 yr	Atkinson et al. 1975
	296	$< 0.5 \times 10^{-15}$			Howard & Evenson 1976a
	293	$< 10^{-17}$			Cox et al. 1976
	298	$< 1.0 \times 10^{-17}$			Atkinson 1989

(Continued)

TABLE 5.1.5.5 (Continued)

Compound	Atmospheric fate rate (photooxidation in air)			Lifetime, τ	Reference
	T/K	$k_{OH}^*/(\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1})$	Temp. range**		
Fluoroethane				60 yr	Brown et al. 1990
				182–635 yr	Cooper et al. 1992
				0.2–1 yr	Cooper et al. 1992
	298	5.1×10^{-14}	293–425 K		Clyne et al. 1978
	295	3.4×10^{-14}			Atkinson 1989
1,1-Difluoroethane	303	5.6×10^{-14}	230–423 K	1.5 yr	Brown et al. 1990
	298	4.2×10^{-14}	243–400 K	1.5 yr	Liu et al. 1990
				1–1.68 yr	Cooper et al. 1992
				0.58–0.8 yr	Cooper et al. 1992
1,2-Difluoroethane					Clyne et al. 1978
1,1,1-Trifluoroethane	298	1.5×10^{-15}	293–425 K		Talukdar et al. 1991
	298	1.35×10^{-15}	223–374	72–74 yr	Brown et al. 1990
1,1,2-Trifluoroethane				6.3 yr	Cooper et al. 1992
				20–45 yr	Clyne et al. 1978
	298	4.9×10^{-14}	293–425		Cooper et al. 1992
				1–3.8 yr	Clyne et al. 1978
1,1,2,2-Tetrafluoroethane	298	6.9×10^{-15}	293–425		Atkinson 1989
	298	8.54×10^{-15}	249–473 K		Cooper et al. 1992
1,1,1,2-Tetrafluoroethane				2–12.3 yr	Clyne et al. 1978
	298	6.9×10^{-15}	293–425		Brown et al. 1990
	301	6.9×10^{-15}	231–423 K	10.7 yr	Liu et al. 1990
	298	5.18×10^{-15}	243–400 K	14.4 yr	Franklin 1993
Pentafluoroethane				13.1–15.5 yr	Cooper et al. 1992
	298	5.0×10^{-15}	293–425 K		Clyne et al. 1978
	303	2.9×10^{-15}	226–423 K	22.1 yr	
	298	1.9×10^{-15}	220–364 K	47–48 yr	Talukdar et al. 1991
1-Chloro-1,1-difluoroethane				17–28.1 yr	Cooper et al. 1992
	298	6.74×10^{-15}	293–425 K		Clyne et al. 1978
	298	3.58×10^{-15}	273–375 K		Atkinson 1989
	303	3.7×10^{-15}	231–423 K	15.4 yr	Brown et al. 1990
1-Chloro-1,1,2-trifluoroethane	298	4.02×10^{-15}	243–400 K	17.8 yr	Liu et al. 1990
	298	1.5×10^{-14}	293–425 K		Clyne et al. 1978
	298	1.61×10^{-14}	263–373 K		Atkinson 1989

1-Chloro-1,2,2,2-tetrafluoroethane	298	1.02×10^{-14}	250–375 K		Atkinson 1989
1,1-Dichloro-1-fluoroethane	298	7.1×10^{-15}	243–400 K	6.7 yr	Liu et al. 1990
	297	1.61×10^{-14}	238–426 K	4.3 yr	Brown et al. 1990
	298	5.92×10^{-15}	233–393 K	13–14 yr	Talukdar et al. 1991
	298	2.61×10^{-14}	249–473 K		Atkinson 1989
1,2-Dichloro-1,1-difluoroethane	298	4.2×10^{-14}	293–425 K		Clyne et al. 1978
1,1-Dichlorotrifluoroethane	298	3.34×10^{-14}	245–375 K		Atkinson 1989
	303	5.9×10^{-14}	232–425 K	1.0 yr	Brown et al. 1990
	298	3.52×10^{-14}	270–400 K	1.4 yr	Liu et al. 1990
1,1,2,2,3-Pentafluoropropane	298	2×10^{-14} , 4×10^{-14}		2, 1.3 yr	Cooper et al. 1993
1,1,1,2,2-Pentafluoropropane	298	7×10^{-15} , 8×10^{-15}		7 yr	Cooper et al. 1993
1,1,1,2,3,3-Hexafluoropropane	298	4×10^{-15} , 6×10^{-15}		10, 9 yr	Cooper et al. 1993
1,1,1,3,3,3-Hexafluoropropane	298	5×10^{-16} , 2×10^{-16}		77, 218 yr	Cooper et al. 1993
1,1,1,2,3,3,3-Heptafluoropropane	298	7×10^{-16}		63, 72 yr	Cooper et al. 1993

* k_{OH} = second order reaction rate constant with hydroxyl radicals

** For temperature dependence equation, see [reference](#).

5.1.5 FLUOROALKANES AND FLUOROALKENES

TABLE 5.2.1

Summary of physical properties of halogenated hydrocarbons

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M	
							cm ³ /mol	
							MW/ρ at 20°C	Le Bas
Chloroalkanes:								
Chloromethane (Methyl chloride)	74-87-3	CH ₃ Cl	50.488	−97.7	−24.09	1	54.79	50.5
Dichloromethane	75-09-2	CH ₂ Cl ₂	84.933	−97.2	40	1	64.07	71.4
Trichloromethane (Chloroform)	67-66-3	CHCl ₃	119.378	−63.41	61.17	1	79.67	92.3
Tetrachloromethane (Carbon tetrachloride)	56-23-5	CCl ₄	153.823	−22.62	76.8	1	96.50	113.2
Chloroethane (Ethyl chloride)	75-00-3	C ₂ H ₅ Cl	64.514	−138.4	12.3	1	72.00	72.7
1,1-Dichloroethane	75-34-3	C ₂ H ₄ Cl ₂	98.959	−96.9	57.3	1	84.18	93.6
1,2-Dichloroethane	107-06-2	C ₂ H ₄ Cl ₂	98.959	−35.7	85.3	1	79.04	93.6
1,1,1-Trichloroethane	71-55-6	C ₂ H ₃ Cl ₃	133.404	−30.01	74.09	1	99.70	114.5
1,1,2-Trichloroethane	79-00-5	C ₂ H ₃ Cl ₃	133.404	−36.3	113.8	1	92.69	114.5
1,1,1,2-Tetrachloroethane	630-20-6	C ₂ H ₂ Cl ₄	167.849	−70.2	130.2	1	108.95	135.4
1,1,2,2-Tetrachloroethane	79-34-5	C ₂ H ₂ Cl ₄	167.849	−42.4	145.2	1	105.27	135.4
Pentachloroethane	76-01-7	C ₂ HCl ₅	202.294	−28.78	162.0	1	120.36	156.3
Hexachloroethane	67-72-1	C ₂ Cl ₆	236.739				113.22	177.2
1-Chloropropane (<i>n</i> -Propyl chloride)	540-54-5	C ₃ H ₇ Cl	78.541	−122.9	46.5	1	88.26	94.9
2-Chloropropane	75-29-6	C ₃ H ₇ Cl	78.541	−117.18	35.7	1	91.15	94.9
1,2-Dichloropropane	78-87-5	C ₃ H ₆ Cl ₂	112.986	−100.53	96.4	1	97.74	115.8
1,2,3-Trichloropropane	96-18-4	C ₃ H ₅ Cl ₃	147.431	−14.7	157	1	106.59	136.7
1-Chlorobutane (<i>n</i> -Butyl chloride)	109-69-3	C ₄ H ₉ Cl	92.567	−123.1	78.4	1	104.51	117.1
2-Chlorobutane	78-86-4	C ₄ H ₉ Cl	92.567	−131.3	68.2	1	106.01	117.1
1-Chloropentane (<i>n</i> -Amyl chloride)	543-59-6	C ₅ H ₁₁ Cl	106.594	−99.0	108.4	1	120.85	139.3
1-Chlorohexane	544-10-5	C ₆ H ₁₃ Cl	120.620	−94.0	135.1	1	137.30	161.5
1-Chloroheptane	629-06-1	C ₇ H ₁₅ Cl	134.647	−69.5	160.4	1	153.74	183.7
1-Chlorooctane	111-85-3	C ₈ H ₁₇ Cl	148.674	−57.8	183.5	1	170.15	205.9
1-Chlorononane	2473-01-0	C ₉ H ₁₉ Cl	162.700	−39.4	205.2	1	206.31	228.1
1-Chlorodecane	1002-69-3	C ₁₀ H ₂₁ Cl	176.727	−31.3	225.9	1	203.02	250.3

Chloroalkenes:

Chloroethene (Vinyl chloride)	75-01-4	C ₂ H ₃ Cl	62.498	-153.84	-13.8	1	68.63	65.3
1,1-Dichloroethene	75-35-4	C ₂ H ₂ Cl ₂	96.943	-122.56	31.6	1	79.91	86.2
<i>cis</i> -1,2-Dichloroethene	156-59-2	C ₂ H ₂ Cl ₂	96.943	-80.0	60.1	1	75.52	86.2
<i>trans</i> -1,2-Dichloroethene	156-60-5	C ₂ H ₂ Cl ₂	96.943	-49.8	48.7	1	77.15	86.2
Trichloroethylene	79-01-6	C ₂ HCl ₃	131.388	-84.7	87.21	1	89.73	107.1
Tetrachloroethylene	127-18-4	C ₂ Cl ₄	165.833	-22.3	121.3	1	120.19	128.0
<i>cis</i> -1,3-Dichloropropene	10061-01-5	C ₃ H ₄ Cl ₂	110.970		104.3		91.18	108.4
<i>trans</i> -1,3-Dichloropropene	10061-02-6	C ₃ H ₄ Cl ₂	110.970		112		90.66	108.4
Chloroprene	126-99-8	C ₄ H ₅ Cl	88.536	-130	59.4	1	92.39	102.3
Hexachloro-1,3-butadiene	87-68-3	C ₄ Cl ₆	260.761	-21	215	1	155.03	206.8
Hexachlorocyclopentadiene	77-47-4	C ₅ H ₆	272.772	-9	239	1	160.27	210.1

Bromoalkanes and bromoalkenes:

Bromomethane	74-83-9	CH ₃ Br	94.939	-93.68	3.5	1	56.66	52.9
Dibromomethane	74-95-3	CH ₂ Br ₂	173.835	-52.5	97	1	69.62	76.2
Tribromomethane	75-25-2	CHBr ₃	252.731	8.69	149.1	1	87.42	99.5
Bromoethane (Ethyl bromide)	74-96-4	C ₂ H ₅ Br	108.965	-118.6	38.5	1	75.12	75.1
1,2-Dibromoethane	106-93-4	C ₂ H ₄ Br ₂	187.861	9.84	131.6	1	86.21	98.4
1-Bromopropane (<i>n</i> -Propyl bromide)	106-94-5	C ₃ H ₇ Br	122.992	-110.3	71.1	1	90.86	97.3
2-Bromopropane	75-26-3	C ₃ H ₇ Br	122.992	-89.0	59.5	1	93.60	97.3
1,2-Dibromopropane	78-75-1	C ₃ H ₆ Br ₂	201.888	-55.49	141.9	1	104.48	120.6
1-Bromobutane (<i>n</i> -Butyl bromide)	109-65-9	C ₄ H ₉ Br	137.018	-112.6	101.6	1	107.40	119.5
1-Bromopentane (<i>n</i> -Amyl bromide)	110-53-2	C ₅ H ₁₁ Br	151.045	-88.0	129.8	1	123.99	141.7
1-Bromohexane	111-25-1	C ₆ H ₁₃ Br	165.071	-83.7	155.3	1	140.56	163.9
1-Bromoheptane	629-04-9	C ₇ H ₁₅ Br	179.098	-56.1	178.9	1	157.10	186.1
1-Bromooctane	111-83-1	C ₈ H ₁₇ Br	193.125	-55.0	200.8	1	173.64	208.3
1-Bromodecane	112-29-8	C ₁₀ H ₂₁ Br	221.178	-29.2	240.6	1	206.67	252.7
1-Bromododecane	143-15-7	C ₁₂ H ₂₅ Br	249.231	-9.5	276	1	239.67	297.1
Bromocyclohexane	108-85-0	C ₆ H ₁₁ Br	163.055	-56.5	166.2	1	122.06	141.5
Vinyl bromide	593-60-2	C ₂ H ₃ Br	106.949	-139.54	15.8	1	71.62	67.7

(Continued)

TABLE 5.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M	
							cm ³ /mol	
							MW/ρ at 20°C	Le Bas
Iodoalkanes:								
Iodomethane (Methyl iodide)	74-88-4	CH ₃ I	141.939	−66.4	42.43	1	62.28	62.9
Iodoethane (Ethyl iodide)	75-03-6	C ₂ H ₅ I	155.965	−111.1	72.3	1	80.57	85.1
1-Iodopropane (<i>n</i> -Propyl iodide)	107-08-4	C ₃ H ₇ I	169.992	−101.3	102.5	1	97.20	107.3
2-Iodopropane	75−30−9	C ₃ H ₇ I	169.992	−90	89.5	1	99.75	107.3
1-Iodobutane (<i>n</i> -Butyl iodide)	542-69-8	C ₄ H ₉ I	184.018	−103	130.5	1	113.91	129.5
1-Iodopentane	628−17−1	C ₅ H ₁₁ I	198.045	−85.6	157.0	1	130.63	151.7
Mixed halogenated hydrocarbons:								
Bromochloromethane	74-97-5	CH ₂ BrCl	129.384	−87.9	68.0	1	66.89	73.8
Bromodichloromethane	75-27-4	CHBrCl ₂	163.829	−57	90	1	83.12	94.7
Dibromochloromethane	124-48-1	CHBr ₂ Cl	208.280	−20	120	1	84.98	97.1
Chlorodifluoromethane (HCFC-22)	75-45-6	CHClF ₂	86.469	−157.42	−40.7	1	71.25	60.5
Dichlorodifluoromethane (CFC-12)	75-71-8	CCl ₂ F ₂	120.914	−158	−29.8	1	90.97	81.4
Trichlorofluoromethane (CFC-11)	75-69-4	CCl ₃ F	137.368	−110.44	23.7	1	92.32	97.3
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	76-13-1	C ₂ F ₃ Cl ₃	187.375	−36.22	47.7	1	119.84	129.5
1,1,2,2-Tetrachloro-1,2-difluoroethane (CFC-112)	76−12−0	C ₂ F ₂ Cl ₄	203.830	24.8	92.8	1		145.4

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 5.2.2

Summary of selected physical-chemical properties of halogenated hydrocarbons at 25°C

Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility			log K _{OW}	H/(Pa·m³/mol)	
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)		calcd P/C	exptl
Chloroalkanes:								
Chloromethane	570000	570000	5325	105.5	105.5	0.91	960.7*	894
Dichloromethane	58000	58000	13200	155.4	155.4	1.25	373.2	300
Trichloromethane	26200	26200	8200	68.69	68.69	1.97	381.4	427
Tetrachloromethane	15250	15250	800	5.200	5.200	2.83	2932	2989
Chloroethane	16000	16000	5700	88.35	88.35	1.43	181.1	1023
1,1-Dichloroethane	30260	30260	5040	50.93	50.93	1.79	594.1	569
1,2-Dichloroethane	10540	10540	8600	86.90	86.90	1.48	121.3	143
1,1,1-Trichloroethane	16500	16500	1290	9.670	9.670	2.49	1706	1763
1,1,2-Trichloroethane	3220	3220	4590	34.41	34.41	2.38	93.59	92.2
1,1,1,2-Tetrachloroethane	1580	1580	1070	6.375	6.375		247.8	
1,1,2,2-Tetrachloroethane	793	793	2830	16.86	16.86	2.39	47.03	25.7
Pentachloroethane	590	590	490	2.422	2.422	3.22	243.6	
Hexachloroethane	50	1923	50	0.2112	8.123	4.14	236.7	846
1-Chloropropane	46000	46000	2500	31.83	31.83	2.04	1445	
2-Chloropropane	68700	68700	3000	38.20	38.20	1.90	1798	
1,2-Dichloropropane	6620	6620	2740	24.25	24.25	2.00	273.0	287
1,2,3-Trichloropropane	492	492	1896	12.86	12.86		38.26	
1-Chlorobutane	13700	13700	615	6.644	6.644	2.64	2062	1537
2-Chlorobutane	20210	20210	1000	10.80	10.80		1871	2267
1-Chloropentane	4142	4142	198	1.858	1.858		2230	2375
Chloroalkenes:								
Chloroethene	354600	354600	2763	44.21	44.21	1.38	8021	2685
1,1-Dichloroethene	80500	80500	3344	34.49	34.49	2.13	2334	2624
<i>cis</i> -1,2-Dichloroethene	27000	27000	3500	36.10	36.10	1.86	747.8	460
<i>trans</i> -1,2-Dichloroethene	44400	44400	6260	64.57	64.57	1.93	687.6	958
Trichloroethylene	9900	9900	1100	8.372	8.372	2.53	1182	1034
Tetrachloroethylene	2415	2415	150	0.904	0.904	2.88	2670	1733

(Continued)

TABLE 5.2.2 (Continued)

Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility			log K _{ow}	H/(Pa·m ³ /mol)	
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		calcd P/C	exptl
1,3-Dichloropropene						1.98		
Chloroprene	23194	23194				2.03		
Hexachloro-1,3-butadiene	20.0	20.0	3.2	0.013	0.013	4.70	1630	
Hexachlorocyclopentadiene	10.9	10.9	1.80	0.0066	0.0066	5.04	1652	
Bromoalkanes and bromoalkenes:								
Bromomethane	217700	217700	15223	160.3	160.3	1.19	631.9*	
Dibromomethane	6034	6034	11442	65.82	65.82	2.50	91.67	86.13
Tribromomethane	727	727	3100	12.27	12.27	2.38	59.27	46.61
Bromoethane	62500	62500	8939	82.04	82.04	1.6	1235*	
1,2-Dibromoethane	1500	1500	4152	22.10	22.10		67.87	65.86
1-Bromopropane	18440	18440	598	4.862	4.862	2.1	3792	
2-Bromopropane	31940	31940	3086	25.09	25.09	1.9	1273	
1,2-Dibromopropane	1040	1040	1428	7.073	7.073		147.0	
1-Bromobutane	5500	5500				2.6		
Vinyl bromide	140476	140476						
Iodoalkanes:								
Iodomethane	54000	54000	13894	97.89	97.89	1.5	551.6	541
Iodoethane	18160	18160	4041	25.91	25.91	2	700.9	
1-Iodopropane	5745	5745	1051	6.183	6.183	2.5	929.2	
1-Iodobutane	1848	1848	182	0.989	0.989	3	1868	
Mixed halogenated hydrocarbons:								
Bromochloromethane	19600	19600	14778	114.2	114.2	1.41	171.6	
Bromodichloromethane	6670	6670	4500	27.47	27.47	2.1	242.8	162
Dibromochloromethane			4000	19.20	19.20	2.24		86.13
Chlorodifluoromethane (HCFC-22)	1044000	1044000	2899	33.53	33.53		3022*	
Dichlorodifluoromethane (CFC-12)	651000	651000	300	2.481	2.481	2.16	40840*	
Trichlorofluoromethane (CFC-11)	102200	102200	1080	7.862	7.862	2.53	12890*	10243
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	48320	48320	166	0.886	0.886	3.16	114375*	32323

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H (Pa·m³/mol) = 101325 Pa/C^S mol/m³.

TABLE 5.2.3

Suggested half-life classes of halogenated hydrocarbons in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Cycloalkanes and cycloalkenes:				
Dichloromethane	6	6	7	8
Trichloromethane	6	6	7	8
Tetrachloroethane	8	6	7	8
Chloroethane	6	6	7	8
1,2-Dichloroethane	6	6	7	8
1,1,2,2-Tetrachloroethane	8	6	7	8
Pentachloroethane	8	6	7	8
Hexachloroethane	8	6	7	8
1,2-Dichloropropane	5	6	7	8
1,2,3-Trichloropropane	5	6	7	8
Chloroethene (Vinyl chloride)	3	5	6	7
Trichloroethylene	4	6	7	8
Tetrachloroethylene	5	6	7	8
Chloroprene	3	5	6	7
Bromoalkanes and bromoalkenes:				
Tribromomethane	6	6	7	8
Mixed halogenated hydrocarbons:	5	5	6	7
Bromodichloromethane	5	5	6	7
Trichlorofluoromethane (CFC-11)	8	8	9	9
Class	Mean half-life (h)		Range (h)	
1	5		< 10	
2	17 (~ 1 d)		10–30	
3	55 (~ 2 d)		30–100	
4	170 (~ 1 week)		100–300	
5	550 (~ 3 weeks)		300–1,000	
6	1700 (~ 2 months)		1,000–3,000	
7	5500 (~ 8 months)		3,000–10,000	
8	17000 (~ 2 yr)		10,000–30,000	
9	55000 (~ 6 yr)		> 30,000	

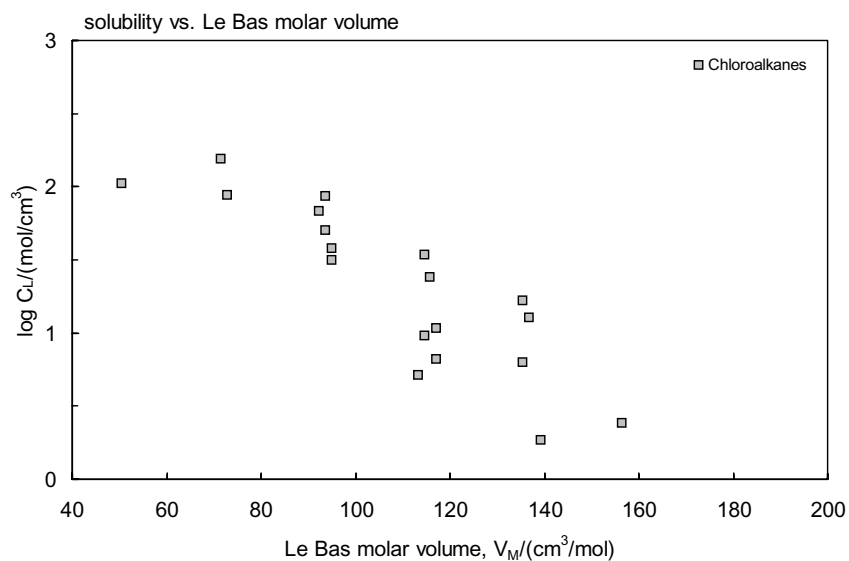


FIGURE 5.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for chloroalkanes.

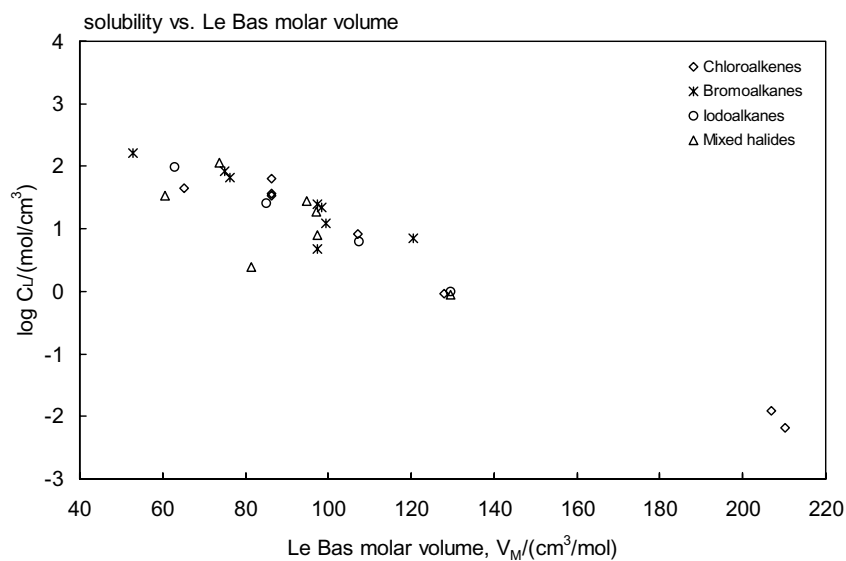


FIGURE 5.2.2 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

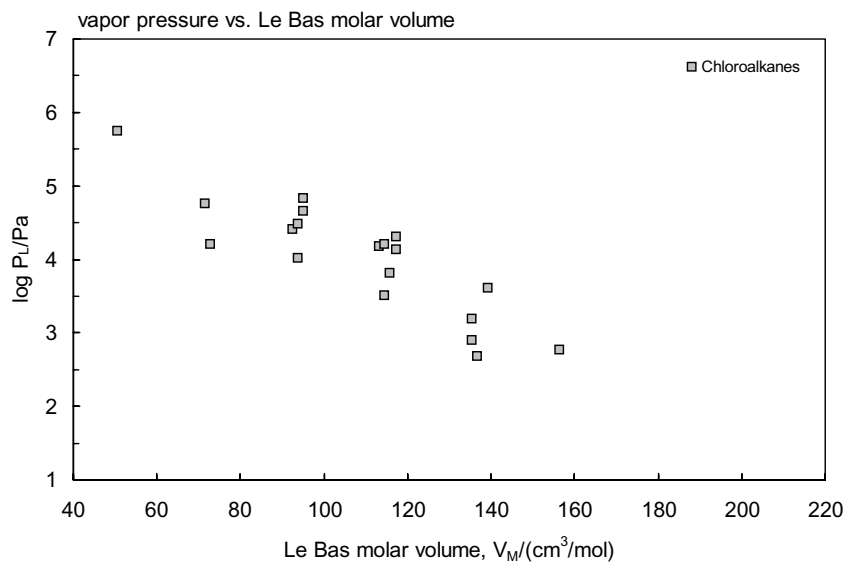


FIGURE 5.2.3 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for chloroalkanes.

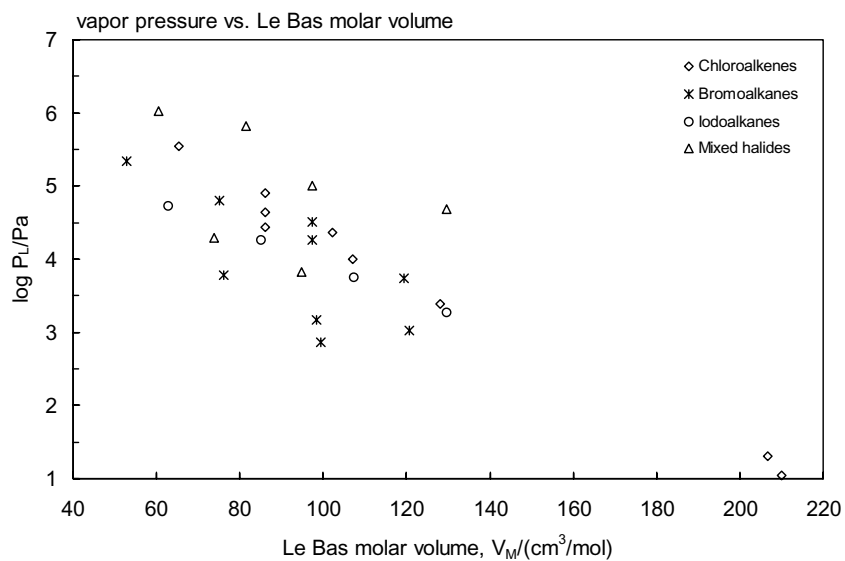


FIGURE 5.2.4 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

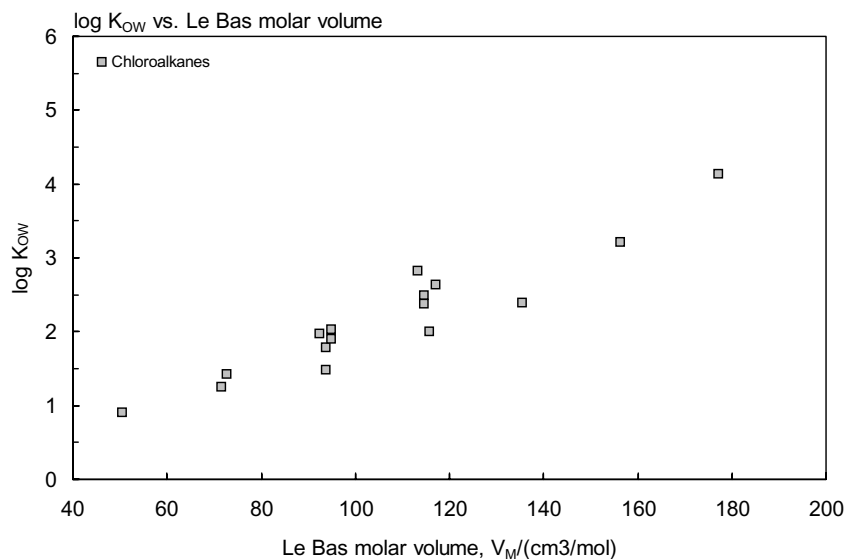


FIGURE 5.2.5 Octanol-water partition coefficient versus Le Bas molar volume for chloroalkanes.

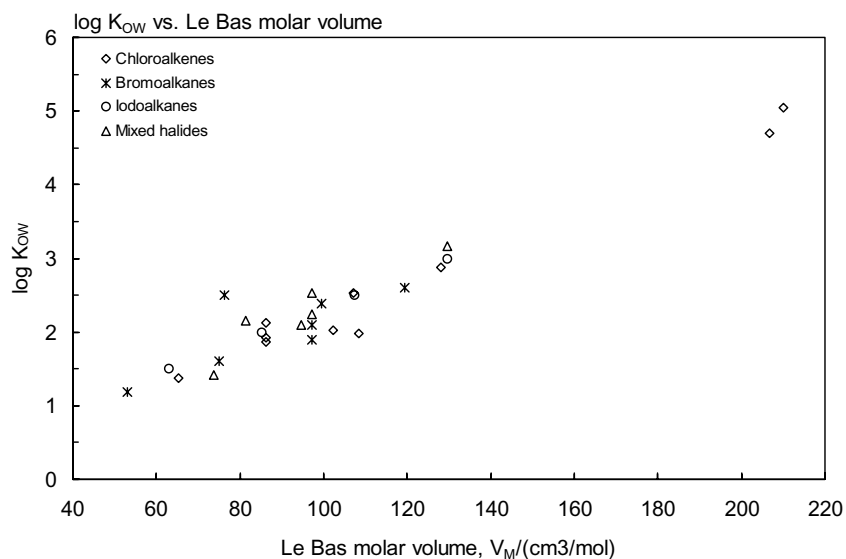


FIGURE 5.2.6 Octanol-water partition coefficient versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

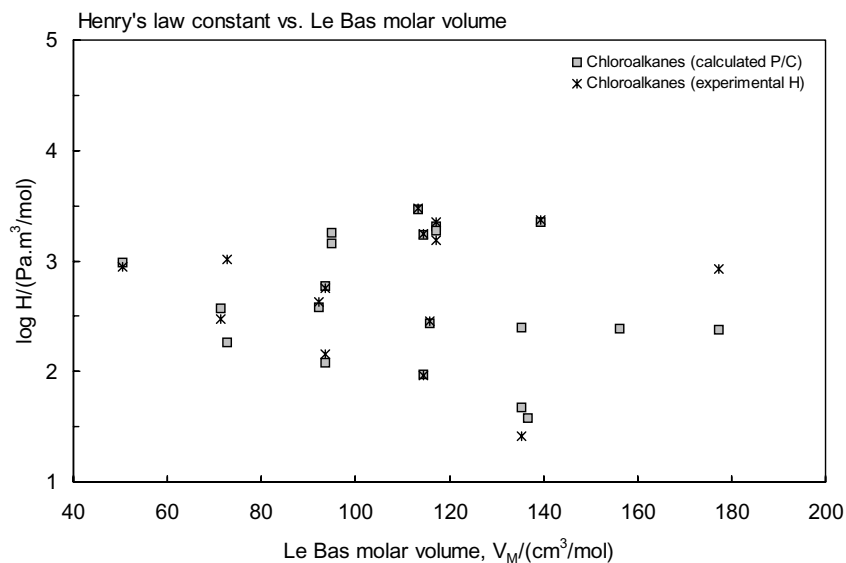


FIGURE 5.2.7 Henry's law constant versus Le Bas molar volume for chloroalkanes.

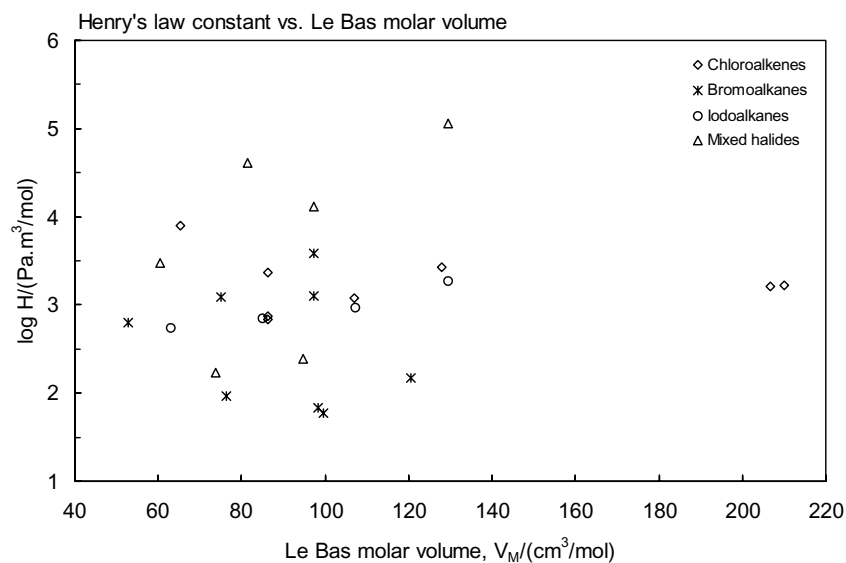


FIGURE 5.2.8 Henry's law constant versus Le Bas molar volume for halogenated aliphatic hydrocarbons.

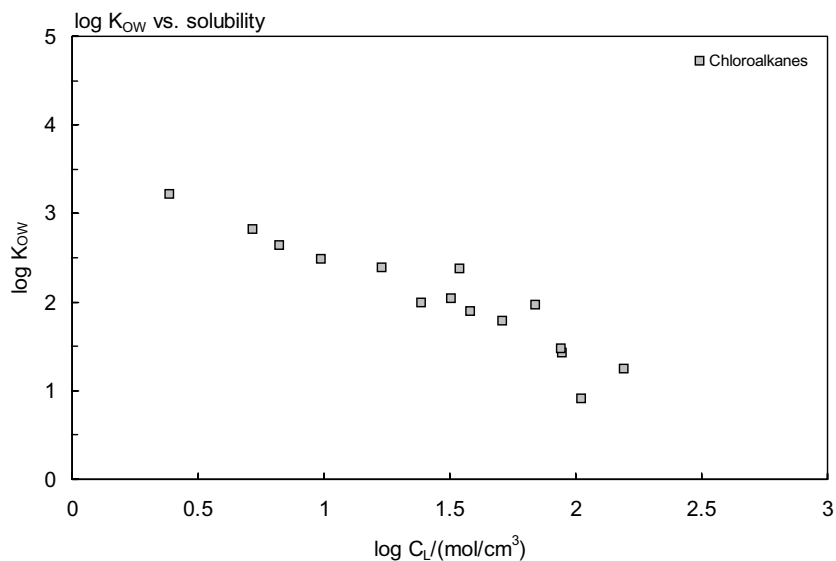


FIGURE 5.2.9 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for chloroalkanes.

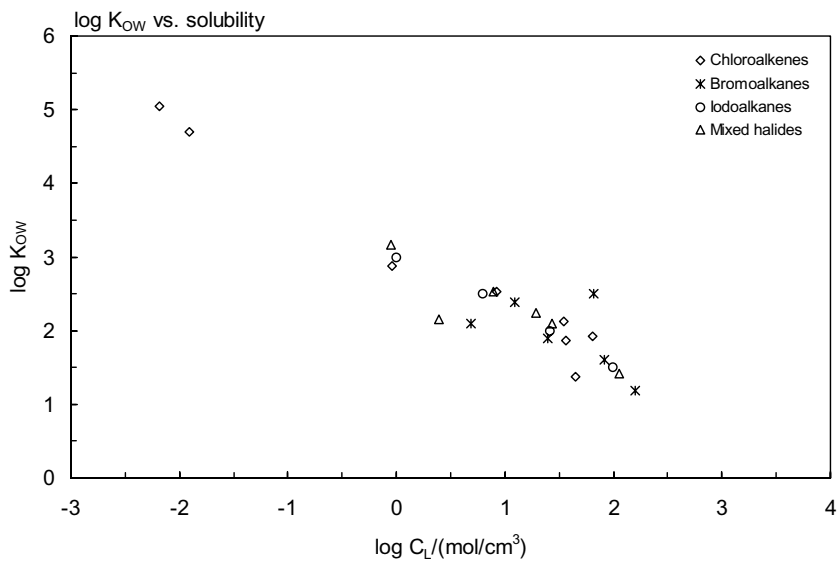


FIGURE 5.2.10 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for halogenated aliphatic hydrocarbons.

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6 Chlorobenzenes and Other Halogenated Mononuclear Aromatics

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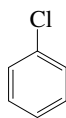
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6.1 LIST OF CHEMICALS AND DATA COMPILATIONS

6.1.1 CHLOROBENZENES

6.1.1.1 Chlorobenzene



Common Name: Chlorobenzene

Synonym: monochlorobenzene, benzene chloride, phenyl chloride

Chemical Name: chlorobenzene

CAS Registry No: 108-90-7

Molecular Formula: C_6H_5Cl

Molecular Weight: 112.557

Melting Point ($^{\circ}C$):

−45.31 (Lide 2003)

Boiling Point ($^{\circ}C$):

131.72 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1058 (Weast 1972–73; Lide 2003)

Molar Volume (cm^3/mol):

101.8 ($20^{\circ}C$, calculated-density)

116.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.49 (Dean 1985)

11.88 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

488 ($30^{\circ}C$, shake flask-interferometer, Gross & Saylor 1931)

551 (Landolt-Börnstein 1951)

488 (Seidell 1941)

< 200 (residue-volume method, Booth & Everson 1948)

500 (shake flask-UV, Andrews & Keefer 1950)

490* ($30^{\circ}C$, shake flask, Kisarov 1962)

546, 523; 534 ($21^{\circ}C$, generator column-GC; mean value, Chey & Calder 1972)

463 (shake flask-UV, Vesala 1974)

100 (Stephen & Stephen 1963)

106.8* (shake flask-GC, measured range $5-45^{\circ}C$, Nelson & Smit 1978)

472 (shake flask-GC, Aquan-Yuen et al. 1979)

472 (shake flask-GC, Mackay et al. 1979, 1980, 1982b)

503 (shake flask-UV, Yalkowsky et al. 1979)

420, 450* ($20^{\circ}C$; elution chromatography, UV adsorption, measured range $10-30^{\circ}C$, Schwarz & Miller 1980)

295 (generator column-HPLC/UV, Tewari et al. 1982)

498 (recommended, Horvath 1982)

499 (generator column-HPLC/UV, Wasik et al. 1983)

508 (HPLC- k' correlation, converted from reported γ_w , Hafkenscheid & Tomlinson 1983a)

295 (generator column-GC, Miller et al. 1984, 1985)

495* (recommended, temp range $10-70^{\circ}C$, IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(\text{g/kg}) = 11.3351 - 3.0290 \times 10^{-2} \cdot (T/K) - 1.8716 \times 10^{-4} \cdot (T/K)^2 + 0.559466 \times 10^{-6} \cdot (T/K)^3$; temp range 283–363 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

490 (30°C, quoted, Dean 1985)

502 (shake flask-HPLC/UV, Banerjee 1984)

348 (shake flask-radiometric method, Lo et al. 1986)

428 (vapor phase saturation-GC, temp range 15–45°C, Sanemasa et al. 1987)

482* (20°C vapor-liquid equilibrium-activity coefficient, measured range 20–50°C, Cooling et al. 1992)

477 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

333 (shake flask-GC, Boyd et al. 1998)

496 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)

$\ln x = -41.9062 + 6054.03/(T/K) + 1.3692 \times 10^{-4} \cdot (T/K)^2$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

470* (shake flask-GC, measured range 5–45°C, Ma et al. 2001)

426, 427, 511 (5, 15, 35°C, estimated-RP-HPLC- k' correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

1333* (22.2°C, summary of literature data, temp range –13.0 to 132.2°C, Stull 1947)

$\log(P/\text{mmHg}) = 7.18473 - 1556.6/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

$\log(P/\text{mmHg}) = 6.94504 - 1413.12/(216.0 + t/^\circ\text{C})$; temp range 40–200°C (Antoine eq. for liquid state, Dreisbach 1955)

7605* (56.28°C, ebulliometry, measured range 56.28–131.70°C, Dreisbach & Shrader 1949)

9657* (62.04°C, ebulliometry, measured range 62.04–131.7°C, Brown 1952)

1580 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 10098.0/(T/K)] + 8.5000$; temp range –35 to –15°C (Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 9067.3/(T/K)] + 7.717535$; temp range –13 to 249.8°C (Antoine eq., Weast 1972–73)

1596, 1610 (extrapolated-Antoine eq., Boublik et al. 1973; 1984)

$\log(P/\text{kPa}) = 6.10416 - 1431.813/(217.655 + t/^\circ\text{C})$; temp range 62.04–131.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.07963 - 1419.045/(216.633 + t/^\circ\text{C})$; temp range 56.2–131.7°C (Antoine eq. from reported exptl. data of Derisbach & Shrader 1949, Boublik et al. 1984)

1586 (Daubert & Danner 1985)

1596 (extrapolated, Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 6.97808 - 1431.05/(217.65 + t/^\circ\text{C})$; temp range 62–131.7°C (Antoine eq., Dean 1985, 1992)

1600 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.11512 - 1438.86/(-54.72 + T/K)$; temp range 333–405 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.62988 - 1897.41/(5.21 + T/K)$; temp range 405–597 K (Antoine eq.-II, Stephenson & Malanowski 1987)

1410* (gas saturation-GC, measured range –14.2 to 40°C, Liu & Dickhut 1994)

1828; 1560 (supercooled liquid P_L , GC-Kovács retention indices correlation; quoted lit., Spiessma et al. 1994)

$\log(P/\text{mmHg}) = 19.4343 - 2.5801 \times 10^3/(T/K) - 3.9391 \cdot \log(T/K) - 4.4005 \times 10^{-11} \cdot (T/K) + 4.9583 \times 10^{-7} \cdot (T/K)^2$; temp range 228–632 K (Yaws 1994)

$\log P/\text{kPa} = 6.11512 - 1438.86/(T/K - 54.72)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

451 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

441 (calculated-bond contribution, Hine & Mookerjee 1975)

382 (batch stripping-GC, Mackay et al. 1979)

379 (calculated P/C , Mackay et al. 1979)

330* (equilibrium cell-concentration ratio, measured range 1.0–23.0°C, Leighton & Calo 1981)

$\ln(k_H/\text{atm}) = 16.83 - 3466/(T/K)$; temp range 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

314 (batch air stripping-GC, Mackay & Shiu 1981)

- 398 (gas stripping-GC, Warner et al. 1987)
 319 (20°C, EPICS-GC, Yurteri et al. 1987)
 273 (20°C, calculated-P/C, Yurteri et al. 1987)
 365* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = 3.469 - 2689/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 460 (computer value, Yaws et al. 1991)
 324* (extrapolated from equilibrium headspace-GC data, measured range 45–80°C, Ettre et al. 1993)
 $\log (1/K_{\text{AW}}) = -2.9050240 + 1129.8083/(T/K)$; temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)
 288 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 315 (gas stripping-GC, Shiu & Mackay 1997)
 293 (headspace equilibrium-GC, de Wolf & Lieder 1998)
 277.2 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)
 537 (modified EPICS method-GC, Ryu & Park 1999)
 297 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 4.225 - 1507/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
 384* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)
 $\ln K_{\text{AW}} = 10.04 - 3359.7/(T/K)$; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 2.84 (Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1985)
 2.81 (calculated-fragment constant, Rekker 1977)
 2.18 (¹⁴C- LSC, Lu & Metcalf 1975)
 2.84, 2.46, 2.18 (Hansch & Leo 1979)
 2.79 (HPLC-RT correlation, Veith et al. 1979b)
 2.84 (HPLC- k' correlation, Könemann et al. 1979)
 2.80 (HPLC- k' correlation, Hanai et al. 1981)
 2.81 (HPLC- k' correlation, D'Amboise & Hanai 1982)
 2.83 (shake flask-HPLC, Hammers et al. 1982)
 2.18 (HPLC- k' correlation, Miyake & Terada 1982)
 2.80 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983a)
 2.98 (generator column-HPLC/UV, Wasik et al. 1983)
 2.98 (generator column-GC/ECD, Miller et al. 1984; 1985)
 2.81–2.84 (HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)
 2.49 (HPLC- k' correlation, Haky & Young 1984)
 3.00 (HPLC- k' correlation, De Kock & Lord 1987)
 2.898 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 2.784 ± 0.061 , 2.898 ± 0.004 (shake flask methods, interlaboratory studies, Brooks et al. 1990)
 2.65, 2.73; 2.84 (25°C, 60°C, shake flask-UV/VIS; quoted lit. at 25°C, Kramer & Henze 1990)
 2.86, 3.02 (centrifugal partition chromatography, Gluck & Martin 1990)
 2.84 (recommended, Sangster 1993)
 2.89 (recommended, Hansch et al. 1995)
 2.98 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
 2.96 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
 3.05* (estimated-RP-HPLC- k' correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.45* (20°C, HPLC- k' correlation, measured range 10–50°C, Su et al. 2002)
 $\log K_{\text{OA}} = 43910/(2.303\cdot\text{RT}) - 4.107$; temp range 10–50°C (HPLC- k' correlation, Su et al. 2002)

Bioconcentration Factor, $\log \text{BCF}$:

- 2.65 (fathead minnow, Veith et al. 1979b, 1980)
 1.30 (Kenaga 1980a)

- 1.08 (fish, flowing water, Kenaga & Goring 1980)
- 2.21 (microorganisms-water, Mabey et al. 1982)
- 1.70 (algae, Freitag et al. 1984, 1985; Halfon & Reggiani 1986)
- 1.88 (fish, Freitag et al. 1984; Halfon & Reggiani 1986)
- 3.23 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
- 1.85 (fish, Freitag et al. 1985)
- 3.23 (activated sludge, Freitag et al. 1985)
- 1.93 (fish, calculated, Figueroa & Simmons 1991)

Sorption Partition Coefficient, log K_{OC} :

- 2.52 (sediment, Mabey et al. 1982)
- 2.18 (Kenaga 1980a)
- 2.59 (field data, Roberts et al. 1980; Schwarzenbach & Westall 1981; quoted, Voice & Weber 1985)
- 1.84 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 1.73–2.99 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 2.44, 2.50 (calculated from K_{OW} , Schwarzenbach & Westall 1981)
- 2.73 (soil, calculated- K_{OW} , Calamari et al. 1983)
- 2.10 (calculated-MCI χ , Koch 1983)
- 2.92 (calculated- K_{OW} , Yoshida et al. 1983b)
- 2.60 (Offshore Grand Haven sediment, batch equilibrium-sorption isotherm, Voice & Weber, Jr. 1985)
- 2.44 (calculated-MCI χ , Bahnick & Doucette 1988)
- 1.92–2.59 (soil, Howard 1989)
- 2.50; 2.17 (Captina silt loam, OC 1.49%, pH 4.17; McLaurin sandy loam, OC 0.66%, pH 4.42, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 2.34 (calculated-MCI χ , Sabljic et al. 1995)
- 2.19, 2.20 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 1.97, 2.14, 1.77 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM} :

- 1.68 (Woodburn soil, organic matter 1.9%, batch equilibrium-sorption isotherm-GC/ECD, Chiou et al. 1983)
- 2.10, 2.32 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: estimated $t_{1/2} \sim 1$ –12 h from a flowing stream (Cadena, 1984; selected, Howard 1989);
 $k = 0.033 \text{ d}^{-1}$ with $t_{1/2} = 21 \text{ d}$ in spring at 8–16°C, $k = 0.152 \text{ d}^{-1}$ with $t_{1/2} = 4.6 \text{ d}$ in summer at 20–22°C,
 $k = 0.053 \text{ d}^{-1}$ with $t_{1/2} = 13 \text{ d}$ in winter at 3–7°C for periods when volatilization appears to dominate, and
 $k = 0.08 \text{ d}^{-1}$ with $t_{1/2} = 8.9 \text{ d}$ with HgCl_2 in September 9–15, 1980 in marine mesocosm experiments;
estimated half-lives from soil: $t_{1/2} = 0.3 \text{ d}$ of 1-cm depth and $t_{1/2} = 12.6 \text{ d}$ for 10 cm depth (Wakeham et al. 1983).
- Photolysis: not environmentally significant or relevant (Mabey et al. 1982);
photolysis $k = 1.1 \times 10^{-5} \text{ d}^{-1}$ with an estimated $t_{1/2} \sim 170 \text{ yr}$ by sunlight in surface water at 40°N in the summer (Dulin et al. 1986)
 $t_{1/2} = 21 \text{ d}$ under sunlight in water (Mansour & Feicht 1994).
- Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
photooxidation $t_{1/2} = 1553$ –62106 h in water, based on a measured rate for hydroxy radicals in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)
 $k_{OH} = 9.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 13 d, loss of 7.4% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)
 $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 radical (Mabey et al. 1982)
 $k = (0.75 \pm 0.2)3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k = 2.88 \times 10^{-3} \text{ h}^{-1}$ in air (Yoshida et al. 1983b; selected, Mackay et al. 1985)

$k_{\text{OH}} = (8.8 \pm 1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with estimated atmospheric lifetime $\tau = 13 \text{ d}$ and $k_{\text{O}_3} < 5 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with lifetime $\tau > 8.8 \text{ yr}$ at room temp. (relative rate method, Atkinson et al. 1985)

$k_{\text{OH}}(\text{obs.}) = 9.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{\text{OH}}(\text{calc}) = 1.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}} = (5.5 \pm 4.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 23.5°C with an atmospheric lifetime $\tau = 21 \text{ d}$ (relative rate method, Edney et al. 1986)

$k_{\text{OH}} = 9.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 17 \text{ d}$ for reaction with OH radical, concn of $5.0 \times 10^5 \text{ molecule/cm}^3$ at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs}) = 0.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^* = (7.41 \pm 0.94) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{\text{OH}} = 7.41 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 9.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k = (4.3\text{--}4.6) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{\text{OH}} = 7.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982);

base rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ with $t_{1/2} > 900 \text{ yr}$, based on assumed base mediated 1% disappearance after 16 d at 85°C and pH 9.7 (Ellington et al. 1988).

$t_{1/2} > 879 \text{ yr}$ based on rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Ellington et al. 1988)

Biodegradation: significant degradation on anaerobic environment with $k = 0.5 \text{ d}^{-1}$ (Tabak et al. 1981; Mills et al. 1982)

$k = 1.88 \times 10^{-4} \text{ h}^{-1}$ in air, and $k = 3.83 \times 10^{-4} \text{ h}^{-1}$ in sediments (Lee & Ryan 1979; selected, Mackay et al. 1985)

$k = 0.24 \text{ L d}^{-1}$ in air, no degradation in water and on the ground (Neely 1982);

$k = 0.07\text{--}0.3 \text{ d}^{-1}$ in river water; $k = 0.04\text{--}0.2 \text{ d}^{-1}$ in estuary water; and $k = 0.01 \text{ d}^{-1}$ in marine water (Bartholomew & Pfaender 1983; selected, Battersby 1990)

$k = 0.033 \text{ d}^{-1}$, $t_{1/2} = 21 \text{ d}$ in spring at 8–16°C, $k = 0.152 \text{ d}^{-1}$, $t_{1/2} = 4.6 \text{ d}$ in summer at 20–22°C, $k = 0.053 \text{ d}^{-1}$, $t_{1/2} = 13 \text{ d}$ in winter at 3–7°C, and $k = 0.08 \text{ d}^{-1}$, $t_{1/2} = 8.9 \text{ d}$ with HgCl_2 in September 9–15, 1980 in marine mesocosm system (Wakeham et al. 1983)

$t_{1/2} = 4.6\text{--}21 \text{ d}$ in marine mesocosm (Wakeham et al. 1983);

$t_{1/2} = 7.9 \text{ d}$ in activated sludge (estimated, Freitag et al. 1985, quoted, Anderson et al. 1991);

$k = 0.07 \text{ yr}^{-1}$ with $t_{1/2} = 37 \text{ d}$ (Olsen & Davis 1990)

$t_{1/2}(\text{aq. aerobic}) = 1632\text{--}3600 \text{ h}$, based on unacclimated aerobic river dieaway tests; $t_{1/2}(\text{aq. anaerobic}) = 6528\text{--}14400 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation: $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1), and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photodecomposition $t_{1/2} = 8.7 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976); residence time of 13 d, loss of 7.4% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

estimated atmospheric lifetime $\tau = 13 \text{ d}$ due to reaction with OH radical and $\tau > 8.8 \text{ yr}$ due to reaction with O_3 (Atkinson et al. 1985);

$t_{1/2} = 72.9\text{--}729 \text{ h}$, based on photooxidation half-life in air (Howard et al. 1991).

Surface Water: $t_{1/2} = 0.3 \text{ d}$ in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 75 \text{ d}$ for an estuarine river with near natural conditions at 22°C (Lee & Ryan 1976);

rate constants: $k = 0.033 \text{ d}^{-1}$, $t_{1/2} = 21 \text{ d}$ in spring at 8–16°C, $k = 0.152 \text{ d}^{-1}$, $t_{1/2} = 4.6 \text{ d}$ in summer at 20–22°C, $k = 0.053 \text{ d}^{-1}$, $t_{1/2} = 13 \text{ d}$ in winter at 3–7°C for periods when volatilization appears to dominate, and $k = 0.08 \text{ d}^{-1}$, $t_{1/2} = 8.9 \text{ d}$ with HgCl_2 in September 9–15, 1980 in marine mesocosm experiments (Wakeham et al. 1983)

$t_{1/2} = 1632\text{--}3600$ h, based on unacclimated aerobic river dieaway tests (Howard et al. 1991)

photolysis $t_{1/2} = 21$ d under sunlight in water (Mansour & Feicht 1994).

Groundwater: $t_{1/2} = 3264\text{--}7200$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} = 75$ d (Lee & Ryan 1976, 1979; quoted, Anderson et al. 1991).

Soil: disappearance $t_{1/2} = 2.1$ d from testing soils (Anderson et al. 1991);

$t_{1/2} = 1632\text{--}3600$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 6.1.1.1.1

Reported aqueous solubilities of chlorobenzene at various temperatures

1.

Kisarov 1962		Nelson & Smit 1978		Schwarz & Miller 1980		Horvath & Getzen 1985	
shake flask		vapor equil.-UV spec.		elution chromatography		recommended values	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
30	490	5	40	10	440	10	454
40	705	25	106.8	20	420	15	452
50	960	35	400.5	30	490	20	466
60	1100	45	471.3	shake flask UV		25	495
70	1605			10	460	30	539
80	1805			20	450	35	600
90	2500			30	500	40	677
						45	771
						50	882
						55	1011
						60	1158
						65	1324
						70	1509
						75	1713
						80	1937
						90	2447

2.

Cooling et al. 1992		Ma et al. 2001		Finizio & Di Guardo 2001	
shake flask-GC/MS		shake flask-GC		RP-HPLC- k' correlation	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	482	5	496	5	426
30	608	15	429	15	427
40	840	25	470	35	511
50	1263	35	538		
		45	546		

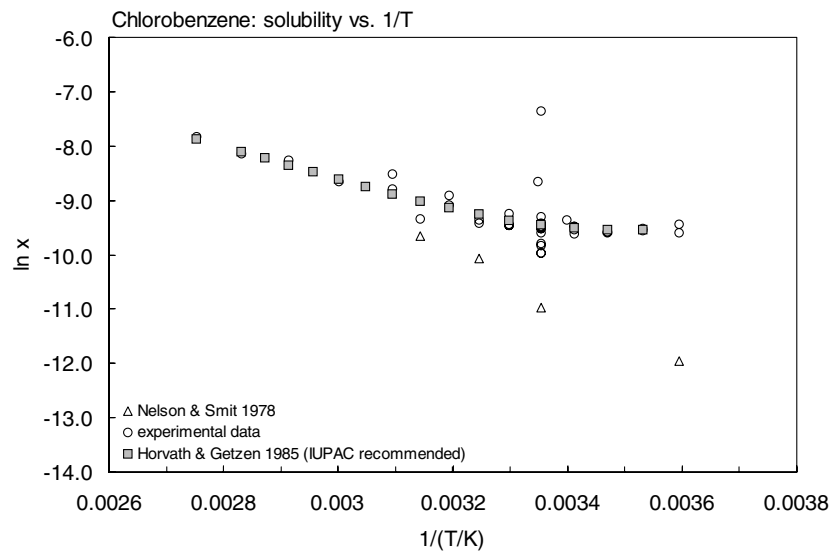


FIGURE 6.1.1.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.2
Reported vapor pressures of chlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Dreisbach & Shrader 1949		Brown 1952		Liu & Dickhut 1994	
summary of lit. data		ebulliometry		ebulliometry		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−13.0	133.3	56.28	7605	62.04	9657	−14.2	66.9
10.6	666.6	63.05	10114	62.06	9663	−5.0	167
22.2	1333	75.22	16500	66.38	11558	10	501
35.3	2666	101.85	42066	74.13	15720	25	1410
49.7	5333	117.30	67661	89.06	27246	40	3270
58.3	7999	131.70	101325	94.04	32276		
70.0	13332			98.79	37961		
89.4	26664			110.35	54794	$\Delta H_v = 35.6 \text{ kJ/mol}$	
110	53329	mp/°C	−45.58	121.1	69774		
132.2	101325	bp/°C	131.67	126.18	87018	$\Delta H_{\text{subl}} = 35.6 \text{ kJ/mol}$	
				130.37	97684		
mp/°C	−45.2	eq. 2	P/mmHg	131.7	101263		
		A	7.18473				
		B	1556.6	eq. 2	P/mmHg		
		C	230	A	6.99893		
				B	1444.75		
				C	219.13		

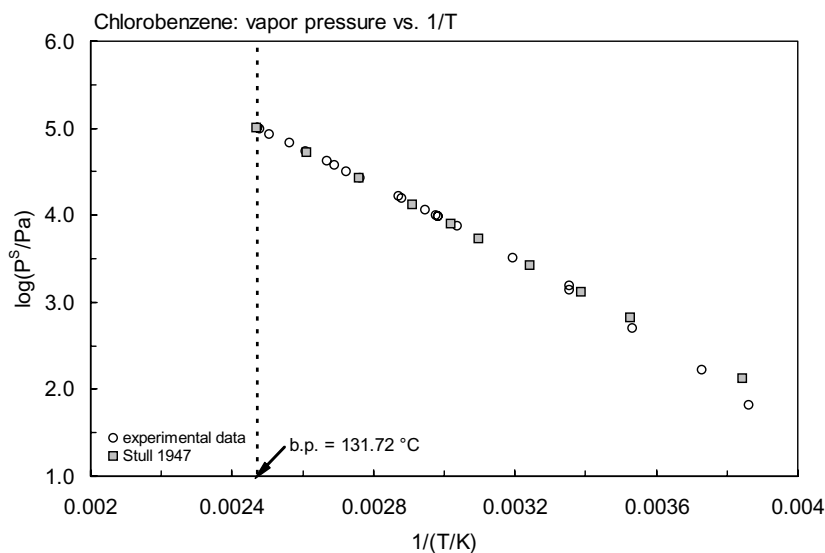


FIGURE 6.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.3

Reported Henry's law constants of chlorobenzene at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln k_H = A - B/(T/K)$	(3)	$\log k_H = A - B/(T/K)$	(3a)
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

1.

Leighton & Calo 1981		Ashworth et al. 1988		Ettre et al. 1993		Görgényi et al. 2002	
equilibrium cell-concn ratio		EPICS-GC		equilibrium headspace-GC		EPICS-SPME method	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
1	124	10	247	45	621	2	112
3	125	15	285	60	863	6	155.5
12.4	190	20	346	70	1114	10	183.6
12.5	206	25	365	80	1579	18	283.2
17.9	243	30	479			25	384
19.1	280					30	472.8
22.7	271	eq. 4	H/(atm m ³ /mol)	eq. 2a	1/K _{AW}	40	755.8
23	321	A	3.469	A	2.905024	50	1046
		B	2689	B	1129.8083	60	1420
eq. 3	k _H /atm					70	1804
A	18.46					eq. 1	K _{AW}
B	3751					A	10.04
						B	3359.7

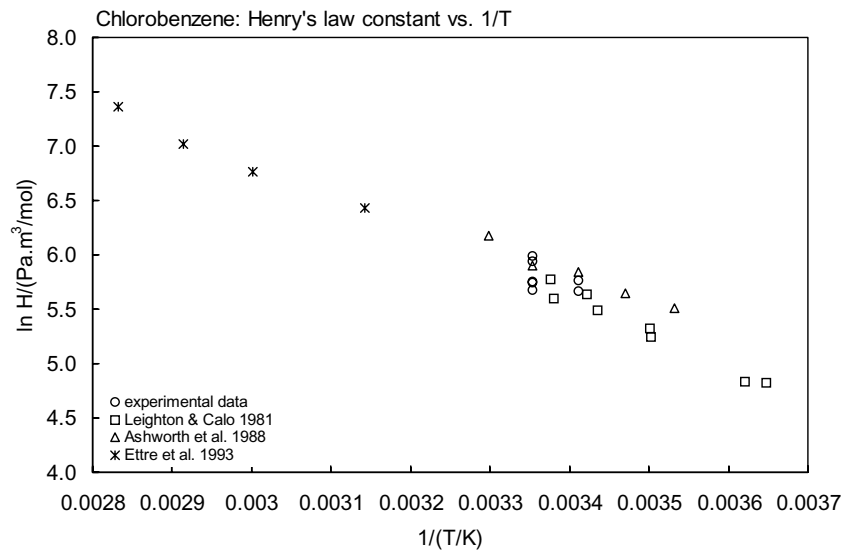


FIGURE 6.1.1.1.3 Logarithm of Henry’s law constant versus reciprocal temperature for chlorobenzene.

TABLE 6.1.1.1.4
Reported octanol-water and octanol-air partition coefficients of chlorobenzene at various temperatures

log K _{OW}		log K _{OA}	
Finizio & Di Guardo 2001		Su et al. 2002	
GC-RT correlation		GC-RT correlation	
t/°C	log K _{OW}	t/°C	log K _{OA}
5	3.19	10	3.76
15	3.15	20	3.45
25	3.05	30	3.17
35	3.04	40	2.90
		50	2.65
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 43.91$			
$\log K_{OA} = A + B/T$			
A		− 4.107	
B		43910	

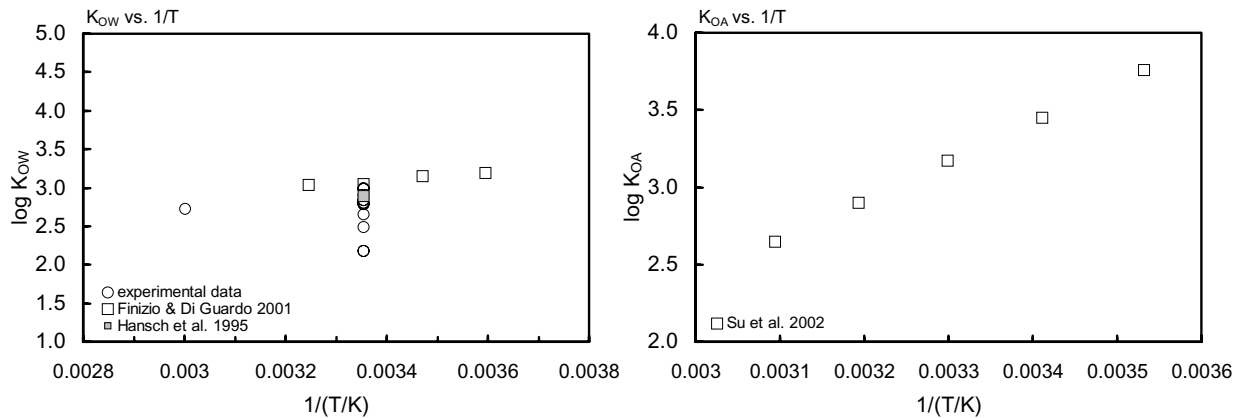
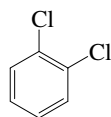


FIGURE 6.1.1.1.4 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for chlorobenzene.

6.1.1.2 1,2-Dichlorobenzene



Common Name: 1,2-Dichlorobenzene

Synonym: *o*-dichlorobenzene, dowerm E

Chemical Name: 1,2-dichlorobenzene

CAS Registry No: 95-50-1

Molecular Formula: $C_6H_4Cl_2$

Molecular Weight: 147.002

Melting Point ($^{\circ}C$):

-17.0 (Pirsch 1956; Dreisbach 1955; Weast 1972-73; 1982-83; Lide 2003)

Boiling Point ($^{\circ}C$):

180 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.3048 (Weast 1972-73; Horvath 1982)

1.3059 (Lide 2003)

Molar Volume (cm^3/mol):

112.6 ($20^{\circ}C$, calculated-density)

137.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.93 (Weast 1972-73)

Entropy of Fusion, ΔS_{fus} (J/mol K):

50.46 (Pirsch 1956)

50.63 (Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$, F: 1.0 (Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

145* (volumetric, measured range $20-60^{\circ}C$, Klemenc & Low 1930; Seidell 1941)

< 260 (residue-volume method, Booth & Everson 1948)

92.7 (Landolt-Börnstein 1951)

79.0 (shake flask-radiolabeled ^{14}C -LSC, Metcalf et al. 1975)

148* ($20^{\circ}C$, shake flask-GC/ECD, measured $0-34^{\circ}C$, Chiou & Freed 1977)

92.8 (shake flask-UV, Yalkowsky et al. 1979)

154 (shake flask-LSC/ ^{14}C , Veith et al. 1980)

128, 124* ($20^{\circ}C$; elution chromatography, UV, Schwarz & Miller 1980)

155.8 (shake flask-LSC, Banerjee et al. 1980; Banerjee 1985)

99.1 (shake flask-GC, Könemann 1981)

92.6 (recommended, Horvath 1982)

154 (shake flask-GC, Chiou et al. 1982, 1983; Chiou 1981, 1985; Chiou & Schmedding 1981)

125 (quoted average, Yalkowsky et al. 1983)

92.3 (generator column-GC, Miller et al. 1984, 1985)

137 (shake flask-HPLC, Banerjee 1984)

147* (recommended, temp range $0-60^{\circ}C$, IUPAC Solubility Data Series, Hovath & Getzen 1985)

$S/(g/kg) = 19.2314 - 1.81140 \times 10^{-1} \cdot (T/K) + 5.6509 \times 10^{-4} \cdot (T/K)^2 - 5.77683 \times 10^{-7} \cdot (T/K)^3$, temp range 273-333 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

169 (shake flask-radiometry, Lo et al. 1986)

156 (quoted lit. average, Riddick et al. 1986; Howard 1989)

31* ($19.5^{\circ}C$, shake flask-GC/TC, measured range $0-90^{\circ}C$, Stephenson 1992)

145 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)

- 159.2 (shake flask-GC/ECD, Tam et al. 1996)
 144 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 109 (shake flask-GC, Boyd et al., 1998)
 92, 93, 137; 97 (quoted lit. values; solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
 $\ln x = -31.5289 + 3834/(T/K) + 8.7172 \times 10^{-5} \cdot (T/K)^2$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 149* ± 8.2 (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)
 140, 124, 158 (5, 15, 25°C, estimated-RP-HPLC- k' correlation, Finizio & Di Guardo 2001)
 93.7* (generator column-GC/ECD, measured range 15–55°C, Oleszek-Kudlak et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 137* (20°C, summary of literature data, Stull 1947)
 $\log (P/\text{mmHg}) = 7.32585 - 1824.6/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)
 5010* (56.28°C, ebulliometry, measured range 87.02–180.48°C, Dreisbach & Shrader 1949)
 171 (calculated by formula., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 6.92400 - 1538.3/(200.0 + t/^\circ\text{C})$; temp range 80–250°C (Antoine eq. for liquid state, Dreisbach 1955)
 25234* (130.82°C, ebulliometry, measured range 130.82–181.62°C, McDonald et al. 1959)
 196 (extrapolated, Antoine eq., Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 10943.0/(T/K)] + 8.185275$; temp range 20–179°C (Antoine eq., Weast 1972–73)
 174, 197 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
 224.87*; 132, 188 (27.8°C reported; 20°C, 25°C, extrapolated-Antoine eq. from gas saturation-GC measurement, temp range 27.8–70°C, Grayson & Fosbraey 1982)
 $\log (P/\text{Pa}) = 25.4 - 6013/(T/K)$, temp range 27.8–70°C (gas saturation-GC, Grayson & Fosbraey 1982)
 $\log (P/\text{kPa}) = 6.13305 - 1599.034/(206.964 + t/^\circ\text{C})$; temp range 87.2–180.5°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.26861 - 1704.435/(219.409 + t/^\circ\text{C})$; temp range 130.8–181.62°C (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1984)
 197 (extrapolated, Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.14378 - 1704.49/(219.42 + t/^\circ\text{C})$; temp range 131–181°C (Antoine eq., Dean 1985, 1992)
 201.4 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
 198 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.26918 - 1705.55/(-52.56 + T/K)$; temp range 373–453 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
 164* (gas saturation, measured range –15 to 40°C, Liu & Dickhut 1994)
 137.3*; 188 (pressure gauge measured at 20.35°C, 25°C, interpolated from reported Antoine eq., Polednicek et al. 1996)
 $\ln (P/\text{Pa}) = 21.5929 - 4053.86/[(T/K) - 50.2328]$; temp range 256–422 K (Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
 252; 185 (supercooled liquid P_L , GC-Kovács retention indices correlation; quoted lit., Spieksma et al. 1994)
 $\log (P/\text{mmHg}) = 31.3614 - 3.5226 \times 10^3/(T/K) - 7.8886 \cdot \log (T/K) - 2.2250 \times 10^{-10} \cdot (T/K) + 1.1842 \times 10^{-6} \cdot (T/K)^2$, temp range 256–705 K (Yaws 1994)
 5729* (90.193°C, comparative ebulliometry, measured range 90.193–181.633°C, Roháč et al. 1998)
 133.8* (20°C, recommended, summary of literature data, temp range 263.15–463.15 K, Roháč et al. 1999)
 $\ln [(P/\text{Pa})/6.80] = [1 - (T/K)/256.10] \cdot \exp\{3.359374 - 8.5641422 \times 10^{-4} \cdot (T/K) + 6.0235167 \times 10^{-7} \cdot (T/K)^2\}$; temp range 256–445 K (Cox eq., recommended, Roháč et al. 1999)
 $\log (P/\text{kPa}) = 19.40 - 6013/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 248 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 375 (calculated-bond contribution, Hine & Mookerjee 1975)
 193 (batch air stripping-GC, Mackay & Shiu 1981)
 122 (20°C, gas stripping-GC, Oliver 1985)

- 197 (gas stripping, Warner et al. 1987)
 159* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = -1.518 - 1422/(T/K)$; temp range 10–30°C (EPICS-GC/FID, Ashworth et al. 1988)
 299 (computer value, Yaws et al. 1991)
 141 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 195 (gas stripping-GC, Shiu & Mackay 1997)
 212.7 (modified EPICS method-GC, Ryu & Park 1999)
 133 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 7.045 - 2636/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 3.55 (Hansch et al. 1968)
 3.38 (Leo et al. 1971; Hansch & Leo 1979, 1985)
 3.57 (calculated-fragment constants, Rekker 1977)
 3.55, 3.39 (shake flask-GC, HPLC- k' , Könemann et al. 1979)
 3.40; 3.75 (concentration ratio; HPLC-RT correlation, Veith et al. 1980)
 3.40 (shake flask-LSC, Banerjee et al. 1980)
 3.71, 3.18–4.36 (shake flask method: mean, range of mean values, OECD 1981)
 3.34 (shake flask-HPLC, Hammers et al. 1982)
 3.40 (shake flask-GC, Watarai et al. 1982)
 3.19, 3.19, 3.31, 3.53, 3.60, 3.84, 4.15, 4.36; 3.61 (shake flask; results of OECD/EEC laboratory comparison tests; mean value, Harnisch et al. 1983)
 3.34, 3.20; 3.61 (HPLC methods; OECD/EEC shake-flask method; Harnisch et al. 1983)
 3.61 (OECD/EEC shake-flask method, Harnisch et al. 1983)
 3.38 (generator column-HPLC/UV, Wasik et al. 1983)
 3.38 (generator column-GC, Miller et al. 1984, 1985)
 3.56 (HPLC-RV correlation, Garst 1984)
 3.433 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 3.49 (shake flask-GC, Pereira et al. 1988)
 3.38 (recommended, Sangster 1993)
 3.43 (recommended, Hansch et al. 1995)
 3.29 \pm 0.05 (shake flask-GC/ECD, Bahadur et al. 1997)
 3.29* (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)
 $\log K_{OW} = 0.1831 + 17800/[2.303\cdot R(T/K)]$; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
 3.447 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
 3.70 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 4.36*, 4.41 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
 $\log K_{OA} = -4.30 + 2574.0/(T/K)$; $\Delta H_{OA} = 49.3$ kJ/mol (generator column-GC, Harner & Mackay 1995)
 4.68 (solid-phase microextraction SPME-GC, Treves et al. 2001)
 $\log K_{OA} = -7.90 + 3304/(T/K)$, $\Delta H_{OA} = 63.3$ kJ/mol (SPME-GC, Treves et al. 2001)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

- 1.95 (bluegill sunfish, Veith et al. 1979b; 1980)
 2.19–2.48 (fish, calculated, Veith et al. 1980)
 1.95 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
 2.86 (microorganisms-water, Mabey et al. 1982)
 2.40–2.48 mean 2.43; 2.60–2.85 mean 2.74 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
 3.51–3.80 (rainbow trout, lipid-basis, Oliver & Niimi 1983)
 2.43–2.75 (fish, Oliver 1984)
 1.95 (correlated-flow through method, bluegill sunfish, Davis & Dobbs 1984)

- 1.60 (fish-normalized, Tadokoro & Tomita 1987)
 1.89 (fish, calculated-MCI χ , Sabljic 1987b)
 3.94, 4.46, 3.79, 3.82 (field data: Atlantic croaker, blue crabs, spotted sea trout, blue catfish, lipid-based, Pereira et al. 1988)
 2.4 \pm 0.1 (guppies, steady-state conditions, rate const. ratio k_1/k_2 , 96-h exposure, Sijm et al. 1993)
 3.5 \pm 0.1 (guppies, lipid normalized BCF, Sijm et al. 1993)
 2.70 (fathead minnow, steady-state conditions, rate const. ratio k_1/k_2 , 96-h exposure, Sijm et al. 1993)
 3.90 (fathead minnow, lipid normalized BCF, Sijm et al. 1993)
 1.95; 2.43, 2.75 (*Lepomis macrochirus*; *Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
 2.40; 2.70 (*Poecilla reticulata*; *Pimephales promelas*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
 2.43, 3.51; 2.333, 2.549 (quoted: whole fish, lipid content; calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)
 3.86; 3.84 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 2.26 (Willamette silt loam soil, 1.6% organic matter, equilibrium sorption isotherm measurement, Chiou et al. 1979)
 3.0, 2.96, 2.62 (calculated- K_{OW} , solubility C_L , C_S , Karickhoff 1981)
 4.60; 4.60; 3.00 (field data of sediment trap material, Niagara River organic matter, calculated from K_{OW} , Oliver & Charlton 1984)
 2.34, 2.59 (Lula aquifer 0.032% OC, Apalachee soil 1.4% OC, batch equilibrium-sorption isotherm, Stauffer & MacIntyre 1986)
 2.45 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 3.27, 2.04 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.43 (untreated Marlette soil B_t horizon, OC 0.30%, batch equilibrium, Lee et al. 1989)
 3.64, 3.52 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
 2.45–3.51 (aquifer materials, Stauffer et al. 1989)
 3.10, 2.90; 2.99 (Captina silt loam, OC 1.49% and pH 4.97, McLaurin sandy loam, OC 0.66%, pH 4.43; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
 2.36–2.61 (16 U.S. soils, 1.03–6.09% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
 2.37–2.51 (16 Chinese soils, 0.16–5.61% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
 2.48–2.76 (14 U.S. bed sediments, 0.4–2.20% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
 2.62–2.78 (21 Chinese bed sediments, 0.11–4.73% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
 2.36–2.63 (suspended solids from four U.S. rivers, 1.78–2.87% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
 2.48 (suspended solids from Yellow River, China, 0.30% OC, batch equilibrium-sorption isotherm, Kile et al. 1995)
 2.39, 2.40 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 3.69 \pm 0.74 (suspended particulate in coastal waters, Masunaga et al. 1996)
 2.50, 2.50, 2.47 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, 0.1 \leq OC $<$ 0.5%, average, Delle Site 2001)
 2.70, 2.69, 2.71 (sediments, organic carbon OC \leq 0.1%, OC \leq 0.5%, 0.1 \leq OC $<$ 0.5%, average, Delle Site 2001)

Sorption Coefficient, log K_{OM} :

- 2.25 (Willamette silt loam soil, 1.6% organic matter, equilibrium isotherm, Chiou et al. 1979; quoted, Howard 1989)
 2.27 (Woodburn silt loam soil, 1.9% organic matter, batch equilibrium-sorption isotherm-GC/ECD, Chiou et al. 1983)
 2.50 (soil, Chiou et al. 1983)
 2.26, 2.54 (quoted, calculated-MCI χ , Sabljic 1984)

- 2.89 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.47, 3.17 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.97 (untreated Marlette soil B_t horizon, OM 0.60%, equilibrium isotherm, Lee et al. 1989)
- 3.97, 3.50, 2.87 (organic cations treated Marlette soil B_t horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: experimental evaporation rate into air, $1.18 \times 10^{-6} \text{ g cm}^{-2} \text{ s}^{-1}$ (Chiou et al. 1980); estimated $t_{1/2} = 4.4 \text{ h}$ for a model river of 1-m depth with a flow rate of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: not environmentally significant (Mabey et al. 1982); rate constant $k = 1.22 \times 10^{-4} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO^- in the gas (Dilling et al. 1988).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical, and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} \sim 3.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $\ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 radical (Mabey et al. 1982)

$k_{\text{OH}} = (4.2 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{\text{O}_3} = 2.0 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K measured range 298–323 K (Atkinson & Carter 1984)

k_{OH} (obs.) = $4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and k_{OH} (calc) = $4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

k_{OH} (calc) = $4.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, k_{OH} (obs) = $4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = 4.07 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 22–27°C (Dilling et al. 1988)

$k = (3.7\text{--}4.0) \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

k_{OH} (calc) = $4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous solutions (Haag & Yao 1992)

k_{OH} (calc) = $0.48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982).

base rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C with a calculated $t_{1/2} > 900 \text{ yr}$ at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

Biodegradation: $t_{1/2}$ (aq. aerobic) = 672–4320 h, based on unacclimated soil grab sample data, and aerobic screening test data (Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 2880–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

significant degradation in an aerobic environment with $k = 0.05 \text{ d}^{-1}$ (Tabak et al. 1981; Mills et al. 1982); in a continuous flow of activated sludge system; virtually 100% (78% biodegradation and 22% stripping) was observed (Kincannon et al. 1983; selected, Howard 1989).

Biotransformation: $1 \times 10^{-10} \text{ ml cell}^{-1} \text{ h}^{-1}$ (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1), and Elimination (k_2) Rate Constants:

$k_1 = 870 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 3.90 \text{ d}^{-1}$ (guppy, 96-h exposure., Sijm et al. 1993)

$k_1 = 635 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 1.40 \text{ d}^{-1}$ (fathead minnow, 96-h exposure, Sijm et al. 1993)

Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 152.8\text{--}1528 \text{ h}$, based on the photooxidation half-life in air. (Howard et al. 1991)

Surface water: $t_{1/2} = 1.2\text{--}37 \text{ d}$ estimated from field data at various locations in the Netherlands, $t_{1/2} = 0.3\text{--}3 \text{ d}$ for river, $t_{1/2} = 3\text{--}30 \text{ d}$ for lakes (Zoeteman et al. 1980)

$t_{1/2} = 672\text{--}4320 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Groundwater: $t_{1/2} = 30\text{--}300 \text{ d}$, estimated from persistence in water (Zoeteman et al. 1980);

$t_{1/2} \sim 1$ yr estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)

$t_{1/2} = 1344\text{--}8640$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on unacclimated aerobic screening test data (Howard et al. 1991)

disappearance $t_{1/2} = 4.0$ d in testing soils (Anderson et al. 1991).

Biota: $t_{1/2} < 1$ d in fish (Veith et al. 1980);

$t_{1/2} < 1$ d bluegill sunfish. (Barrows et al. 1980);

$t_{1/2} < 5$ d in worms at 8°C (Oliver 1987a);

biological half-lives: $t_{1/2} < 1$ d in trout muscle, $t_{1/2} < 1$ d in sunfish and $t_{1/2} < 1$ d in guppy for dichlorobenzenes (Niimi 1987).

TABLE 6.1.1.2.1

Reported aqueous solubilities of 1,2-dichlorobenzene at various temperatures

1.

Klemenc & Löw 1930		Chiou & Freed 1977		Schwarz & Miller 1980		Horvath & Getzen 1985	
volumetric method		shake flask-GC		elution chromatography		recommended values	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	134	0	133	10	169	0	142
25	145	20	148	20	128	5	135
30	161	34	162	shake flask-UV		10	133
35	183			10	156	15	134
40	194			20	124	20	139
45	203					25	147
55	223					30	157
60	232					35	169
						40	182
						45	197
						50	212
						55	228
						60	243

2.

Stephenson 1992		Ma et al. 2001		Finizio & Di Guardo 2001		Oleszek-Kudlak et al. 2004	
shake flask-GC		shake flask-GC/FID		RP-HPLC- k' correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
0	50	5	127	5	140	25	93.7
19.5	31	15	132	15	124	25	94.4
40	17	25	149	35	158	35	108.0
50	24	35	162			45	122.7
60.5	54	45	204			55	130.1
70.7	55						
80.0	91						
90.5	83						

$\Delta H_{\text{sol}} = 10.49$ kJ/mol

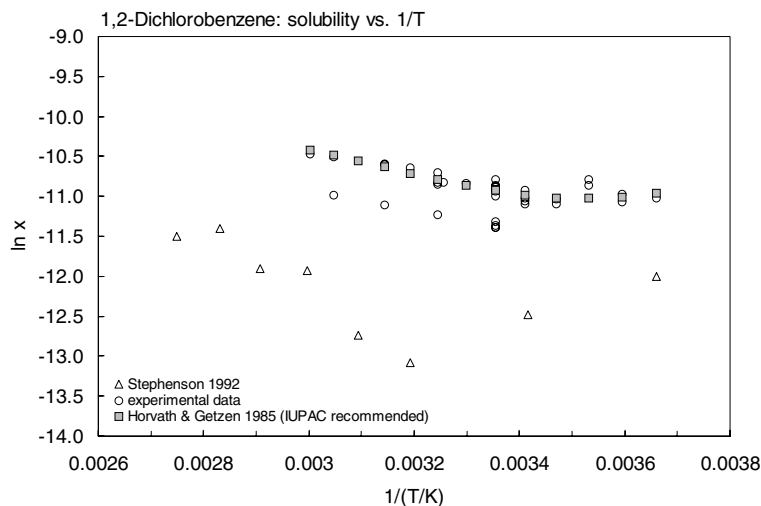


FIGURE 6.1.1.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,2-dichlorobenzene.

TABLE 6.1.1.2.2

Reported vapor pressures of 1,2-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln (P/\text{Pa}) = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_0) = (1 - T/T_0) \cdot \exp[\sum A_i T^i]$	(5) - Cox eq.		

1.

Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959		Grayson & Fosbraey 1982	
summary of lit. data		ebulliometry		ebulliometry		gas saturation-GC	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
20	133.3	87.02	5010	130.82	25234	20.0	132
46	666.6	97.66	7605	154.83	51778	27.8	224.8
59.1	1333	104.94	10114	178.66	96998	32.0	282.8
73.4	2666	118.32	16500	179.73	99614	41.5	599.3
89.4	5333	147.6	42066	180.54	101655	48.6	780.1
99.5	7999	164.65	67661	181.62	104322	56.3	1253
112.9	13332	180.48	101325			61.1	1645
133.4	26664			mp/ $^{\circ}\text{C}$	-17.0	70.0	2636
155.8	53329						
180	101325	eq. 2	P/mmHg	eq. 2	P/mmHg		
		A	7.32585	A	7.07028	eq. 1	P/Pa
mp/ $^{\circ}\text{C}$	-17.6	B	1824.6	B	1649.55	A	25.4
		C	230	C	213.314	B	6013

TABLE 6.1.1.2.2 (Continued)

2.

Liu & Dickhut 1994		Polednicek et al. 1996		Roháč et al. 1998		Roháč et al. 1999	
gas saturation-GC		pressure gauge		comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
-14.2	7.73	-16.65	7.056	90.193	5729	263.15	12.9
-5.0	14.7	-16.65	7.042	99.529	8333	273.15	30.1
10	56.1	-9.75	13.175	99.53	8335	283.15	65.4
25	164	-9.75	13.195	107.0	11074	283.15	133.8
40	448	0.30	30.815	113.265	13917	303.15	259.1
		10.32	67.088	118.61	16800	313.15	477.9
		20.35	137.3	118.61	16799	232.15	843.3
$\Delta H_v/(\text{kJ mol}^{-1}) = 51.2$		30.28	264.39	124.14	20290	333.15	1430
		40.24	485.45	129.935	24569	343.25	2338
exptl data fitted to the		50.15	848.67	135.547	29394	353.15	3699
modified Watson correlation		60.15	1440.7	141.024	34818	363.15	5681
		60.15	1442.0	146.292	40757	373.15	8491
		70.05	2313.0	146.292	40761	383.15	12380
		70.05	2318.6	151.657	47825	393.15	17640
		80.02	3660.3	160.102	60273	403.15	24630
		80.03	3661.2	168.184	74765	413.15	33720
		88.75	5428.4	176.912	93403	423.15	45370
		88.75	54284	178.845	97970	433.15	60070
		89.94	5606.9	181.633	104893	443.15	78370
		89.94	5601.2			453.15	10080
		98.79	8102.5	bp/°C	180.190	463.15	12810
		98.79	8104.0				
		108.76	11826	eq. 3	P/kPa	Cox eq.	
		118.8	16870	A	6.16161	eq. 5	
		128.19	23583	B	1612.27	A ₀	3.359374
		138.83	32396	C	-64.447	10 ⁻⁴ A ₁	-8.5641422
		148.91	43690			10 ⁻⁷ A ₂	6.0235167
						T ₀ /K	256.10
		eq. 3a	P/Pa			P ₀ /Pa	6.80
		A	21.5929			bp/K	453.35
		B	4053.86			temp range	256–445 K
		C	-50.2358				

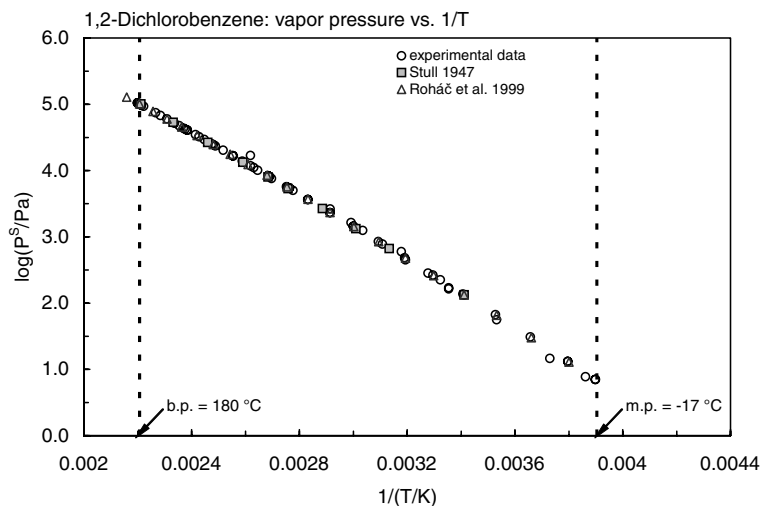


FIGURE 6.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2-dichlorobenzene.

TABLE 6.1.1.2.3

Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,2-dichlorobenzene at various temperatures and temperature dependence equations

Henry's law constant		log K_{OW}		log K_{OA}			
Ashworth et al. 1988		Bahadur et al. 1997		Harner & Mackay 1995		Su et al. 2002	
EPICS		shake flask-GC/ECD		generator column-GC		GC-RT correlation	
t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OW}	t/°C	log K_{OA}	t/°C	log K_{OA}
10	165	5	3.51	-10	5.51	10	4.6
15	145	15	3.41	0	5.16	20	4.27
20	170	25	3.29	10	4.82	30	3.96
20	159	35	3.2	20	4.51	40	3.67
30	240	45	3.09			50	3.4
ln H = A - B/(T/K)		enthalpy of transfer		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 49.3$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 57.02$	
		$\Delta H/(\text{kJ mol}^{-1}) = -17.8$.			
H/(atm m ³ /mol)				log $K_{OA} = A + B/RT$		log $K_{OA} = A + B/2.303RT$	
A	-1.518	log $K_{OW} = A - \Delta H/2.303RT$		A	-4.3	A	-5.856
B	1422	A		B	2574	B	57020
		ΔH					
		-17800					

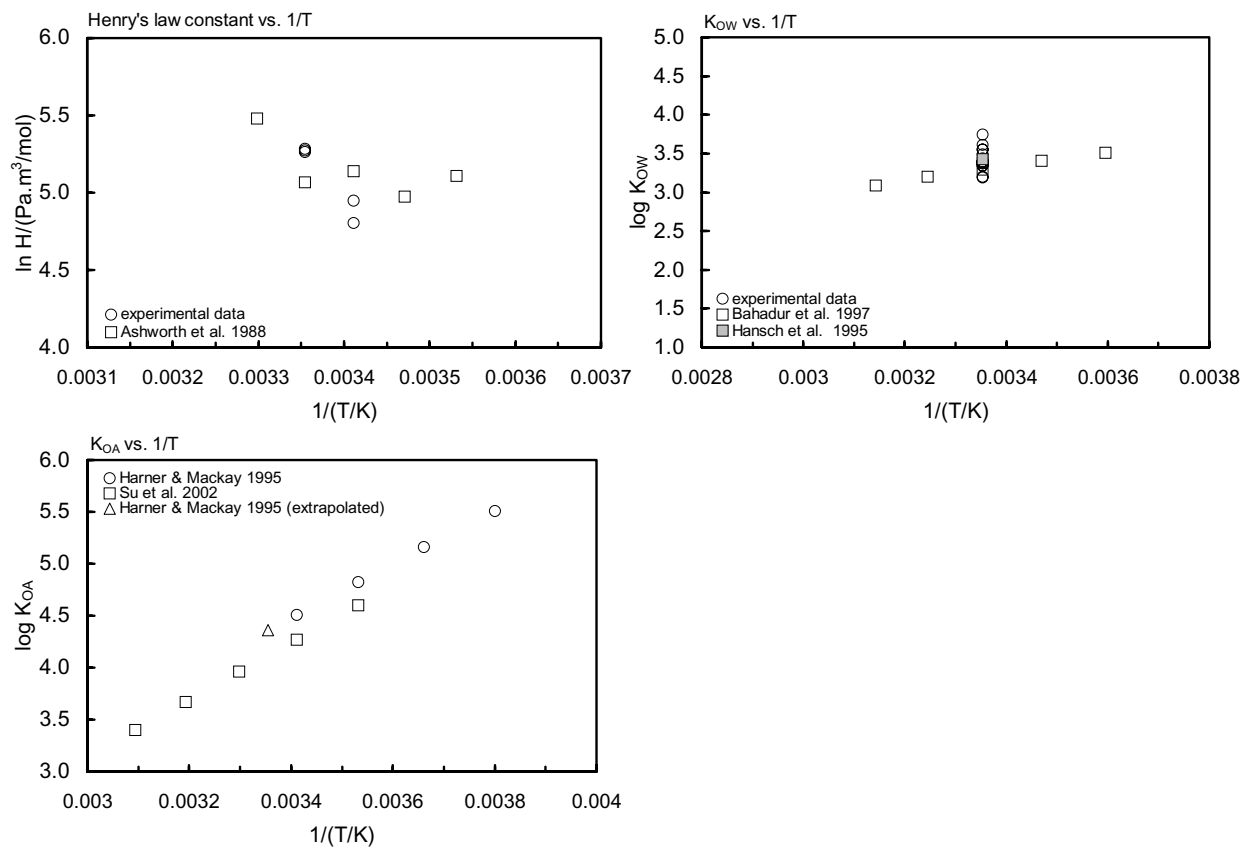
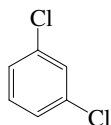


FIGURE 6.1.1.2.3 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for 1,2-dichlorobenzene.

6.1.1.3 1,3-Dichlorobenzene



Common Name: 1,3-Dichlorobenzene

Synonym: *m*-dichlorobenzene

Chemical Name: 1,3-dichlorobenzene

CAS Registry No: 541-73-1

Molecular Formula: C₆H₄Cl₂

Molecular Weight: 147.002

Melting Point (°C):

-24.8 (Lide 2003)

Boiling Point (°C):

173 (Lide 2003)

Density (g/cm³ at 20°C):

1.2884 (Dreisbach 1955; Weast 1972–73; Horvath 1982; Lide 2003)

Molar Volume (cm³/mol):

114.1 (20°C, calculated-density)

137.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.64 (Weast 1972–73)

Entropy of Fusion, ΔS_{fus} (J/mol K):

50.63 (Pirsch 1956)

51.46 (Yalkowsky 1979)

51.05 (Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

123* (volumetric, measured range 20–60°C, Klemenc & Löw 1930)

123.5 (Ginnings et al. 1939)

124 (Landolt-Börnstein 1951)

101.26* (shake flask-UV, measured range 10–35°C, Vesala 1973)

102.9 (shake flask-UV, Vesala 1974)

119.5 (shake flask-UV, Yalkowsky et al. 1979)

131 (shake flask-LSC-¹⁴C, Veith et al. 1980)

144*, 149 (23.5°C, elution chromatography, measured range 10–30°C, Schwarz 1980)

111, 89, 113, 101 (20°C, quoted, UV, elution chromatography, average exptl. value, Schwarz & Miller 1980)

133.5 (shake flask-LSC, Banerjee et al. 1980)

68.6 (shake flask-GC, Könemann 1981)

134 (shake flask-GC/ECD, Chiou & Schmedding 1981; Chiou et al. 1982, 1983; Chiou 1985)

124 (recommended, Horvath 1982)

124.5 (generator column-GC/ECD, Miller et al. 1984, 1985)

143 (shake flask-HPLC, Banerjee 1984)

106* (recommended, temp range 10–60°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)

S/(g/kg) = 27.6827 – 2.61597 × 10⁻¹·(T/K) + 8.19706 × 10⁻⁴·(T/K)² – 8.4698 × 10⁻⁷·(T/K)³, temp range 283–333 K
(regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

110 (Dean 1985)

111 (20°C, Riddick et al. 1986)

130 (20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

123; 138 (quoted lit.; shake flask-GC, Boyd et al. 1998)

126* \pm 6.1 (shake flask-GC/FID, measured range 5–45°C, Ma et al. 2001)

71, 104, 132, 166 (5, 15, 25, 35°C, estimated-RP-HPLC- k' correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (12.1°C, summary of literature data, Stull 1947)

$\log(P/\text{mmHg}) = 7.30364 - 1782.4/(C + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

7605* (90.72°C, ebulliometry, measured range 90.72–173.0°C, Dreisbach & Shrader 1949)

252 (calculated by formula., Dreisbach 1955)

$\log(P/\text{mmHg}) = 6.88045 - 1496.2/(201.0 + t/^\circ\text{C})$; temp range 75–240°C (Antoine eq. for liquid state, Dreisbach 1955)

307 (extrapolated, Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 10446.8/(T/K)] + 8.017555$; temp range 12.1–173°C (Antoine eq., Weast 1972–73)

266 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.17083 - 1611.121/(213.817 + t/^\circ\text{C})$; temp range 90.7–173°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

179.3 (gas saturation, interpolated from reported graph, Rordorf 1985)

265 (extrapolated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 7.0401 - 1607.05/(213.38 + t/^\circ\text{C})$; temp range 91–173°C (Antoine eq., Dean 1985, 1992)

243 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.00535 - 1496.2/(-72.15 + T/K)$; temp range 348–513 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

236 (supercooled liquid P_L , GC-Kovács retention indices correlation; Spieksma et al. 1994)

190.4* (20.39°C, static-pressure gauge, measured range –25 to 159°C, Polednicek et al. 1996)

$\ln(P/\text{Pa}) = 21.6433 - 4031.27/[(T/K) - 47.5846]$; temp range 249–432 K (Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)

$\log(P/\text{mmHg}) = 3.2904 - 2.5839 \times 10^3/(T/K) + 3.893 \cdot \log(T/K) - 9.5398 \times 10^{-3} \cdot (T/K) + 4.6397 \times 10^{-6} \cdot (T/K)^2$, temp range 248–684 K, (Yaws 1994)

5731* (84.353°C, comparative ebulliometry, measured range 84.353–175.207°C, Roháč et al. 1998)

185.0* (20°C, recommended, summary of literature data, temp range 263.15–463.15 K, Roháč et al. 1999)

$\ln[(P/\text{Pa})/4.85] = [1 - (T/K)/248.39] \cdot \exp\{3.366439 - 8.3811530 \times 10^{-4} \cdot (T/K) + 5.9337577 \times 10^{-7} \cdot (T/K)^2\}$; temp range 250–448 K (Cox eq., recommended, Roháč et al. 1999)

$\log(P/\text{Pa}) = 21.6433 - 4031.27/[(T/K) - 47.5846]$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

472 (calculated as $1/K_{AW} \cdot C_W/C_A$, reported as exptl., Hine & Mookerjee 1975; selected exptl., Nirmalakhandan & Speece 1988a)

375 (calculated-bond contribution, Hine & Mookerjee 1975)

182 (20°C, batch air stripping-GC, Oliver 1985)

267 (gas stripping-GC, Warner et al. 1987)

289* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

$\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 2.882 - 2564/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

328 (computer value, Yaws et al. 1991)

216 (20°C, equilibrium gas stripping-GC, Hovorka & Dohnal 1997)

269 (21°C, headspace equilibrium-GC, de Wolf & Lieder 1998)

288 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 2.436 - 986/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.55 (Hansch et al. 1968)

3.38 (Leo et al. 1971; Hansch & Leo 1979)

3.57, 3.55 (calculated-fragment constants, Rekker 1977)

- 3.60 (shake flask-GC, Könemann et al. 1979)
- 3.62 (HPLC- k' correlation, Könemann et al. 1979)
- 3.44 (shake flask-LSC, Banerjee et al. 1980)
- 3.44 (shake flask-LSC, Veith et al. 1980; Oliver & Niimi 1983)
- 3.95 (HPLC-RT correlation, Veith et al. 1980)
- 3.53 (shake flask-GC, Watarai et al. 1982)
- 3.46 (shake flask-HPLC, Hammers et al. 1982)
- 3.38–3.62, 3.52 (range, mean, shake flask method, Eadsforth & Moser 1983)
- 3.62–3.95, 3.73 (range, mean, HPLC method, Eadsforth & Moser 1983)
- 3.48 (generator column-HPLC/UV, Wasik et al. 1983)
- 3.48 (generator column-GC/ECD, Miller et al. 1984; 1985)
- 3.57 (HPLC-RV correlation, Garst 1984)
- 3.60 (Hansch & Leo 1985)
- 3.55* (19°C, shake flask-GC, measured range 13–33°C, Opperhuizen et al. 1988)
- 3.50 (shake flask-GC, Pereira et al. 1988)
- 3.525 (slow stirring, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 3.52 (recommended, Sangster 1993)
- 3.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:

- 4.36 (calculated- S_{oct} and vapor pressure, Abraham et al. 2001)
- 4.27* (20°C, HPLC- k' correlation, measured range 10–50°C, Su et al. 2002)
- $\log K_{OA} = 57020/(2.303 \cdot RT) - 5.856$; temp range 10–50°C (HPLC- k' correlation, Su et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 1.82 (bluegill sunfish, Veith et al. 1979b; 1980)
- 1.82 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
- 2.86 (microorganisms-water, Mabey et al. 1982)
- 2.57–2.68 mean 2.62; 2.74–2.96 mean 2.87 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
- 3.70–4.02 (rainbow trout, lipid base, Oliver & Niimi 1983)
- 2.62–2.87 (fish, Oliver 1984)
- 1.99 (fathead minnow, flowing water, Carlson & Kosian 1987)
- 3.77, 3.78, 3.83, 3.84 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
- 3.60, 3.86, 3.25, 3.40 (field data-lipid based: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
- 1.82; 2.62, 2.87 (*Lepomis macrochirus*; *Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
- 3.78 (*Poecilia reticulata*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
- 2.62, 3.70; 2.553, 2.305 (quoted: whole fish, lipid content; calculated-QSPR-MCI χ , K_{OW} , Lu et al. 1999)
- 3.79; 3.75 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.50; 4.10 (field data of sediment trap material; Niagara River-organic matter, Oliver & Charlton 1984)
- 2.14 (soil, Lee et al. 1989)
- 2.48 (soil, calculated-QSAR-MCI χ , Sabljic et al. 1995)
- 2.43, 2.58, 2.88 (RP-HPLC- k' correlation on three different stationary phases, Szabo et al. 1995)
- 2.60, 2.60 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 3.47 \pm 0.74 (suspended particulate in coastal waters, Masunaga et al. 1996)
- 2.49, 2.53 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, $\log K_{OM}$:

- 2.23 (Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm, Chiou et al. 1983)
 3.88 (micelle-water, Valsaraj & Thibodeaux 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 4.1$ h from a model river of 1 m depth with a current of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982);

$k = 1.9 \times 10^{-4} \text{ h}^{-1}$ with H_2O_2 at 25°C in F-113 solution and with HO• in the gas (Dilling et al. 1988);
 pseudo-first-order direct photolysis $k(\text{exptl}) = (0.008 \pm 0.001) \text{ min}^{-1}$ with $t_{1/2} = (92.3 \pm 6.4) \text{ min}$ in aqueous solution (Peijnenburg et al. 1992)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} \sim 3.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 radical (Mabey et al. 1982)

$k_{OH} = (7.2 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{OH}(\text{obs.}) = 7.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{OH}(\text{calc.}) = 11.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{OH}(\text{calc.}) = 1.01 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 0.72 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k(\text{aq.}) = (0.57 \pm 0.005) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} = 16$ h at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = (5.4\text{--}5.9) \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{HO\cdot}(\text{aq.}) = (5.0 \pm 1.0) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous solutions (Haag & Yao 1992)

$k_{OH} = 0.46 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982)

base rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C with a calculated $t_{1/2} > 900$ yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

first-order $t_{1/2} > 879$ yr, based on rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Howard et al. 1991).

Biodegradation: significant degradation in an aerobic environment with rate constant $k = 0.05 \text{ d}^{-1}$ (Tabak et al. 1981; Mills et al. 1982);

nearly 100% removed by an apparent combination of biodegradation and stripping in a continuous flow activated sludge system (Kincannon et al. 1983; selected, Howard 1989)

$t_{1/2}(\text{aq. aerobic}) = 672\text{--}4320$ h, estimated from unacclimated soil grab sample data; $t_{1/2}(\text{aq. anaerobic}) = 2688\text{--}17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 200.6\text{--}2006$ h, based on photooxidation half-life in air (Howard et al. 1991).

Surface Water: $t_{1/2} = 0.9\text{--}50$ d, various locations in the Netherlands in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980)

$t_{1/2} = 672\text{--}4320$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

measured rate constant $k = (0.57 \pm 0.05) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} = 16$ h at pH 7 (Yao & Haag 1991)

direct photolysis $t_{1/2} = 92.3$ min in aqueous solution (Peijnenburg et al. 1992).

Groundwater: $t_{1/2} = 1$ yr estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)

$t_{1/2} = 1334\text{--}8640$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on unacclimated aerobic screening test data and aerobic soil grab sample data (Howard et al. 1991).

Biota: $t_{1/2} < 1$ d in bluegill sunfish (Veith et al. 1980; Barrows et al. 1980)

$t_{1/2} < 5$ d in worm at 8°C (Oliver 1987a);

biological half-lives, $t_{1/2} < 1$ d in trout muscle, $t_{1/2} < 1$ d in sunfish, and $t_{1/2} < 1$ d in guppy for dichlorobenzenes (Niimi 1987).

TABLE 6.1.1.3.1

Reported aqueous solubilities of 1,3-dichlorobenzene at various temperatures

1.

Klemenc & Löw 1930		Vesala 1973		Schwarz & Miller 1980		Horvath & Getzen 1985	
volumetric method		shake flask-UV spec.		elution chromatography		recommended values	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	111	10	97.63	10	116	10	103
25	123	15.2	97.76	20	89	15	99.9
30	140	19.6	98.32	30	139	20	101
35	150	25.1	101.26	shake flask-UV		25	106
40	167	30.0	112.74		120	30	114
45	177	35.0	121.13	20	113	35	125
55	196			30	132	40	137
60	201			average		45	151
				10	118	50	165
				20	101	55	179
				30	135	60	192

2.

Ma et al. 2001		Finizio & Di Guardo 2001	
shake flask-GC		RP-HPLC- k' correlation	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
5	114	5	71
15	108	15	104
25	126	25	132
35	134	35	166
45	141		

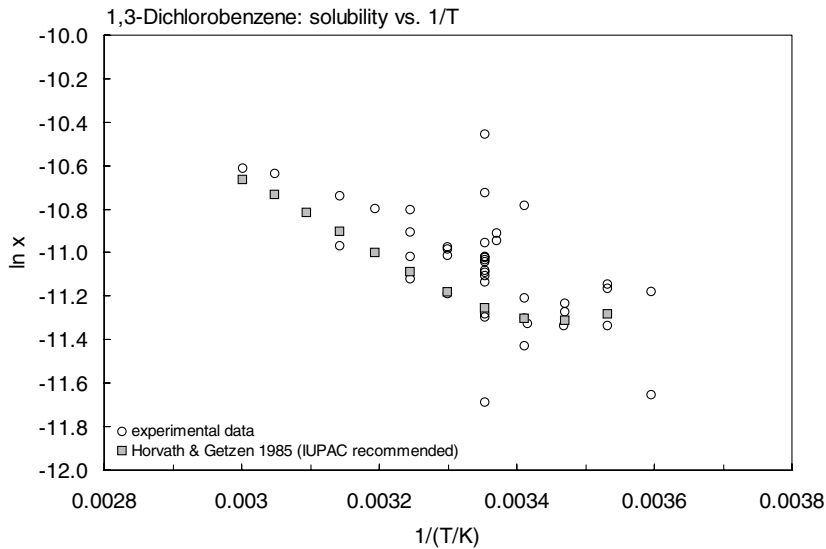


FIGURE 6.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,3-dichlorobenzene.

TABLE 6.1.1.3.2
Reported vapor pressures of 1,3-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_0) = (1 - T/T_0) \cdot \exp[\sum A_i T^i]$	(5) - Cox eq.		

1.

Stull 1947		Dreisbach & Shrader 1949		Poledniecek et al. 1996		Roháč et al. 1998	
summary of literature data		ebulliometry		static method-pressure gauge		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.1	133.3	90.72	7605	−23.55	5.459	84.353	5731
39	666.6	98.05	10114	−19.57	7.987	93.65	8343
52.9	1333	111.49	16500	−19.57	7.973	97.99	11076
66.2	2666	140.49	42060	−9.7	19.355	107.17	13922
82	5333	157.37	67660	0.3	44.17	112.433	16799
92.2	7999	173.0	101325	10.34	94.451	117.892	20292
105	13332			10.35	9.459	117.893	20291
125.9	26664	mp/°C	−24.76	20.39	190.4	123.625	24569
149	53329	bp/°C	173.0	30.28	360.02	129.141	29396
173	101325			40.26	652.82	134.535	34819
		eq. 2	P/mmHg	50.15	1122.2	139.715	40761
mp/°C	−24.2	A	7.30364	50.16	1125.0	144.993	47623
		B	1782.4	60.18	1872.9	144.993	47623
		C	230	60.18	1875.7	153.301	60276
				70.03	2980.9	161.253	74765
				70.03	2978.4	169.859	93403
				80.0	4661.7	172.047	98670

(Continued)

TABLE 6.1.1.3.2 (Continued)

Stull 1947		Dreisbach & Shrader 1949		Poledniecek et al. 1996		Roháč et al. 1998	
summary of literature data		ebulliometry		static method-pressure gauge		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				89.94	7042.6	174.92	105933
				89.94	7049.0	175.207	106716
				98.86	10180		
				108.83	14713	bp/°C	173.095
				118.87	20859		
				128.93	28986	eq. 3	P/kPa
				138.94	39411	A	6.16151
				149.05	52842	B	1595.19
				159.06	69604	C	-62.398
				eq. 3a	P/Pa		
				A	21.6433		
				B	4031.27		
				C	-47.5846		

2.

Roháč et al. 1999	
recommended	
T/K	P/Pa
253.15	7.70
263.15	18.9
273.15	43.1
283.15	92.0
283.15	185.0
303.15	352.9
313.15	641.6
232.15	1117
333.15	1871
343.25	3016
353.15	4737
363.15	7205
373.15	10670
383.15	15420
393.15	21810
403.15	30210
413.15	41080
423.15	54920
433.15	72270
443.15	93730
453.15	12000
Cox eq.	
eq. 5	P/Pa
A ₀	3.366439
10 ⁻⁴ A ₁	-8.3811530

TABLE 6.1.1.3.2 (Continued)

Roháč et al. 1999	
recommended	
T/K	P/Pa
$10^{-7}A_2$	5.9337577
T_o/K	248.39
P_o/Pa	4.85
bp/K	446.25
temp range 250–448 K	

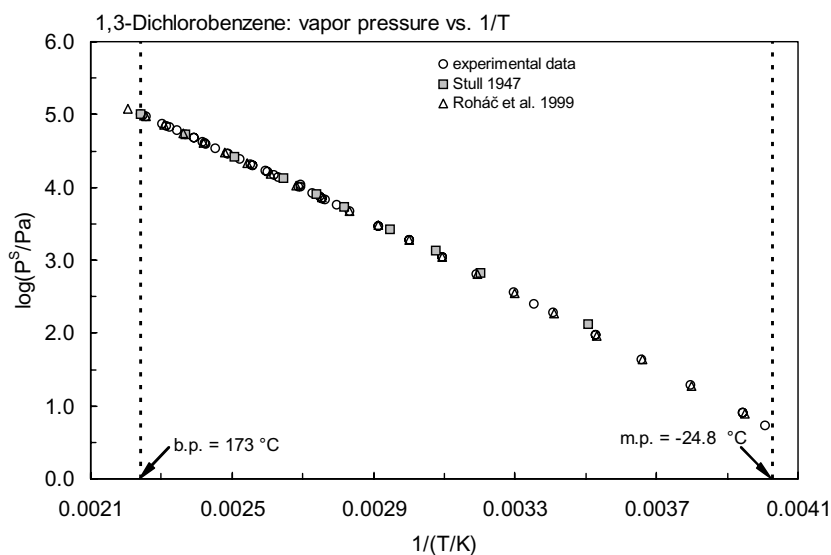


FIGURE 6.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3-dichlorobenzene.

TABLE 6.1.1.3.3

Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,3-dichlorobenzene at various temperatures and temperature dependence equations

Henry's law constant		log K_{OW}		log K_{OA}	
Ashworth et al. 1988		Oppenhuizen et al. 1988		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
$t/^{\circ}C$	$H/(Pa \text{ m}^3/\text{mol})$	$t/^{\circ}C$	log K_{OW}	$t/^{\circ}C$	log K_{OA}
10	224	13	3.72	10	4.6
15	234	19	3.55	20	4.27
20	298	28	3.48	30	3.96
20	289	33	3.42	40	3.67
30	428			50	3.4
		$\Delta H/(kJ \text{ mol}^{-1}) = -15.0$		$\Delta H_{OA}/(kJ \text{ mol}^{-1}) = 57.02$	
$\ln H = A - B/(T/K)$				$\log K_{OA} = A + B/2.303RT$	
	$H/(\text{atm m}^3/\text{mol})$				
A	-2.882			A	-5.856
B	2564			B	57020

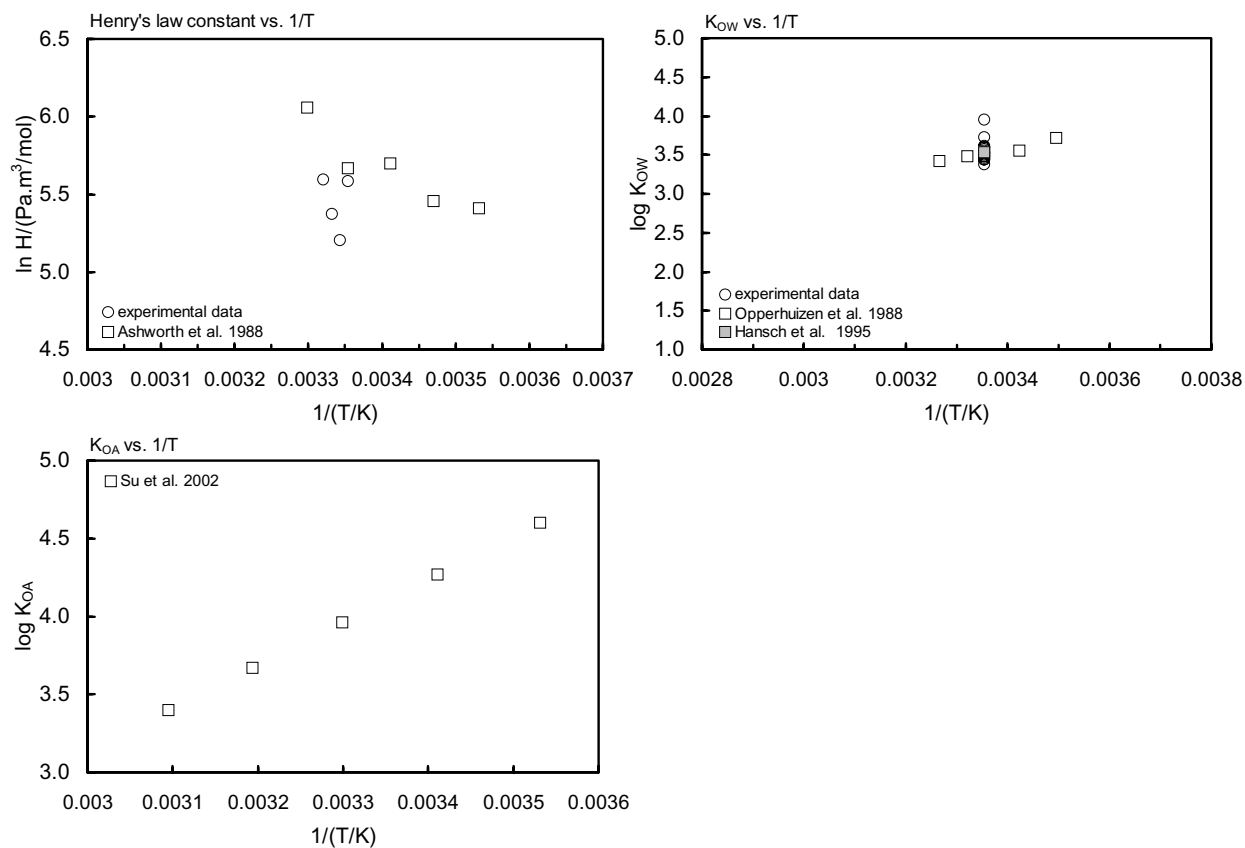
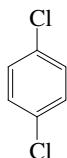


FIGURE 6.1.1.3.3 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for 1,3-dichlorobenzene.

6.1.1.4 1,4-Dichlorobenzene



Common Name: 1,4-Dichlorobenzene

Synonym: *p*-dichlorobenzene, paradichlorobenzene

Chemical Name: 1,4-dichlorobenzene

CAS Registry No: 106-46-7

Molecular Formula: $C_6H_4Cl_2$

Molecular Weight: 147.002

Melting Point ($^{\circ}C$):

53.09 (Lide 2003)

Boiling Point ($^{\circ}C$):

174 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2457 (Dreisbach 1955; Weast 1972–73; Horvath 1982)

Molar Volume (cm^3/mol):

118.0 ($20^{\circ}C$, calculated-density)

137.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.72 (Dreisbach 1955)

17.882 (Weast 1972–73)

18.16, 18.70 (Wauchope & Getzen 1972)

18.20 (Tsonopoulos & Prausnitz 1971; Dean 1985)

19.0 (Miller et al. 1984)

17.153 (Ruelle et al. 1993)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56.484 (Pirsch 1956)

55.65 (Tsonopoulos & Prausnitz 1971)

54.81 (Weast 1976–77; Amidon & Williams 1982; Yalkowsky 1979)

56.07 (Yalkowsky & Valvani 1980)

58.16 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.53 (mp at $53.09^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

79.1* (volumetric method, measured range 20 – $60^{\circ}C$, Klemenc & Löw 1930)

77 ($30^{\circ}C$, shake flask-interferometer, Gross & Saylor 1930)

< 500 (residue-volume method, Booth & Everson 1948)

76 (shake flask-UV, Andrew & Keefer 1950)

89.8 (Landolt-Börnstein 1951)

83.4* ($24.6^{\circ}C$, shake flask-UV, measured 22.2 – $73.4^{\circ}C$, Wauchope & Getzen 1972)

85.5 (shake flask-UV, Vesala 1974)

56.9 ($20^{\circ}C$, shake flask-GC/ECD, Chiou & Freed 1977)

34 (shake flask-GC, Jones et al. 1977/1978)

87.2 (shake flask-GC, Aqun-Yuen et al. 1979)

90.6 (shake flask-UV, Yalkowsky et al. 1979)

73.7 (shake flask-LSC, Veith et al. 1980)

73.8 (shake flask-LSC, Banerjee et al. 1980)

48.7 (shake flask-GC, Könnemann 1981)

73, 137 (shake flask-GC, solid, supercooled liquid, Chiou et al. 1982)

90.0	(recommended, Horvath 1982)
25	(calculated-UNIFAC activity coefficients, Arbuckle 1983)
175	(calculated-HPLC- k' , converted from reported γ_w , Hafkenscheid & Tomlinson 1983a)
154	(30°C, shake flask-GC, McNally & Grob 1983)
30.9	(generator column-GC, Miller et al. 1984, 1985)
65.3	(shake flask-HPLC, Banerjee 1984)
158	(30°C, shake flask-GC, McNally & Grob 1984)
82.9*	(recommended, temp range 10–75°C, IUPAC Solubility Data Series, Horvath & Getzen 1985)
$S/(g/kg) = 13.974 - 8.5829 \times 10^{-2} \cdot (T/K) + 1.3365 \times 10^{-4} \cdot (T/K)^2$; temp range 328–348 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)	
100	(Dean 1985)
141	(20°C, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)
81.4* \pm 1.5	(shake flask-GC/ECD, measured range 5–45°C, Shiu et al. 1997)
42.0	(shake flask-GC, Boyd et al. 1998)
$\ln x = -4.178 - 2186.7/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)	

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1333*	(54.8°C, summary of literature data, temp range 54.8–173.9°C, Stull 1947)
$\log (P/\text{mmHg}) = 7.30697 - 1788.7/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)	
7605*	(92.0°C, ebulliometry, measured range 92.0–174.12°C, Dreisbach & Shrader 1949)
235	(calculated by formula., Dreisbach 1955; quoted, Hine & Mookerjee 1975; Riddick et al. 1986; Howard 1989)
$\log (P/\text{mmHg}) = 6.89797 - 1507.3/(201.0 + t/^\circ\text{C})$; temp range 75–240°C (Antoine eq. for liquid state, Dreisbach 1955)	
8514*	(94.8°C, ebulliometry, measured range 94.8–174.04°C, McDonald et al. 1959)
93.33*	(20.4°C, α - <i>p</i> -dichlorobenzene, manometry, measured range 20.4–39.6°C, Walsh & Smith 1961)
402.6*	(37.9°C, β - <i>p</i> -dichlorobenzene, manometry, measured range 37.9–52.5°C, Walsh & Smith 1961)
90.2	(solid vapor pressure, extrapolated, Antoine eq., Weast 1972–73)
$\log (P/\text{mmHg}) = [-0.2185 \times 17260.5/(T/K)] + 12.4800$; temp range 30–50°C, (Antoine eq., Weast 1972–73)	
$\log (P/\text{mmHg}) = [-0.2185 \times 10611.0/(T/K)] + 8.073632$; temp range 54.8–173.9°C (Antoine eq., Weast 1972–73)	
137.2*	(diaphragm pressure gauge, measured range: 0–20°C, De Kruif et al. 1981)
128	(extrapolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 5.94201 - 1668.355/(186.212 + t/^\circ\text{C})$; temp range 164.7–237.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)	
158*	(gas saturation-GC, measured range 20–100°C, Rordorf 1985)
243	(extrapolated-Antoine eq., Dean 1985)
$\log (P/\text{mmHg}) = 7.0208 - 1590.9/(210.2 + t/^\circ\text{C})$, temp range 95–174°C (Antoine eq., Dean 1985, 1992)	
86.7	(20°C, gas saturation, Chiou & Shoup 1985)
134	(interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_s/\text{kPa}) = 10.472 - 3382.9/(T/K)$; temp range 293–313 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)	
$\log (P_s/\text{kPa}) = 10.181 - 3290.4/(T/K)$; temp range 310–336 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)	
$\log (P_L/\text{kPa}) = 6.12695 - 1578.51/(-64.22 + T/K)$; temp range 341–448 K (liquid, Antoine eq., Stephenson & Malanowski 1987)	
133*	(gas saturation-GC, measured range –15 to 40°C, Liu & Dickhut 1994)
216; 257	(supercooled liquid P_L , GC-Kovács retention indices correlation; quoted lit., Spieksma et al. 1994)
$\log (P/\text{mmHg}) = 36.2276 - 3.6756 \times 10^3/(T/K) - 9.6308 \cdot \log (T/K) - 1.3372 \times 10^{-9} \cdot (T/K) + 1.9905 \times 10^{-6} \cdot (T/K)^2$; temp range 326–685 K (vapor pressure eq., Yaw et al. 1994)	
135*	(25°C; pressure gauge measurement; interpolated from reported Antoine eq., Poledniecek et al. 1996)
$\ln (P_s/\text{Pa}) = 28.4986 - 6272.86/[(T/K) - 32.2741]$; temp range 273–323 K (Antoine eq. from exptl data, pressure gauge measurement, solid, Poledniecek et al. 1996)	
$\ln (P_L/\text{Pa}) = 21.0472 - 3665.96/[(T/K) - 62.3849]$; temp range 333–442 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Poledniecek et al. 1996)	

- 5729* (85.139°C, comparative ebulliometry, measured range 85.139–175.626°C, Roháč et al. 1998)
 87.0* (20°C, recommended, summary of literature data, temp range 273.15–453.15 K, Roháč et al. 1999)
 $\ln [(P_s/P_a)/1280] = [1 - (T/K)/326.3] \cdot \exp\{3.251427 - 2.853921 \times 10^{-4} \cdot (T/K)\}$; temp range 273–323 K (Cox eq. solid, recommended, Roháč et al. 1999)
 $\ln [(P_L/P_a)/1280] = [1 - (T/K)/326.3] \cdot \exp\{3.100023 - 1.0557743 \times 10^{-3} \cdot (T/K) + 7.816354 \times 10^{-7} (T/K)^2\}$; temp range 328–449 K (Cox eq., liquid, recommended, Roháč et al. 1999)
 $\log (P/P_a) = 11.63209 - 2829.32/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 330 (equilibrium cell-GC, concentration ratio, Leighton & Calo 1981)
 240 (gas stripping-GC, Mackay & Shiu 1981)
 152 (20°C, gas stripping-GC, Oliver 1985)
 276 (gas stripping-GC, Warner et al. 1987)
 321* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 3.373 - 2720/(T/K)$; temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 438 (computer value, Yaws et al. 1991)
 244 (gas stripping-GC, Shiu & Mackay 1997)
 188 (20°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 275 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 2.649 - 1054/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.39 (shake flask, Leo et al. 1971; Hansch & Leo 1979)
 3.57, 3.55 (calculated-fragment constants, Rekker 1977)
 3.38 (Hansch & Leo 1979)
 3.62, 3.39 (shake flask-GC, HPLC-k' correlation, Könnemann et al. 1979)
 3.37, 3.78 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
 3.37 (shake flask-LSC, Banerjee et al. 1980)
 3.46 (HPLC-k' correlation, Hammers et al. 1982)
 3.52 (shake flask-GC, Watarai et al. 1982)
 3.43 (HPLC-k' correlation, Miyake & Terada 1982)
 3.67, 3.90 (calculated-UNIFAC activity coefficients, Arbuckle 1983)
 3.37 (generator column-HPLC/UV, Wasik et al. 1983)
 3.38 (generator column-GC/ECD, Miller et al. 1984; 1985)
 3.37 (HPLC-RV correlation, Garst 1984; Garst & Wilson 1984)
 3.52 (Hansch & Leo 1985)
 3.444 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 3.85–4.30, 4.0 (range, average: round robin work, shake flask or HPLC-k' correlation, Kishi & Hashimoto 1989)
 3.355 ± 0.053, 3.444 ± 0.001 (shake flask methods, interlaboratory studies, Brooke et al. 1990)
 3.45 (recommended, Sangster 1993)
 3.44 (recommended, Hansch et al. 1995)
 3.23* ± 0.03 (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)
 $\log K_{OW} = 0.2338 + 17100/[2.303 \cdot R(T/K)]$; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
 3.65 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 4.46 (calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)
 4.32* (20°C, HPLC-k' correlation, measured range 10–50°C, Su et al. 2002)
 $\log K_{OA} = 55590/(2.303 \cdot RT) - 5.556$; temp range 10–50°C (HPLC-k' correlation, Su et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

- 2.33 (rainbow trout, Neely et al. 1974)
 2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
 1.78 (bluegill sunfish, Veith et al. 1979b, 1980)
 1.78 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
 3.26 (guppy, lipid basis, Könnemann & van Leeuwen 1980)
 2.53–2.59 mean 2.57; 2.79–2.96 mean 2.86 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
 3.64–3.96 (rainbow trout, lipid basis, Oliver & Niimi 1983)
 3.40 (15°C, guppy, Banerjee et al. 1984)
 2.83–2.86 (fish, Oliver 1984)
 2.00, 1.70, 2.75 (algae, fish, activated sludge, Freitag et al. 1984)
 2.0, 1.70, 2.75 (algae, fish, activated sludge, Freitag et al. 1985)
 2.32–2.72 mean 2.71; 2.74–3.15 mean 2.95 (15°C, rainbow trout, wet wt., steady-state BCF on 7- to 96-d laboratory study in two tanks with different water concn, Oliver & Niimi 1985)
 2.04 (fathead minnow, flowing water, Carlson & Kosian 1987)
 5.3–5.6, 5.5 (Niagara River plume, range, mean; Oliver 1987b)
 3.91, 4.53, 4.09, 3.51 (field data-lipid based: Atlantic creakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 3.25 (guppy, lipid weighted-based, 12 to 31 d exposure-GC, Gobas et al. 1989)
 2.47, 3.56 (flagfish: whole fish, lipid, Smith et al. 1990)
 1.7 ± 0.2 (guppy, steady-state conditions, rate const. ratio k_1/k_2 , 96-h exposure, Sijm et al. 1993)
 3.5 ± 0.1 (guppy, lipid normalized BCF, Sijm et al. 1993)
 2.40 (fathead minnow, steady-state conditions, rate const. ratio k_1/k_2 , 96-h exposure, Sijm et al. 1993)
 3.60 (fathead minnow, lipid normalized BCF, Sijm et al. 1993)
 1.78; 2.47; 2.57–2.95 (*Lepomis macrochirus*; *Jordanella floridae*; *Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
 1.70; 2.40 (*Poecilia reticulata*; *Pimephales promelas*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
 2.57, 3.65; 2.517, 2.242 (quoted: whole fish, lipid content; calculated-MCI χ , K_{OW} , Lu et al. 1999)
 3.70; 3.75 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 2.59 (Kenaga 1980a)
 2.78–3.14 (organic carbon, Schwarzenbach & Westall 1981)
 2.29 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
 2.18–3.44 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
 4.80; 5.00 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
 2.82, 2.45 (Aprison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium Southworth & Keller 1986)
 5.30–5.60; 5.50 (Niagara River plume: range; average value; Oliver 1987b)
 2.92; 2.91 (Aldrich humic acid, equilibrium dialysis; Aldrich and Fluka humic acid, Flory-Huggins model, Chin & Weber 1989)
 2.43 (organic polymers in Huron River water, Chin et al. 1990)
 2.88 (HPLC- k' correlation, Szabo et al. 1995)
 2.60, 2.61 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 2.66, 2.57, 2.77 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
 2.99–3.46 (three wetland soils, batch equilibrium-sorption isotherm-LSC, Lee et al. 2003)

Sorption Coefficient, log K_{OM} :

- 2.20 (Woodburn silt loam soil, organic matter 1.9%, equilibrium sorption isotherm, Chiou et al. 1983)

Environmental Fate Rate Constants, k or Half-Lives. $t_{1/2}$:

Volatilization: $t_{1/2} = 4.3$ h from a model river of 1 m depth and with a current of 1 m/s and wind velocity of 3 m/s at 20°C (Lyman et al. 1982);

rate constants: $k = 0.04$ d⁻¹, $t_{1/2} = 18$ d in spring at 8–16°C, $k = 0.068$ d⁻¹, $t_{1/2} = 10$ d in summer at 20–22°C, $k = 0.054$ d⁻¹, $t_{1/2} = 13$ d in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.066$ d⁻¹, $t_{1/2} = 10.6$ d with HgCl₂, and $k = 0.063$ d⁻¹, $t_{1/2} = 11$ d without HgCl₂ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982)

Direct photolysis unimportant (Zepp & Cline 1977; Zepp 1978);

$t_{1/2} = 25$ d under sunlight in water (Mansour & Feicht 1994)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated, *data at other temperatures see reference:

$k = 9.63 \times 10^{-3}$ h⁻¹ in air (Ware & West 1977; selected, Mackay et al. 1985)

$k_{OH} \sim 3.0 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹, residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$k \ll 360$ M⁻¹ h⁻¹ for singlet oxygen and $k \ll 1$ M⁻¹ h⁻¹ for RO₂ radical (Mabey et al. 1982)

$k \ll 3$ M⁻¹ s⁻¹ for the reaction with ozone in water using 0.5 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = (3.2 \pm 0.2) \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

k_{OH} (obs.) = 3.2×10^{-13} cm³ molecule⁻¹ s⁻¹; and k_{OH} (calc) = 4.9×10^{-13} cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1985)

k_{OH} (calc) = 0.41×10^{-12} cm³ molecule⁻¹ s⁻¹, k_{OH} (obs) = 0.32×10^{-12} cm³ molecule⁻¹ s⁻¹ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = (0.32 - .52) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 295–300 K (literature review, Atkinson 1989)

$t_{1/2} = 200.6$ – 2006 h based on vapor phase reaction with OH radicals (Howard et al. 1991)

$k = (5.0 - 5.3) \times 10^9$ M⁻¹ s⁻¹ for the reaction of OH radical with benzene at pH 7 in aqueous solution (Kochany & Bolton 1992)

$k_{HO\cdot} = 4.0 \times 10^9$ M⁻¹s⁻¹ in aqueous solutions (Haag & Yao 1992)

k_{OH} (calc) = 0.44×10^{-12} cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1993).

Hydrolysis: not environmentally significant (Mabey et al. 1982);

base rate constant $k < 0.9$ M⁻¹ h⁻¹ at 25°C with a calculated $t_{1/2} > 900$ yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)

first order $t_{1/2} > 879$ yr, based on rate constant $k < 0.9$ M⁻¹ h⁻¹ extrapolated to pH 7 at 25°C from 1% disappearance after 16 d at 85°C and pH 9.7 (Howard et al. 1991).

Biodegradation:

$k = 1.09 \times 10^{-2}$ h⁻¹ degradation in water (Verschuereen 1977)

$t_{1/2}$ (aq. aerobic) = 672–4320 h, based on unacclimated aerobic screening test data (Canton et al. 1985) and aerobic soil grab sample data (Haider et al. 1981; Howard et al. 1991)

$k = 0.05$ d⁻¹, significant degradation in aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2}$ (aq. anaerobic) = 2688–17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: 1×10^{-10} mL cell⁻¹ h⁻¹ (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 5.67$ h⁻¹; $k_2 = 0.0264$ h⁻¹ (trout muscle, Neely et al. 1974; Neely 1979)

$k_1 = 7.44$ h⁻¹ (10°C, yellow perch, Neely et al. 1974; Neely 1979)

$k_1 = 17.0$ h⁻¹ (25°C, yellow perch, Neely et al. 1974; Neely 1979)

$kk_1 = 1800$ d⁻¹; $k_2 = 1.00$ d⁻¹ (guppy, Könemann & van Leeuwen 1980)

$k_1 = 4.1$ h⁻¹; $1/k_2 = 24$ h (guppy, quoted from Könemann & van Leeuwen 1980, Hawker & Connell 1985)

$k_1 = 5.7$ h⁻¹; $1/k_2 = 38$ h (rainbow trout, quoted from Neely et al. 1974, Hawker & Connell 1985)

$k_1 = 97$ d⁻¹ (fish, quoted, Opperhuizen 1986)

$\log k_2 = 0, -0.2$ d⁻¹ (fish, calculated- K_{OW} , Thomann 1989)

$\log k_1 = 1.99$ d⁻¹; $\log k_2 = 0.0$ (guppy, 12–31 d exposure experiments, Gobas et al. 1989)

$\log k_1 = 1.99$ d⁻¹ (fish, quoted, Connell & Hawker 1988)

$k_1 = 291$ d⁻¹, 4230 d⁻¹; $k_2 = 0.98$ d⁻¹, 1.18 d⁻¹ (American flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 0.98 \text{ d}^{-1}$, 1.46 d^{-1} (American flagfish: bioconcentration exptl., toxicity data, Smith et al. 1990)

$k_1 = 760 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 4.80 \text{ d}^{-1}$ (guppy, 96-h exposure, Sijm et al. 1993)

$k_1 = 600 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 2.50 \text{ d}^{-1}$ (fathead minnow, 96-h exposure, Sijm et al. 1993)

Half-Lives in the Environment:

Air: residence time of 38.6 d, loss of 2.6% in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)

$t_{1/2} = 200.6\text{--}2006 \text{ h}$, based on photooxidation half-life in air (Howard et al. 1991)

Surface Water:

$t_{1/2} = 1.1\text{--}26 \text{ d}$, various locations in the Netherlands in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980);

half-lives from marine mesocosm: $t_{1/2} = 18 \text{ d}$ in the spring at $8\text{--}16^\circ\text{C}$, $t_{1/2} = 10 \text{ d}$ in the summer at $20\text{--}22^\circ\text{C}$ and $t_{1/2} = 31 \text{ d}$ in the winter at $3\text{--}7^\circ\text{C}$ when volatilization dominates, and $t_{1/2} = 10.6 \text{ d}$ and 11 d for experiments with and without HgCl_2 , respectively, in September 9–15 (Wakeham et al. 1983);

hydrolysis $t_{1/2} > 900 \text{ yr}$ at pH 7 and 25°C (Ellington et al. 1988)

$t_{1/2}(\text{aerobic}) = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic screening test data and aerobic soil grab sample data; $t_{1/2}(\text{anaerobic}) = 2688\text{--}17280 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

photolysis $t_{1/2} = 25 \text{ d}$ under sunlight in water (Mansour & Feicht 1994).

Groundwater: $t_{1/2} \sim 1 \text{ yr}$ estimated from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)

$t_{1/2} = 1344\text{--}8640 \text{ h}$, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic screening test data and aerobic soil grab sample data (Howard et al. 1991).

Biota: $t_{1/2} < 1 \text{ d}$ in fish tissues (Veith et al. 1980);

$t_{1/2} < 1 \text{ d}$ in bluegill sunfish (Barrows et al. 1980);

$t_{1/2} = 16 \text{ h}$, clearance from fish (Neely 1980);

$t_{1/2} < 5 \text{ d}$ in worms at 8°C (Oliver 1987a);

biological half-lives, $t_{1/2} < 1 \text{ d}$ in trout muscle, $t_{1/2} < 1 \text{ d}$ in sunfish and $t_{1/2} < 1 \text{ d}$ in guppy for dichlorobenzenes (Niimi 1987);

depuration $t_{1/2} = 0.70 \text{ d}$ for whole fish, $t_{1/2} = 0.59 \text{ d}$ for fish lipid (American flagfish, Smith et al. 1990).

TABLE 6.1.1.4.1
Reported aqueous solubilities of 1,4-dichlorobenzene at various temperatures

Klemenc & Löw 1930		Wauchope & Getzen 1972		Horvath & Getzen 1985		Shiu et al. 1997	
volumetric method		shake flask-UV		recommended values		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
		liquid		liquid			
20	68.1	22.2	77.8	10	51.2	5	48.6
20	79.1	24.6	83.4	15	60.5	15	63.0
30	93.3	25.5	86.9	20	71.0	25	81.4
35	104	30.0	92.6	25	82.9	35	104.5
35	83	34.5	102	30	96.3	45	130
40	101	38.4	121	35	111.3		
45	122	47.5	169	40	128		
55	156	50.1	173	45	147		
60	163	solid		30	167		
		59.2	210	55	190		
		60.7	218	solid			
		65.1	230	55	201		
		65.2	237	60	214		
		73.4	281	65	233		
				70	259		
				75	292		

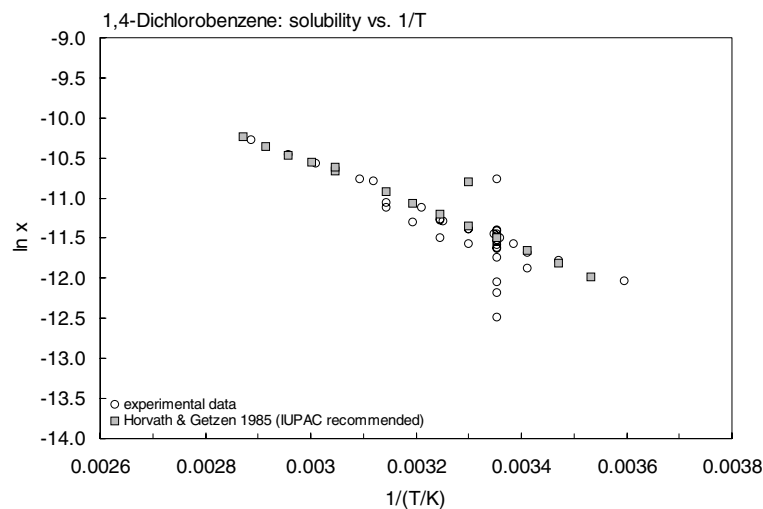


FIGURE 6.1.1.4.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,4-dichlorobenzene.

TABLE 6.1.1.4.2

Reported vapor pressures of 1,4-dichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\ln (P/P_0) = (1 - T/T_0) \cdot \exp[\Sigma A_i T^i]$	(5) - Cox eq.		

1.

Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959		Walsh & Smith 1961	
summary of lit. data		ebulliometry		ebulliometry		manometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
54.8	1333	92.0	7605	94.8	8514	α -p-dichlorobenzene	
69.2	2666	99.41	10114	98.55	9844	20.4	93.33
84.8	5333	112.66	16500	104.81	12444	23.9	121.32
95.2	7999	141.65	42066	116.28	18808	26.8	156.0
108.4	13332	158.52	67660	143.52	44465	29.8	202.65
128.3	26664	174.12	101325	159.79	70117	33.2	269.3
150.2	53329			171.87	95945	33.7	277.3
173.9	101325			174.04	101325	35.0	312.0
						36.4	317.3
						37.3	350.6
mp/ $^{\circ}\text{C}$	53.0			mp/ $^{\circ}\text{C}$	52.90	37.5	382.6
						39.2	440.0
				eq. 2	P/mmHg	39.6	454.6
				A	6.99800		
				B	1575.11	mp/ $^{\circ}\text{C}$	53.23
				C	208.513		
						eq. 1	P/mmHg
						A	11.347
						B	3382.9
						$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 64.79$	

2.

Walsh & Smith 1961		de Kruif et al. 1981		Rordorf 1985		Liu & Dickhut 1994	
manometry		static manometry		gas saturation		gas saturation-GC	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
β -p-dichlorobenzene							
37.9	402.6	1.47	14.14	25	158.1*	-14.5	4.67
39.8	469.3	3.94	18.32	50	1217.6*	-5.0	16.0
40.2	477.3	6.45	23.67	75	6992.7	10	31.7
40.5	490.6	8.43	28.88	100	31774	25	133
40.8	501.3	10.33	34.83	125	119380	40	452
41.1	508.0	12.35	42.44	150	383592		
41.3	522.6	14.3	51.13				
41.7	534.6	16.63	63.79				
42.4	568.0	19.84	85.98		*solid		
42.6	584.0			eq. 1	P/Pa	$\Delta H_v/(\text{kJ mol}^{-1}) = 35.0$	
42.9	593.3			A	13.384		
43.2	597.3	eq. 1	P/Pa	B	3450		

TABLE 6.1.1.4.2 (Continued)

Walsh & Smith 1961		de Kruif et al. 1981		Rordorf 1985		Liu & Dickhut 1994	
manometry		static manometry		gas saturation		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
43.7	629.3	A	13.6459				
44.1	640.0	B	3431.3		liquid		
45.8	727.9			eq. 1	P/Pa		
46.4	766.6			A	10.472		
48.0	859.3	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 65.7$		B	3382.9		
49.4	955.9	11°C					
51.3	955.9			$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 65.40$			
51.7	1135			30–50°C			
52.5	1192						
eq. 1	P/mmHg						
A	11.056						
B	3290.4						
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 63.01$							
3.							
Polednicek et al. 1996				Roháč et al. 1998		Roháč et al. 1999	
pressure gauge				comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
	solid		liquid				
0.34	12.2	60.12	1838.2	85.139	5729	273.15	12.2
0.35	11.98	60.15	1839.6	94.305	8334	283.15	33.8
10.35	34.25	70.03	2948.1	101.656	11074	283.15	87.0
10.35	34.21	80.03	4629.1	107.836	13921	303.15	209.3
20.35	88.75	80.04	4627.7	113.103	16800	313.15	474.2
20.35	88.61	89.99	7038.6	118.564	20290	232.15	1017
30.31	214.6	90.0	7041.4	118.568	20292	333.15	1817
40.25	485.5	98.72	9904.2	124.29	24570	343.25	2941
50.15	1037	108.68	1434.2	129.822	29388	353.15	4611
25	135.0	118.73	20385	135.223	34809	363.15	7020
	interpolated	128.78	28351	140.416	40752	373.15	10410
		138.8	38541	145.702	47615	383.15	15060
for solid:		148.28	51728	154.032	60269	393.15	21310
eq. 3a	P/Pa	158.9	68186	154.033	60271	403.15	29550
A	28.4986	168.93	88642	162.009	74759	413.15	40220
B	6272.86			170.622	93393	423.15	53800
C	–32.2741			172.86	98793	433.15	70850
		for liquid:		175.626	105783	443.15	91950
		eq. 3a	P/Pa			453.15	11780
		A	21.0472	bp/°C	173.864		
		B	3665.96			Cox eq.	for solid
		C	–62.3849	eq. 3	P/kPa	eq. 5	P _s /Pa
				A	6.13050	A ₀	3.251427
				B	1575.69	10 ^{–4} A ₁	–2.8153921
				C	–65.007	A ₂	0
						temp range 273–323 K	

(Continued)

TABLE 6.1.1.4.2 (Continued)

Poledniecek et al. 1996				Roháč et al. 1998		Roháč et al. 1999	
pressure gauge				comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						eq. 5	P _L /Pa
						A ₀	3.100023
						10 ⁻³ A ₁	-1.0557743
						10 ⁻⁷ A ₂	7.8161354
						T ₀ /K	326.3
						P ₀ /Pa	1280.0
						bp/K	447.01
						temp range	328–449 K

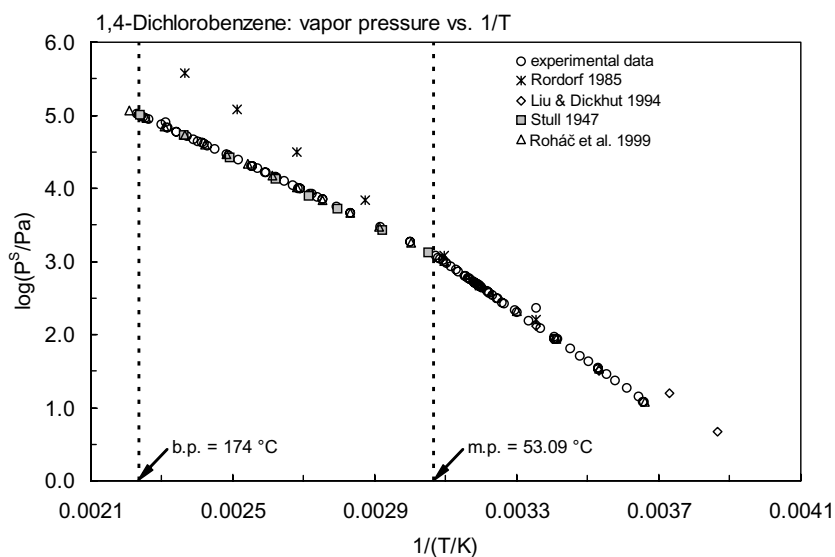


FIGURE 6.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for 1,4-dichlorobenzene.

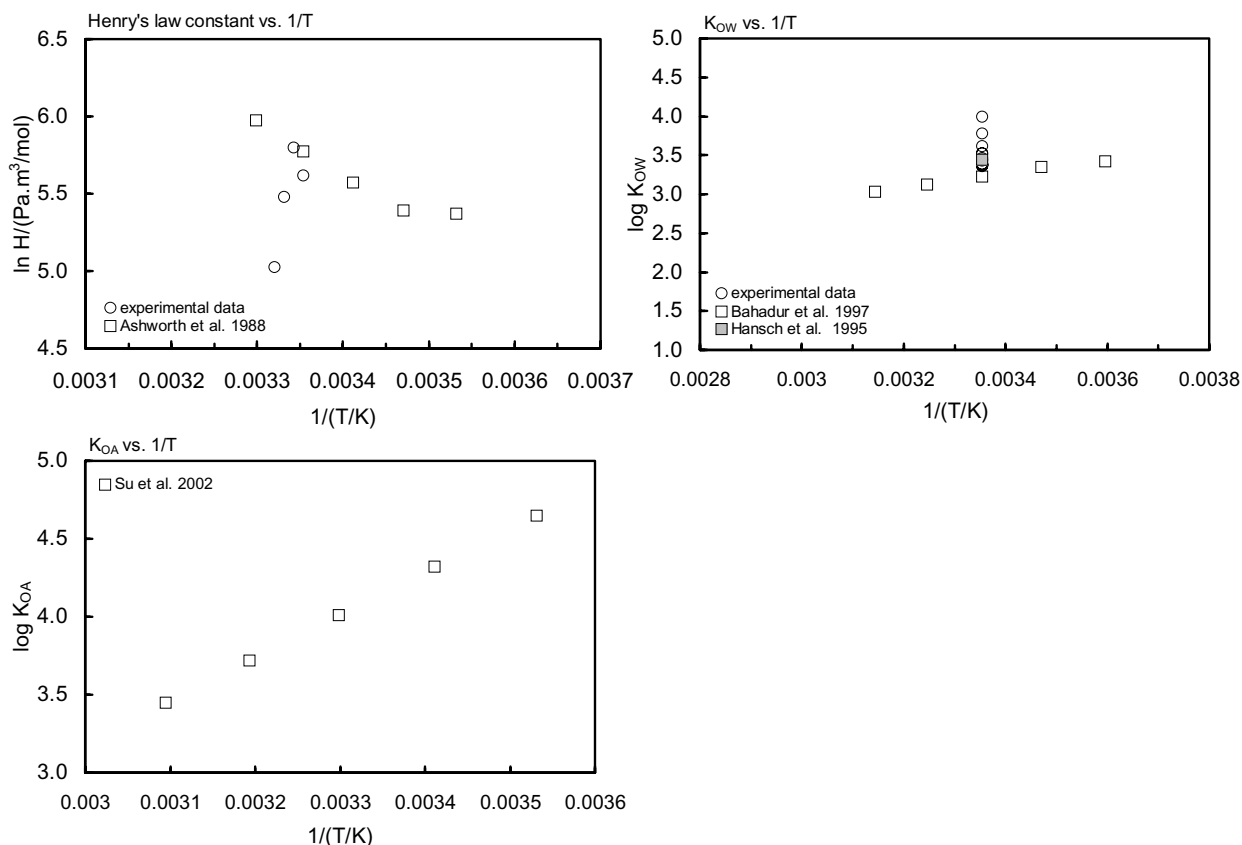
TABLE 6.1.1.4.3

Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,4-dichlorobenzene at various temperatures

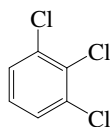
Henry's law constant		log K _{OW}		log K _{OA}	
Ashworth et al. 1988		Bahadur et al. 1997		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OW}	t/°C	log K _{OA}
10	215	5	3.42	10	4.65
15	220	15	3.35	20	4.32
20	262	25	3.23	30	4.01
20	321	35	3.12	40	3.72
30	394	45	3.03	50	3.45

TABLE 6.1.1.4.3 (Continued)

Henry's law constant		log K_{OW}		log K_{OA}	
Ashworth et al. 1988		Bahadur et al. 1997		Su et al. 2002	
EPICS-GC		shake flask-GC/ECD		GC-RT correlation	
t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OW}	t/°C	log K_{OA}
$\ln H = A - B/(T/K)$		enthalpy of transfer $\Delta H/(\text{kJ mol}^{-1}) = -17.1$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 55.59$	
	H/(atm m ³ /mol)				
A	3.373	$\log K_{OW} = A - \Delta H/2.303RT$		$\log K_{OA} = A + B/2.303RT$	
B	2720	A	0.2338	A	-5.556
		ΔH	-17100	B	55590

FIGURE 6.1.1.4.3 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for 1,4-dichlorobenzene.

6.1.1.5 1,2,3-Trichlorobenzene



Common Name: 1,2,3-Trichlorobenzene

Synonym: vic-trichlorobenzene

Chemical Name: 1,2,3-trichlorobenzene

CAS Registry No: 81-61-6

Molecular Formula: $C_6H_3Cl_3$

Molecular Weight: 181.447

Melting Point ($^{\circ}C$):

51.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

218.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4533 ($40^{\circ}C$, Weast 1972–73; Horvath 1982)

1.4533 ($25^{\circ}C$, Lide 2003)

1.69 (Dean 1985, 1992)

Molar Volume (cm^3/mol):

124.9 ($25^{\circ}C$, calculated-density)

158.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.364 (Tsonopoulos & Prausnitz 1971)

17.99 (Miller et al. 1984)

17.153 (Ruelle et al. 1993)

20.50 (Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

53.14 (Tsonopoulos & Prausnitz 1971)

56.90 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.552 (mp at $51.3^{\circ}C$)

0.53 ($25^{\circ}C$, mp at $53^{\circ}C$, Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

25.1 (Tsonopoulos & Prausnitz 1971)

31.5 (shake flask-UV, Yalkowsky et al. 1979, 1983)

16.6 (shake flask-GC, Mackay & Shiu 1981)

12.0 (shake flask-GC, Könemann 1981)

31.6 (recommended, Horvath 1982)

12.27 (generator column-GC/ECD, Miller et al. 1984, 1985)

18.0 (shake flask-HPLC, Banerjee 1984)

16.3 ($23^{\circ}C$, shake flask-GC, Chiou 1985)

18.0 (shake flask-GC, Chiou et al. 1986; Chiou et al. 1991)

$19.3^* \pm 0.24$; 23.7 ± 1.3 (generator column-GC/ECD; shake flask-GC/ECD, measured range 5 – $45^{\circ}C$, Shiu et al. 1997)

13.0 (shake flask-GC, Boyd et al. 1998)

$\ln x = -1.773 - 3418.9/(T/K)$, temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

19.71, 14.8, 21.04, 40.25 (5, 15, 25, $35^{\circ}C$, estimated- RP-HPLC- k' correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($40^{\circ}C$, summary of literature data, Stull 1947)

- 52.4 (extrapolated-Antoine eq., supercooled liquid P_L , Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 11349.5/(T/K)] + 7.91649$; temp range 40–218.5°C (Antoine eq., Weast 1972–73)
 28.0 (selected-converted from reported P_L , with fugacity ratio, Mackay & Shiu 1981)
 25.1 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
 17.7 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_S/\text{kPa}) = 9.787 - 3440/(T/K)$; temp range 289–303 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.23008 - 2624.09/(10.506 + T/K)$; temp range 343–492 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 11.20* (gas saturation-GC, measured range –15 to 40°C, Liu & Dickhut 1994)
 8.82* (20.35°C, static method-pressure gauge measurement; Antoine eq., measured range 0.36–169°C, Polednicek et al. 1996)
 $\ln (P_S/\text{Pa}) = 33.2977 - 9327.37/[(T/K) + 6.13445]$; temp range 272–3 (Antoine eq. from exptl data, pressure gauge measurement, solid, Polednicek et al. 1996)
 $\ln (P_L/\text{Pa}) = 21.1681 - 4077.21/[(T/K) - 71.6539]$; temp range 334–2 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Polednicek et al. 1996)
 44.1 (supercooled liquid P_L , GC-Kováš retention indices correlation; Spijksma et al. 1994)
 8.50* (20°C, recommended, summary of literature data, temp range 233.15–503.15 K, Roháč et al. 1999)
 $\ln [(P_S/\text{Pa})/173.0] = [1 - (T/K)/325.6] \cdot \exp\{3.380608 - 2.5802866 \times 10^{-4} \cdot (T/K)\}$; temp range 273–323 K (Cox eq., solid, recommended, Roháč et al. 1999)
 $\ln [(P_L/\text{Pa})/173.0] = [1 - (T/K)/325.6] \cdot \exp\{3.274398 - 1.0923018 \times 10^{-3} \cdot (T/K) + 7.8603029 \times 10^{-7} \cdot (T/K)^2\}$; temp range 333–448 K (Cox eq., liquid, recommended, Roháč et al. 1999)
 $\log (P/\text{kPa}) = 9.787 - 3440/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

- 127 (gas stripping-GC, Mackay & Shiu 1981)
 90.0 (gas stripping-GC, Oliver 1985)
 72.0 (20°C, gas stripping-GC, ten Hulscher et al. 1992)
 147 (equilibrium air stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 4.27 (Leo et al. 1971; Hansch & Leo 1979)
 4.11, 3.99 (shake flask-GC, HPLC- k' correlation, Könemann et al. 1979)
 4.02 (HPLC- k' correlation, McDuffie 1981)
 3.97 (shake flask-GC, Watarai et al. 1982)
 3.96 (HPLC- k' correlation, Hammers et al. 1982)
 4.04 (generator column-GC, Miller et al. 1984, 1985)
 4.14 (shake flask-GC, Chiou 1985)
 4.14 (shake flask-GC, Pereira et al. 1988)
 4.139 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 4.05 (recommended, Sangster 1993)
 4.14 (recommended, Hansch et al. 1995)
 3.81* (estimated- RP-HPLC- k' correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 5.19*, 5.11 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
 6.491, 6.073, 5.699, 5.385 (–10, 0, 9.88, 19.85°C, generator column-GC, Harner & Mackay 1995)
 $\log K_{OA} = -4.6 + 20 - 8.7/(T/K)$; $\Delta H_{OA} = 55.7 \text{ kJ/mol}$ (Harner & Mackay 1995)
 5.19 (calculated- S_{oct} and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 4.11 (guppy, lipid basis, Könemann & van Leeuwen 1980)
 3.00–3.20 mean 3.08; 3.34–3.52 mean 3.41 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

- 4.15–4.47 (rainbow trout, lipid basis, Oliver & Niimi 1983)
 3.08–3.42 (fish, Oliver 1984)
 4.35 (rainbow trout, hatching, 3.2% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
 4.11 (guppy, 5.4% lipid, wet wt basis, Geyer et al. 1985)
 4.11 (guppy, lipid weight base, 12 to 31-d exposure studies, Gobas et al. 1987, 1989)
 2.85 (fish, calculated-concentration ratio C_B/C_W or rate constant ratio k_1/k_2 , Connell & Hawker 1988)
 3.28 (guppy, Van Hoogan & Opperhuizen 1988)
 4.76, 4.90, 3.54, 4.68 (field data-lipid based: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 3.30 (guppy, steady-state conditions, rate const. ratio k_1/k_2 , 96-h exposure, Sijm et al. 1993)
 4.50 (guppy, lipid normalized BCF, Sijm et al. 1993)
 2.99 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption, Koelmans et al. 1993)
 2.90, 3.28; 3.08, 3.41 (*Poecilla reticulata*; *Oncorhynchus mykiss*, quoted lit., flow through conditions, Devillers et al. 1996)
 2.94–3.23 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
 3.08, 4.16; 2.812, 3.055 (quoted: whole fish, lipid content; calculated- MCI χ , K_{OW} , Lu et al. 1999)
 3.68; 3.72 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 2.85 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
 2.73–4.00 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
 4.70; 4.10 (field data of Lake Ontario sediment trap material; Niagara River-organic matter, Oliver & Charlton 1984)
 3.0, 2.0 (Sanhedron soil humic acid, Suwannee River humic acid, batch equilibrium-sorption isotherm, GC/ECD, Chiou et al. 1986)
 2.3, 2.0 (Sanhedron soil fulvic acid, Suwannee River fulvic acid, batch equilibrium-sorption isotherm, GC/ECD, Chiou et al. 1986)
 3.21, 3, 14 (Riddles soil: top layer 1.84% OC; below top layer, batch equilibrium-sorption isotherm, Boyd et al. 1990)
 3.18, 3.38, 3.43, 3.26, 3.23 (five soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
 3.91 (Isora soil 1.87% OC, batch equilibrium, GC, Paya-Perez et al. 1991)
 3.81 (lake sediment 2.5% OC, batch equilibrium, Schrap et al. 1994)
 3.61 \pm 0.39 (suspended particulates in coastal waters, Masunaga et al. 1996)
 3.16 (HPLC-screening method; Müller & Kördel 1996)
 3.48, 3.37 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)

Environment Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} \sim 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

$k(aq.) \leq 0.06 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 3 and 21°C, with $t_{1/2} > 6 \text{ d}$ at pH 7 (Yao & Haag 1991).

$k_{HO}(\text{calc}) = 4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous solutions (Haag & Yao 1992)

Hydrolysis: base rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C with a calculated $t_{1/2} > 900 \text{ yr}$ at pH 7 (Ellington et al. 1988)

Biodegradation: dechlorination pseudo-first order rate constant $k = 0.387 \text{ d}^{-1}$ with $t_{1/2} = 1.8 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 8300 \text{ d}^{-1}$; $k_2 = 0.45 \text{ d}^{-1}$ (guppy, exptl., Könemann & van Leeuwen 1980)

$k_2 = 0.45 \text{ d}^{-1}$ (guppy, exptl., Könemann & van Leeuwen 1980)

$k_1 = 18.7 \text{ h}^{-1}$; $1/k_2 = 53 \text{ h}$ (guppy, quoted, Hawker & Connell 1985)
 $\log k_1 = 2.50 \text{ d}^{-1}$; $\log k_2 = -0.35 \text{ d}^{-1}$ (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)
 $k_1 = 780 \text{ mL g}^{-1} \cdot \text{d}^{-1}$; $k_2 = 0.42 \text{ d}^{-1}$ (guppy, Van Hoogan & Opperhuizen 1988)
 $k_1 = 780 \pm 220 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.42 \pm 0.06 \text{ d}^{-1}$ (guppy, 96-h exposure studies, Sijm et al. 1993)
 $k_1 = (23\text{--}29) \text{ mL g}^{-1} \text{ d}^{-1}$, $k_2 = (5\text{--}3) \text{ d}^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in one day or 12 sunlit hour at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

Surface Water: $t_{1/2} = 1.9\text{--}30 \text{ d}$, surface waters in various locations in the Netherlands in case of first order reduction process may be assumed (estimated, Zoeteman et al. 1980)

hydrolysis $t_{1/2} > 900 \text{ yr}$ at pH 7 and 25°C (Ellington et al. 1988)

$k(\text{exptl}) \leq 0.006 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with $t_{1/2} > 6 \text{ d}$ at pH 7 (Yao & Haag 1991)

Groundwater:

Sediment: dechlorination $t_{1/2} = 1.8 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota: biological $t_{1/2} < 1 \text{ d}$ in trout, $t_{1/2} = 2 \text{ d}$ in sunfish and $t_{1/2} = 2 \text{ d}$ in guppy for trichlorobenzenes (Niimi 1987)
 $t_{1/2} < 5 \text{ d}$ in worm at 8°C (Oliver 1987a).

TABLE 6.1.1.5.1

Reported aqueous solubilities, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,3-trichlorobenzene at various temperatures

Aqueous solubility		log K_{OW}		log K_{OA}	
Shiu et al. 1997		Finizio & Di Guardo 2001		Harner & Mackay 1995	
shake flask-GC		GC-RT correlation		generator column-GC/ECD	
$t/^{\circ}\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$	$t/^{\circ}\text{C}$	log K_{OW}	$t/^{\circ}\text{C}$	log K_{OA}
5	7.66	5	3.91	25	5.19
25	19.31	15	3.84	-10	6.491
50	45.61	25	3.81	0	6.073
		35	2.64	9.88	5.699
				19.85	5.829
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 55.7$					
$\log K_{OA} = A + B/T$					
A					-4.6
B					2909

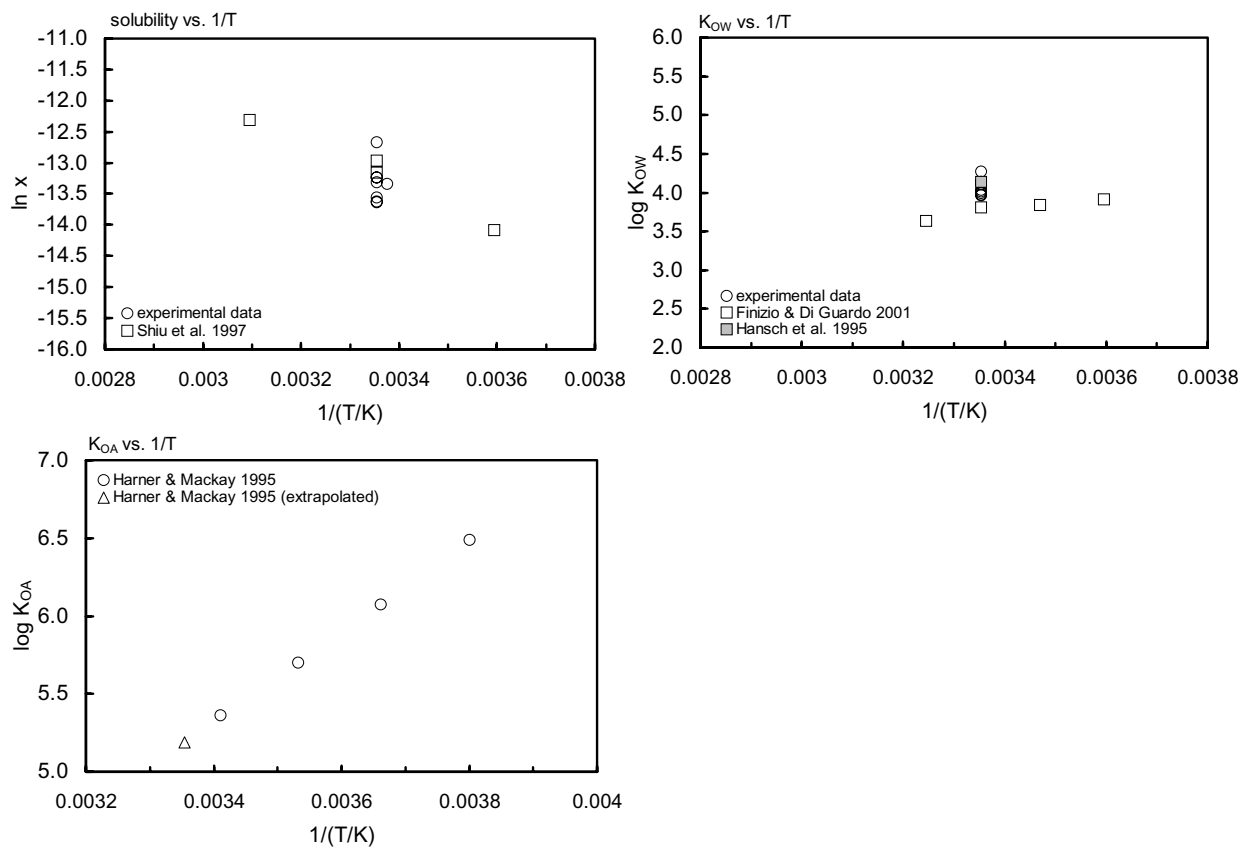


FIGURE 6.1.1.5.1 Logarithm of mole fraction solubility, K_{OW} and K_{OA} versus reciprocal temperature for 1,2,3-trichlorobenzene.

TABLE 6.1.1.5.2

Reported vapor pressures of 1,2,3-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \ln P = A - B/(C + T/K) & (3a) \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & & \\ \ln(P/P_0) &= (1 - T/T_0) \cdot \exp[\Sigma A_i T^i] & (5) - \text{Cox eq.} & & \end{aligned}$$

1.

Stull 1947		Liu & Dickhut 1994		Poledniecek et al. 1996			
summary of lit. data		gas saturation-GC		static method-pressure gauge			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
40	133.3	−15	0.124	0.36	0.94	60.11	268.14
70	666.6	5.0	0.445	0.38	0.955	70.04	472.25
85.5	1333	10	2.80	10.35	2.971	80.01	789.67
101.8	2666	25	11.2	10.36	2.965	80.01	799.36
119.8	5333	40	50.5	20.35	8.820	88.72	1241.7
131.5	7999			20.37	8.834	88.73	1238.8
146.0	13332	$\Delta H_v/(\text{kJ mol}^{-1}) = 54.5$		30.28	23.62	92.95	1305.6
168.2	26664	(−15 to 40°C)		30.28	23.66	98.72	1995.1
193.5	53329			50.12	146.0	108.67	3055.0
218.5	101325	for solid		50.12	145.5	118.69	4618.2
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 72.7$		25	14.07	128.73	6805.3
mp/°C	52.5				interpolated	138.77	9800.6
						138.78	9788.7
					solid	148.88	13815
				eq. 3a	P/Pa	158.88	19090
				A	33.2977	168.95	25970
				B	9327.37		
				C	6.13455		
							liquid
						eq. 3a	P/Pa
						A	21.1681
						B	4077.21
						C	−71.5639

Sears & Hopke 1949	
Rodebush gauge	
t/°C	P/Pa
measure range: 16–30°C	
mp/°C	52.55 to 52.70
eq. 1	P/micron
A	13.662
B	3440.2

2.

Roháč et al. 1999			
recommended			
T/K	P/Pa	T/K	P/Pa
	solid		liquid
233.15	0.003	333.15	272.4
243.15	0.015	343.25	479.4
253.15	0.065	353.15	812.0

(Continued)

TABLE 6.1.1.5.2 (Continued)

Roháč et al. 1999			
recommended			
T/K	P/Pa	T/K	P/Pa
263.15	0.26	363.15	1329
273.15	0.90	373.15	2106
283.15	2.90	383.15	3245
283.15	8.50	393.15	4868
303.15	23.1	403.15	7130
313.15	58.9	413.15	10220
323.15	140.9	423.15	14340
		433.15	19760
Data fitted to Cox eq.		443.15	26760
For solid		453.15	35700
eq. 5	P/Pa	463.15	46860
A_0	3.380608	473.15	6730
$10^{-4}A_1$	-2.5802866	483.15	77730
A_2	0	493.15	98350
T_0/K	325.6	503.15	123100
P_0/Pa	173.0		
bp/K	494.45	Cox eq.	
temp range 273–323 K		eq. 5	P/Pa
		A_0	3.274398
		$10^{-3}A_1$	-1.0923018
		$10^{-7}A_2$	7.8603029
		T_0/K	325.6
		P_0/Pa	173.0
		bp/K	494.45
		temp range 333–448 K	

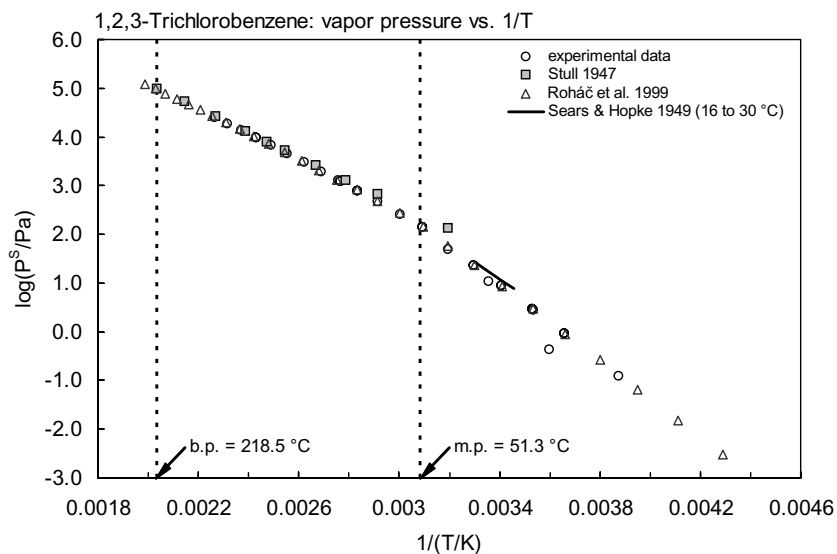
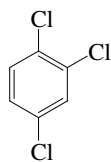


FIGURE 6.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3-trichlorobenzene.

6.1.1.6 1,2,4-Trichlorobenzene



Common Name: 1,2,4-Trichlorobenzene

Synonym: unsym-trichlorobenzene

Chemical Name: 1,2,4-trichlorobenzene

CAS Registry No: 120-82-1

Molecular Formula: $C_6H_3Cl_3$

Molecular Weight: 181.447

Melting Point ($^{\circ}C$):

16.92 (Lide 2003)

Boiling Point ($^{\circ}C$):

213.5 (Weast 1972–73; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4542 (Weast 1972–73)

1.446 (Dean 1985, 1992)

1.459 (Lide 2003)

Molar Volume (cm^3/mol):

124.8 ($20^{\circ}C$, calculated-density)

158.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.48 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

53.56 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio, at $25^{\circ}C$, F: 1.0 (Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

25.03 (Irmann 1965)

34.7 (shake flask-UV, Yalkowsky et al. 1979)

30.0 (Callahan et al. 1979)

19.4 (shake flask-GC, Könemann 1981)

30.0 (recommended, Hovarth 1982)

48.8 ($20^{\circ}C$, shake flask-GC, Chiou & Schmedding 1981; Chiou et al. 1982; 1983)

46.1 (generator column-GC/ECD, Miller et al. 1984; 1985)

31.3 (shake flask-HPLC/UV, Banerjee 1984)

30.9 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

34.6 (shake flask-GC, Chiou 1985)

52.0 (shake flask-GC, Boyd et al. 1998)

36.5 ± 0.36 (shake flask-GC/FID, measured range 5 – $45^{\circ}C$, Ma et al. 2001)

7.71, 10.39, 13.58, 19.82 (5, 15, 25, $35^{\circ}C$, estimated- RP-HPLC- k' correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($38.4^{\circ}C$, summary of literature data, temp range 38.4 – $213^{\circ}C$, Stull 1947)

38.6 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.19608 - 1827.0/(210.0 + t/^{\circ}C)$; temp range 110 – $280^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

60.6 (extrapolated-Antoine eq., supercooled liquid, Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 11425.1/(T/K)] + 8.030523$; temp range 38.4 – $213^{\circ}C$ (Antoine eq., Weast 1972–73)

- 26.4 (gas saturation, Politzki et al. 1982)
 28.5 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
 38.7 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_g/\text{kPa}) = 9.570 - 3254/(T/K)$; temp range 279–290 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.31998 - 1827/(-63.15 + T/K)$; temp range 383–553 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.6802 - 2064.4/(-43.05 + T/K)$; temp range 293–383 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
 53.4 (supercooled liquid P_L , GC-Kovács retention indices correlation; Spijksma et al. 1994)
 $\log (P/\text{mmHg}) = 15.5947 - 2.8920 \times 10^3/(T/K) - 2.5549 \cdot \log (T/K) + 2.0384 \times 10^{-4} \cdot (T/K) - 7.0601 \times 10^{-14} \cdot (T/K)^2$, temp range 290–725 K, (Yaws 1994)
 5728* (118.671°C, comparative ebulliometry, measured range 118.671–215.887°C, Roháč et al. 1998)
 24.2* (20°C, recommended, summary of literature data, temp range 293.15–493.15 K, Roháč et al. 1999)
 $\ln [(P/\text{Pa})/19.0] = [1 - (T/K)/290.07] \cdot \exp\{3.352607 - 9.0343639 \times 10^{-4} \cdot (T/K) + 6.0501757 \times 10^{-7} \cdot (T/K)^2\}$; temp range 294–489 K (Cox eq., recommended, Roháč et al. 1999)
 $\log (P/\text{kPa}) = 9.570 - 3254/(T/K)$; temp range 6–17°C (solid, regression eq. from literature data, Shiu & Ma 2000)
 $\log (P/\text{kPa}) = 6.682 - 2064.4/[(T/K) - 43.5]$; temp range 20–110°C (liquid, regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 122 (gas stripping-GC, Oliver 1985)
 144 (gas stripping-GC, Warner et al. 1987)
 195* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = -16.34 + 3307/(T/K)$; temp range 10–30°C (EPICS-GC/FID, Ashworth et al. 1988)
 101 (gas stripping-GC, ten Hulscher et al. 1992)
 375.2 (modified EPICS method-GC, Ryu & Park 1999)
 172 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 4.381 - 1622/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 4.05 (Leo et al. 1971)
 4.26 (Callahan et al. 1979)
 4.02 (Hansch & Leo 1979; Hansch & Leo 1985)
 3.93 (shake flask-GC, HPLC-k' correlation, Könemann et al. 1979)
 4.02 (20°C, shake flask-GC, Chiou & Schmedding 1981; Chiou et al. 1982; Chiou 1985)
 3.97 (shake flask-GC, Watarai et al. 1982)
 3.96 (HPLC-k' correlation, Hammers et al. 1982)
 3.93–4.18, 4.09 (range, mean, shake flask method, Eadsforth & Moser 1983)
 4.12–4.32, 4.21 (range, mean, HPLC method, Eadsforth & Moser 1983)
 3.98 (generator column-GC/ECD, Miller et al. 1984; 1985)
 4.22 (HPLC-k' correlation, De Kock & Lord 1987)
 4.02 (shake flask-GC, Pereira et al. 1988)
 4.05 (slow stirring-GC, De Bruijn et al. 1989)
 4.02 (recommended, Sangster 1993)
 4.02 (recommended, Hansch et al. 1995)
 3.92* (estimated- RP-HPLC-k' correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.

- 5.10* (20°C, HPLC-k' correlation, measured range 10–50°C, Su et al. 2002)
 $\log K_{OA} = 62080/(2.303 \cdot RT) - 6.031$; temp range 10–50°C (HPLC-k' correlation, Su et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

- 3.32 (fathead minnow, 32-d exposure, Veith et al. 1979b)
- 3.45; 3.37; 2.95 (fathead minnow; green sunfish; rainbow trout, Veith et al. 1979b)
- 2.69 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980a)
- 2.26 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
- 3.52 (microorganism-water, Mabey et al. 1982)
- 3.04–3.11 mean 3.11; 3.43–3.60 mean 3.51 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
- 4.19–4.56 (rainbow trout, lipid base, Oliver & Niimi 1983)
- 3.26–3.61 (fish, Oliver 1984, 1985)
- 2.40 (algae, Geyer et al. 1984)
- 3.15 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
- 2.40, 2.69, 3.15 (algae, fish, sludge, Klein et al. 1984)
- 3.15–3.72 mean 3.36; 3.30–3.75 mean 3.57 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)
- 3.11; 3.08 (rainbow trout, wet wt. basis, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)
- 4.19–4.56 (rainbow trout, lipid base, Oliver & Niimi 1985)
- 2.09; 3.84 (quoted, rainbow trout, 1.8% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
- 2.28, 2.40, 2.34, 2.66 (quoted, carp, 2.2% lipid, wet wt basis, Geyer et al. 1985)
- 3.94, 3.96, 4.0, 4.32 (quoted, carp, 2.2% lipid, lipid basis, Geyer et al. 1985)
- 2.54; 4.04 (quoted, rainbow trout, hatching, 3.2% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
- 2.66, 2.73; 4.02, 4.09 (quoted, carp, 4.4% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
- 2.96; 4.26 (quoted, golden ide, 5.0% lipid, wet wt basis, lipid basis, Geyer et al. 1985)
- 2.86, 2.94; 4.15, 4.19 (quoted, zebra fish, 5.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 2.83, 3.12; 4.12, 4.22 (quoted, tilapia, 5.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 2.98, 3.12; 4.23, 4.36 (quoted, bluegill sunfish, 5.7% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 3.13, 3.14; 4.37, 4.38 (quoted, guppy, 5.8% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 3.11, 3.20; 4.23, 4.38 (quoted, rainbow trout, 7.7%, wet wt basis; lipid basis, Geyer et al. 1985)
- 2.96, 3.03; 4.05, 4.23 (quoted, guppy, 8.2% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 3.11; 4.19 (quoted, rainbow trout, 8.3% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
- 3.32; 4.30 (quoted, fathead minnow, 10.5% lipid, wet wt basis, lipid basis Geyer et al. 1985)
- 2.69; 2.40; 3.15 (fish; algae; activated sludge, Freitag et al. 1985)
- 2.61 (fathead minnow, Carlson & Kosian 1987)
- 4.76, 4.90, 3.54, 4.68 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
- 3.31, 4.25 (American flagfish, whole fish, fish lipid, Smith et al. 1990)
- 2.95–3.57; 3.31; 3.32; 3.36 (*Oncorhynchus mykiss*; *Jordanella floridae*; *Pimephales promelas*; *Lepomis cyanellus*, quoted lit., flow through conditions, Devillers et al. 1996)
- 3.0, 3.06, 3.06 (guppy: k_1/k_2 -best fit exptl. data, k_1/k_2 -slope method, C_f/C_w -steady state, van Eck et al. 1997)
- 3.81; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{oc} :

- 2.80 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 2.68–3.94 (5 soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
- 4.70; 4.40 (field data of sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
- 4.3–5.1, 5.10; 5.10 (suspended sediment, average; algae > 50 μ m, Oliver 1987c)
- 4.8–5.3, 5.0 (Niagara River plume, range, mean, Oliver 1987b)
- 3.91 (untreated Marlette soil A horizon, organic carbon OC 2.59%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.66, 3.40 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48%; DDTMA treated, OC 4.37%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.27 (untreated Marlette soil B₁ horizon, 0.30% OC, equilibrium isotherm, Lee et al. 1989)

- 3.91, 3.64, 3.04 (organic cations treated Marlette soil B_t horizon: HDTMA treated OC 3.72%, DDTMA treated OC 1.98%, NTMA treated, OC 1.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.32 (calculated- K_{OW} , Aldrich or Fluka humic acid polymers, Chin & Weber 1989)
- 3.32; 2.62 (Aldrich humic acid, organic polymers, Chin et al. 1990)
- 4.02 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
- 2.71, 2.71 (RP-HPLC- k' correlation including: MCI-related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 3.86 \pm 0.40 (suspended particulates in coastal waters, Masunaga et al. 1996)
- 3.15, 3.19, 3.10 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, 0.1 \leq OC < 0.5%, average, Delle Site 2001)
- 4.38–3.24 (NIST SRM diesel particulate matter, sorption isotherm, Ngyuen et al. 2004)

Sorption Partition Coefficient, log K_{OM} :

- 2.70 (Woodburn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm, Chiou et al. 1983)
- 2.89 (untreated Marlette soil A horizon, organic matter OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 3.47, 3.17 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03%; DDTMA treated, OM 5.18%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
- 2.97 (untreated Marlette soil B_t horizon, 0.30% OC, equilibrium sorption isotherm, Lee et al. 1989)
- 3.97, 3.50, 2.87 (organic cations treated Marlette soil B_t horizon: HDTMA treated OM 4.85%, DDTMA treated OM 2.73%, NTMA treated, OM 1.74%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: rate constants: $k = 0.032 \text{ d}^{-1}$ with $t_{1/2} = 22 \text{ d}$ in spring at 8–16°C, $k = 0.066 \text{ d}^{-1}$ with $t_{1/2} = 11 \text{ d}$ in summer at 20–22°C, $k = 0.058 \text{ d}^{-1}$ with $t_{1/2} = 12 \text{ d}$ in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.073 \text{ d}^{-1}$ with $t_{1/2} = 9.5 \text{ d}$ with HgCl_2 , and $k = 0.066 \text{ d}^{-1}$ with $t_{1/2} = 10.6 \text{ d}$ without HgCl_2 in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Photolysis: not environmentally relevant (Mabey et al. 1982)

$t_{1/2} = 450 \text{ yr}$ for surface water photolysis at 40°N latitude in the summer (Dulin et al. 1986)

$k = 1.16 \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 at 25°C in F-113 solution and with HO \cdot in the gas (Dilling et al. 1988)

$k = 0.03 \text{ h}^{-1}$, the maximum summer photolysis rate calculated at midday clear sky, the minimum photolytic $t_{1/2} \sim 4 \text{ months}$, but a realistic value is likely to be at least 1 yr (Bunce et al. 1989)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 7.22 \times 10^{-3} \text{ h}^{-1}$ (Simmons et al. 1976; selected, Mackay et al. 1985)

$k_{OH} \sim 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

$k(\text{singlet oxygen}) \ll 360 \text{ M}^{-1} \text{ h}^{-1}$; $k(\text{RO}_2 \text{ radical}) \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982)

$k \ll 1.6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 10 mM *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 5.32 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 273–368 K (flash photolysis-resonance fluorescence, Rinke & Zetzsch 1984)

$k_{OH}(\text{obs.}) = 5.32 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{OH}(\text{calc}) = 3.47 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{OH}(\text{calc}) = 0.29 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs}) = 0.532 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}(\text{aq.}) = 4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous solutions (Haag & Yao 1992)

$k_{OH}(\text{calc}) = 0.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: not environmentally significant (Mabey et al. 1982);

base rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C with a calculated $t_{1/2} > 900 \text{ yr}$ at pH 7 (Ellington et al. 1988)

first-order rate constant $k = 2.3 \times 10^{-5} \text{ h}^{-1}$ with $t_{1/2} = 3.4 \text{ yr}$ at pH 7 and 25°C (Howard et al. 1991).

Biodegradation: $k = 1.92 \times 10^{-2} \text{ h}^{-1}$, degradation in water (Simmons et al. 1976)

$t_{1/2}(\text{aq. aerobic}) = 672\text{--}4320 \text{ h}$ estimated from unacclimated soil grab sample data (Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 2688\text{--}17280 \text{ h}$ based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$k = 0.05 \text{ d}^{-1}$, significant degradation in an aerobic environment (Tabak et al. 1981; Mills 1982)

$k = 0.029 \text{ d}^{-1}$ in river water, $k = 0.026 \text{ d}^{-1}$ in estuarine water, and $k = 0.012 \text{ d}^{-1}$ in marine water (Bartholomew & Pfaender 1983; Battersby 1990)

$t_{1/2}(\text{aerobic}) = 28 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 110 \text{ d}$ in natural waters (Capel & Larson 1995)

$k = 0.035 \text{ d}^{-1}$, the dechlorination pseudo-first order rate constant, with $t_{1/2} = 19.8 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000)

Biotransformation: $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 8300 \text{ d}^{-1}$; $k_2 = 0.45 \text{ d}^{-1}$ (guppy, exptl., Könemann & Van Leeuwen 1980)

$k_1 = 18.7 \text{ h}^{-1}$; $1/k_2 = 53.0 \text{ h}$ (guppy, selected, Hawker & Connell 1985)

$\log k_1 = 2.65 \text{ d}^{-1}$; $\log 1/k_2 = 0.34 \text{ d}$ (guppy, selected, Connell & Hawker 1988)

$\log k_2 = -1.85 \text{ d}^{-1}$; $\log k_2 = 0.23 \text{ d}^{-1}$ (fish, calculated- K_{ow} , fast-biphasic, Thomann 1989)

$k_1 = 1158 \text{ d}^{-1}$, 10140 d^{-1} ; $k_2 = 0.57 \text{ d}^{-1}$, 0.57 d^{-1} (American flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 0.57 \text{ d}^{-1}$, 0.46 d^{-1} (American flagfish: bioconcentration data, toxicity data, Smith et al. 1990)

$k_1 = 492 \pm 234 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.49 \pm 0.22 \text{ d}^{-1}$ (guppy, exptl., van Eck et al. 1997)

Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in one day or 12 sunlit hour at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

calculated minimum photolytic $t_{1/2} \sim 4$ months, but realistically at least 1 yr (Bunce et al. 1989);

tropospheric lifetime of 25 d based on reaction principally with OH radical and other photochemical reactions (Bunce 1991);

$t_{1/2} = 128.4\text{--}1284 \text{ h}$, based on the photooxidation with OH radical (Howard et al. 1991).

Surface Water: $t_{1/2} = 2.1\text{--}28 \text{ d}$ estimated for various locations in the Netherlands, $t_{1/2} = 0.3\text{--}3 \text{ d}$ for river water, $t_{1/2} = 3\text{--}30 \text{ d}$ for lakes estimated from persistence (Zoeteman et al. 1980);

half-lives from marine mesocosm: $t_{1/2} = 22 \text{ d}$ in the spring at $8\text{--}16^\circ\text{C}$, $t_{1/2} = 11 \text{ d}$ in the summer at $20\text{--}22^\circ\text{C}$ and $t_{1/2} = 12 \text{ d}$ in the winter at $3\text{--}7^\circ\text{C}$ when volatilization dominates, and $t_{1/2} = 9.5 \text{ d}$ and 10.6 d for experiments with and without HgCl_2 respectively in September 9–15 (Wakeham et al. 1983)

hydrolysis $t_{1/2} > 900 \text{ yr}$ at pH 7 and 25°C (Ellington et al. 1988)

$t_{1/2}(\text{aerobic}) = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic soil grab sample data; $t_{1/2}(\text{anaerobic}) = 2688\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life; and first order hydrolysis $t_{1/2} = 3.4 \text{ yr}$ (Howard et al. 1991);

$t_{1/2}(\text{aerobic}) = 28 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 110 \text{ d}$ in natural waters (Capel & Larson 1995)

Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 30\text{--}300 \text{ d}$ estimated from persistence (Zoeteman et al. 1980).

Soil: $t_{1/2} < 10 \text{ d}$ (Ryan et al. 1988)

$t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic soil grab sample data (Howard et al. 1991).

Sediment: dechlorination $t_{1/2} = 19.8 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biota: $1 < t_{1/2} < 3 \text{ d}$ in blue bluegill sunfish (Barrows et al. 1980);

biological half-lives, $t_{1/2} < 1 \text{ d}$ in trout, $t_{1/2} = 2 \text{ d}$ in sunfish, and $t_{1/2} = 2 \text{ d}$ in guppy for trichlorobenzenes (Niimi 1987);

$t_{1/2} < 5 \text{ d}$ in worms at 8°C (Oliver 1987a);

depuration $t_{1/2} = 1.21 \text{ d}$ from whole fish, $t_{1/2} = 1.20 \text{ d}$ from fish lipid (American flagfish, Smith et al. 1990).

TABLE 6.1.1.6.1

Reported aqueous solubilities of 1,2,4-trichlorobenzene at various temperatures

Ma et al. 2001		Finizio & Di Guardo 2001	
shake flask-GC		RP-HPLC-k' correlation	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
5	32.9	5	7.71
15	28.5	15	10.39
25	36.5	25	13.58
35	39.8	35	19.82
45	46.5		

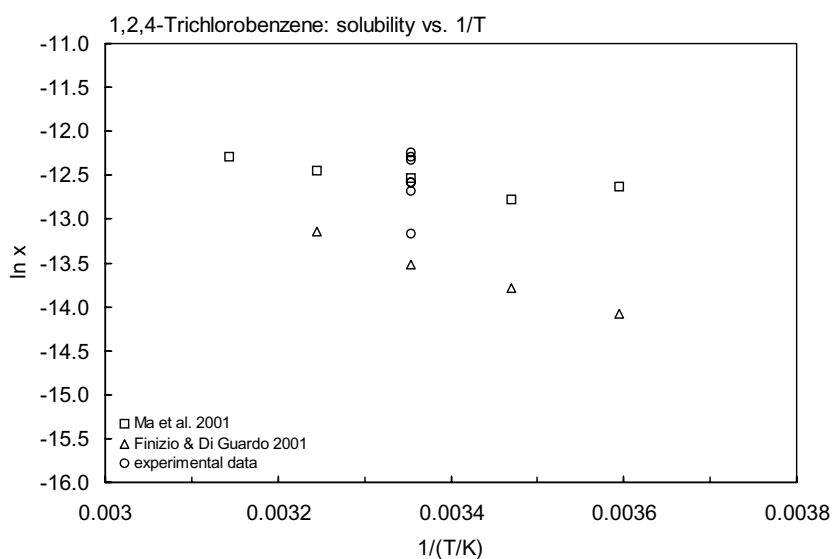


FIGURE 6.1.1.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1,2,4-trichlorobenzene.

TABLE 6.1.1.6.2

Reported vapor pressures of 1,2,4-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)	$\ln P = A - B/(C + T/K)$		(3a)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
$\ln (P/P_o) = (1 - T/T_o) \cdot \exp[\Sigma A_i T^i]$		(5) - Cox eq.					
Stull 1947		Sears & Hopke 1949		Roháč et al. 1998		Roháč et al. 1999	
summary of literature data		Rodebush gauge		comparative ebulliometry		recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
38.4	133.3	measured range: 6–25°C		118.671	5728	293.15	24.2
67.3	666.6			128.383	8331	303.15	51.2
81.7	1333	mp/°C	17.05–17.40	136.228	11070	313.15	102.4
97.2	2666			142.813	13911	232.15	194.7
114.8	5333	for solid:-		142.819	13914	333.15	354.0
125.7	7999	eq. 1	P/micron	148.44	16794	343.25	617.7
140	13332	A	13.445	154.289	20281	353.15	1038
162	26664	B	3254.0	154.308	20290	363.15	1687
187.7	53329			160.441	24566	373.15	2658
213	101325	for liquid:-		166.386	29387	383.15	4071
mp/°C	17.0	eq. 1	P/micron	172.180	34807	393.15	6075
		A	10.682	177.755	40745	403.15	8854
		B	2452.3	183.424	47613	413.15	12630
				192.328	60271	423.15	17650
				192.331	60264	433.15	224210
				200.386	74748	443.15	32650
				209.989	93380	453.15	43360
				212.397	98847	463.15	56740
				215.887	107216	473.15	73260
						483.15	93420
		bp/°C	213.492	493.15	117800		
		eq. 3	P/kPa	eq. 5	P/Pa		
		A	6.11973	A ₀	3.352607		
		B	1677.35	10 ⁻³ A ₁	–9.0343639		
		C	–78.926	10 ⁻⁷ A ₂	6.0501757		
				T _o /K	290.07		
				P _o /Pa	19.0		
				bp/K	486.60		
				temp range 294–489 K			

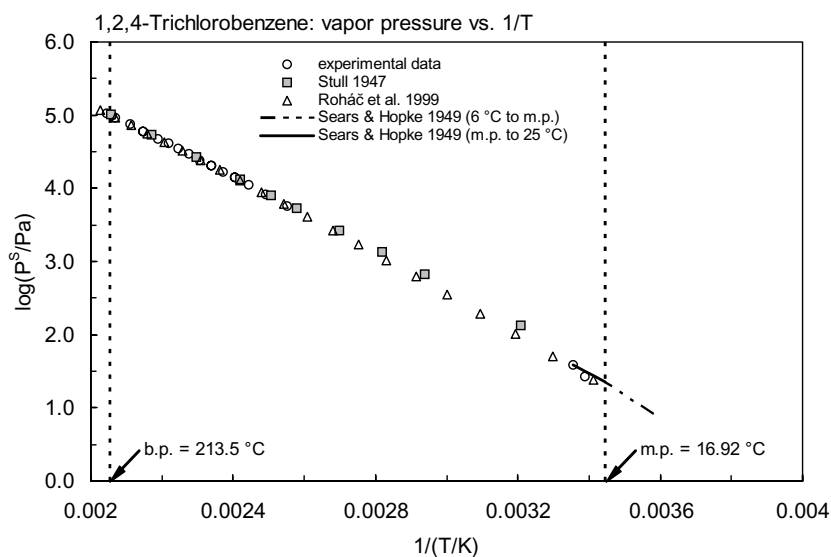


FIGURE 6.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4-trichlorobenzene.

TABLE 6.1.1.6.3

Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,4-trichlorobenzene at various temperatures

Henry's law constant		log K _{OW}		log K _{OA}	
Ashworth et al. 1988		Finizio & Di Guardo 2001		Su et al. 2002	
EPICS-GC		HPLC-RT correlation		GC-RT correlation	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OW}	t/°C	log K _{OA}
10	131	5	4.12	10	5.45
15	106	15	4.02	20	5.1
20	185	25	3.92	30	4.77
20	195	35	3.8	40	4.46
30	301			50	4.17
ln (H/(atm m ³ /mol)) = A - B/(T/K)				ΔH _{OA} /(kJ mol ⁻¹) = 62.08	
A	7.261			log K _{OA} = A + B/2.303RT	
B	4028			A	-6.031
				B	62080

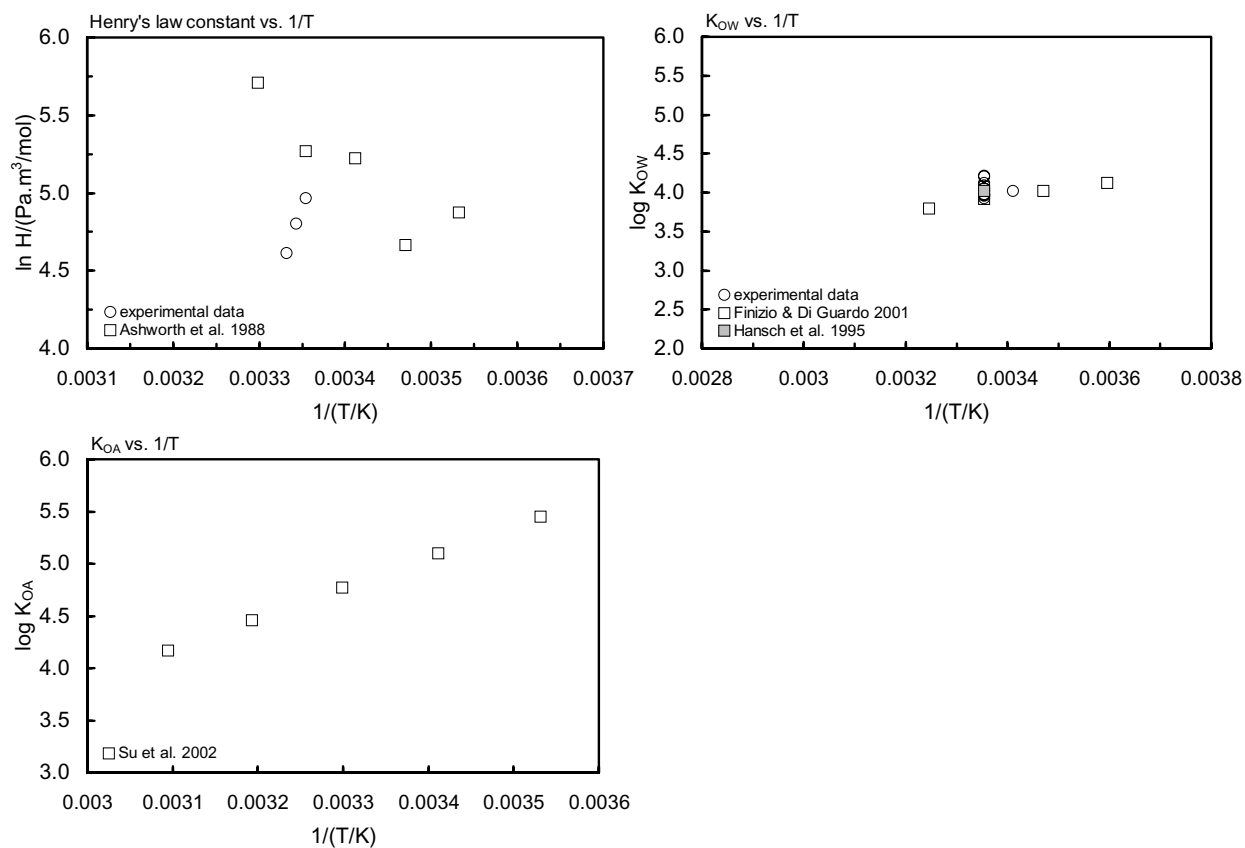
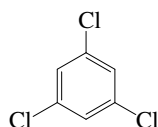


FIGURE 6.1.1.6.3 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for 1,2,4-trichlorobenzene.

6.1.1.7 1,3,5-Trichlorobenzene



Common Name: 1,3,5-Trichlorobenzene

Synonym: sym-trichlorobenzene

Chemical Name: 1,3,5-trichlorobenzene

CAS Registry No: 108-70-3

Molecular Formula: $C_6H_3Cl_3$

Molecular Weight: 181.447

Melting Point ($^{\circ}C$):

62.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

208.0 (Weast 1972–72, 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.3865 ($64^{\circ}C$, Weast 1972–73; Horvath 1982)

Molar Volume (cm^3/mol):

130.9 ($64^{\circ}C$, calculated-density)

125 (calculated-density, liquid molar volume, Chiou 1985)

158.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.622 (Tsonopoulos & Prausnitz 1971)

18.786 (Miller et al. 1984)

18.198 (Ruelle et al. 1993; Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

58.16 (Tsonopoulos & Prausnitz 1971)

56.07 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.426 (mp at $62.8^{\circ}C$)

0.413 ($25^{\circ}C$, Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

25.03 (Tsonopoulos & Prausnitz 1971)

6.59 (shake flask-UV, Yalkowsky et al. 1979)

5.87 (shake flask-GC, Könnemann 1981)

6.61 (recommended, Hovarth 1982)

4.12 (generator column-GC/ECD, Miller et al. 1984, 1985)

6.01 (shake flask-HPLC, Banerjee 1984)

10.6 (shake flask-GC, Chiou 1985)

6.53 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

$8.46^* \pm 0.26$ (generator column-GC/ECD, measured range 5 – $45^{\circ}C$, Shiu et al. 1997)

2.40 (shake flask-GC, Boyd et al. 1998)

$\ln x = -5.083768 - 2650.68/(T/K)$, temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* ($63.8^{\circ}C$, summary of literature data, temp range 63.8 – $208.4^{\circ}C$, Stull 1947)

77 (extrapolated-Antoine eq., supercooled liquid, Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 11211.0/(T/K)] + 7.977218$; temp range 63.8 – $208.4^{\circ}C$ (Antoine eq., Weast 1972–73)

30.23 (gas saturation, interpolated from reported graph, Rordorf 1985)

24.4 (solid, extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 8.301 - 2956/(T/\text{K})$; temp range 282–301 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.43345 - 1932.26/(-45.268 + T/\text{K})$; temp range 336–482 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

124.4 (GC-RT correlation, Watanabe & Tatsukawa 1989)

62.4; 74.9 (supercooled liquid P_L , GC-Kovács retention indices correlation; quoted lit., Spieksma et al. 1994)

$\log (P/\text{mmHg}) = 19.2854 - 4.4976 \times 10^3/(T/\text{K}) - 3.6158 \cdot \log (T/\text{K}) - 5.2495 \times 10^{-9} \cdot (T/\text{K}) + 1.5596 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 398–748 K (Yaws 1994)

12.4, 20.44* (20.35°C pressure gauge measurement, 25°C interpolated from reported Antoine eq. based on exptl. data, Polednicek et al. 1996)

$\ln (P_s/\text{Pa}) = 32.5109 - 8909.70/[(T/\text{K}) + 3.94116]$; temp range 273–333 K (Antoine eq. from exptl data, pressure gauge measurement, solid, Polednicek et al. 1996)

$\ln (P_L/\text{Pa}) = 21.1215 - 3939.96/[(T/\text{K}) - 71.2907]$; temp range 343–442 K (Antoine eq. from exptl data, pressure gauge measurement, liquid, Polednicek et al. 1996)

12.5 (20°C, recommended, summary of literature data, temp range 233.15–483.15 K, Roháč et al. 1999)

$\ln [(P_s/\text{Pa})/565.0] = [1 - (T/\text{K})/337.0] \cdot \exp\{3.305508 - 2.3049477 \times 10^{-4} \cdot (T/\text{K})\}$; temp range 273–333 K (Cox eq., solid, recommended, Roháč et al. 1999)

$\ln [(P_L/\text{Pa})/547.0] = [1 - (T/\text{K})/336.6] \cdot \exp\{3.190854 - 1.0710853 \times 10^{-3} \cdot (T/\text{K}) + 7.5659237 \times 10^{-7} \cdot (T/\text{K})^2\}$; temp range 343–442 K (Cox eq., liquid, recommended, Roháč et al. 1999)

32.3* (29.33°C, static method-diaphragm manometer, measured range 29–142°C, Blok et al. 2001)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

192.5 (20°C, batch stripping-GC, Oliver 1985)

192 (gas stripping-GC/ECD, ten Hulscher et al. 1992)

Octanol/Water Partition Coefficient, $\log K_{ow}$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

4.02 (Leo et al. 1971; Hansch & Leo 1979)

4.15 (shake flask-GC, HPLC- k' correlation, Könemann et al. 1979)

4.17 (shake flask-GC, Watarai et al. 1982)

4.17 (HPLC- k' correlation, Hammers et al. 1982)

4.02 (generator column-GC/ECD, Miller et al. 1984; 1985)

4.18 (HPLC-RV correlation, Garst 1984)

4.31 (shake flask-GC, Chiou 1985)

4.49 (Hansch & Leo 1985)

4.32* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)

4.31 (shake flask-GC, Pereira et al. 1988)

4.189 (slow stirring-GC, De Bruijn et al. 1989)

4.15 (recommended, Sangster 1993)

4.19 (recommended, Hansch et al. 1995)

4.34* ± 0.04 (shake flask-GC/ECD, Bahadur et al. 1997)

$\log K_{ow} = 1.1228 - 18200/[2.303 \cdot R(T/\text{K})]$; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)

4.44 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:

4.85 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

4.89* (20°C HPLC- k' correlation, measured range 10–50°C, Su et al. 2002)

$\log K_{OA} = 68550/(2.303 \cdot RT) - 7.368$; temp range 10–50°C (HPLC- k' correlation, Su et al. 2002)

Bioconcentration Factor, $\log BCF$: at 25°C or as indicated

4.15 (guppy, lipid basis, Könemann & van Leeuwen 1980)

3.15–3.30 mean 3.26; 3.57–3.92 mean 3.61 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

4.34–4.67 (rainbow trout, lipid basis, Oliver & Niimi 1983)

3.26–3.61 (fish, Oliver 1984)

- 4.15 (guppy, female, 5.4% lipid, wet wt basis; lipid basis, Geyer et al. 1985)
 2.39–2.55 (fish, normalized, Tadokoro & Tomita 1987)
 4.14 (guppy-lipid phase, Gobas et al. 1987, 1989)
 2.88 (fish, calculated- C_B/C_W or k_1/k_2 , Connell & Hawker 1988; Hawker 1990)
 4.32, 4.35, 4.38, 4.43 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
 4.40, 4.45, 3.51, 4.22 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 3.26, 3.61; 3.48 (*Oncorhynchus mykiss*; *Poecilia reticula*, quoted lit., flow through conditions, Devillers et al. 1996)
 2.68 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
 3.26, 4.33; 3.271, 2.884 (quoted: whole fish, lipid content; calculated-MCI χ , K_{OW} , Lu et al. 1999)
 3.69; 3.64 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 5.10; 4.20 (field data of Lake Ontario sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
 2.85 (forest soil 0.2% OC, observed, Seip et al. 1986)
 4.13 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
 3.55 \pm 0.47 (suspended particulates in coastal waters, Masunaga et al. 1996)
 3.69 (soil: organic carbon OC \geq 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 4.5$ h from a model river of 1 m depth with water current 1 m/s and wind velocity 3 m/s at 20°C (Lyman et al. 1982).

Photolysis: may be susceptible to direct photolysis by sunlight (Howard 1989)

$t_{1/2} \sim 450$ yr for sunlight photolysis at 40°N in the summer (Dulin et al. 1986)

$k = 0.003 \text{ min}^{-1}$, measured pseudo-first-order direct photolysis reaction with $t_{1/2} = (205.5 \pm 7.5) \text{ min}$ in aqueous solution (Peijnenburg et al. 1992)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} \sim 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, residence time of 116 d, loss of 0.9% in one day or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

photooxidation $t_{1/2} = 6.17$ months, based on a measured rate for the vapor phase reaction with photochemically produced hydroxyl radicals in air (Atkinson et al. 1985).

Hydrolysis: will not hydrolyze under normal environmental conditions (Howard 1989).

Biodegradation: resistant to biodegradation (Tabak et al. 1964; Howard 1989);

dechlorination pseudo-first order rate constant $k = 0.069 \text{ d}^{-1}$ with $t_{1/2} = 10.1 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 8000 \text{ d}^{-1}$; $k_2 = 0.40 \text{ d}^{-1}$ (guppy, Könemann & van Leeuwen 1980)

$k_1 = 18.0 \text{ h}^{-1}$; $1/k_2 = 60 \text{ h}$ (guppy, quoted, Hawker & Connell 1985)

$k_1 = 430 \text{ d}^{-1}$ (fish, quoted, Opperhuizen 1986)

$\log k_1 = 2.63 \text{ d}^{-1}$; $\log k_2 = 0.440 \text{ d}^{-1}$ (fish, quoted, Connell & Hawker 1988)

$\log k_1 = 2.48 \text{ d}^{-1}$; $\log k_2 = -0.40 \text{ d}^{-1}$ (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)

$\log k_2 = -0.40 \text{ d}^{-1}$ (fish, calculated- K_{OW} , Thomann 1989)

$k_1 = 7 \text{ mL g}^{-1} \text{ d}^{-1}$, $k_2 = 3 \text{ d}^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air: residence time of 116 d, loss of 0.9% in 1 d or 12 sunlit hours at 300 K for trichlorobenzenes in urban environments (Singh et al. 1981)

Surface Water: $t_{1/2} = 18 \text{ d}$ under field conditions in the Netherlands in case of first order reduction process may be assumed (estimated, Zoeteman et al. 1980)

direct photolysis $t_{1/2} = 206 \text{ min}$ in aqueous solution (Peijnenburg et al. 1992)

Groundwater:.

Sediment: dechlorination $t_{1/2} = 1.8$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota: biological half-lives, $t_{1/2} < 1$ d in trout, $t_{1/2} = 2$ d in sunfish and $t_{1/2} = 2$ d in guppy for trichlorobenzenes (Niimi 1987);

$t_{1/2} < 5$ d in worms at 8°C (Oliver 1987a).

TABLE 6.1.1.7.1

Reported aqueous solubilities, octanol-water partition coefficients and octanol-air partition coefficients of 1,3,5-trichlorobenzene at various temperatures

Aqueous solubility		log K_{OW}				log K_{OA}	
Shiu et al. 1997		Oppenhuizen et al. 1988		Bahadur et al. 1997		Su et al. 2002	
shake flask-GC		shake flask-GC/ECD		shake flask-GC/ECD		GC-RT correlation	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	log K_{OW}	$t/^{\circ}\text{C}$	log K_{OW}	$t/^{\circ}\text{C}$	log K_{OA}
5	4.62	13	4.40	5	4.52	25	5.23
15	6.29	19	4.32	15	4.43	-10	4.89
25	8.46	28	4.04	25	4.34	0	4.56
35	11.14	33	3.93	35	4.21	10	4.26
45	15.55			45	4.09	18.7	3.98
$\Delta H_{\text{sol}} = 22.04$ kJ/mol		$\Delta H/(\text{kJ mol}^{-1}) = -21.7$		enthalpy of transfer $\Delta H/(\text{kJ mol}^{-1}) = -18.2$		$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 68.55$	
				$\log K_{\text{OW}} = A - \Delta H/2.303RT$		$\log K_{\text{OA}} = A + B/2.303RT$	
				A 1.1228		A -7.368	
				ΔH -18200		B 68500	

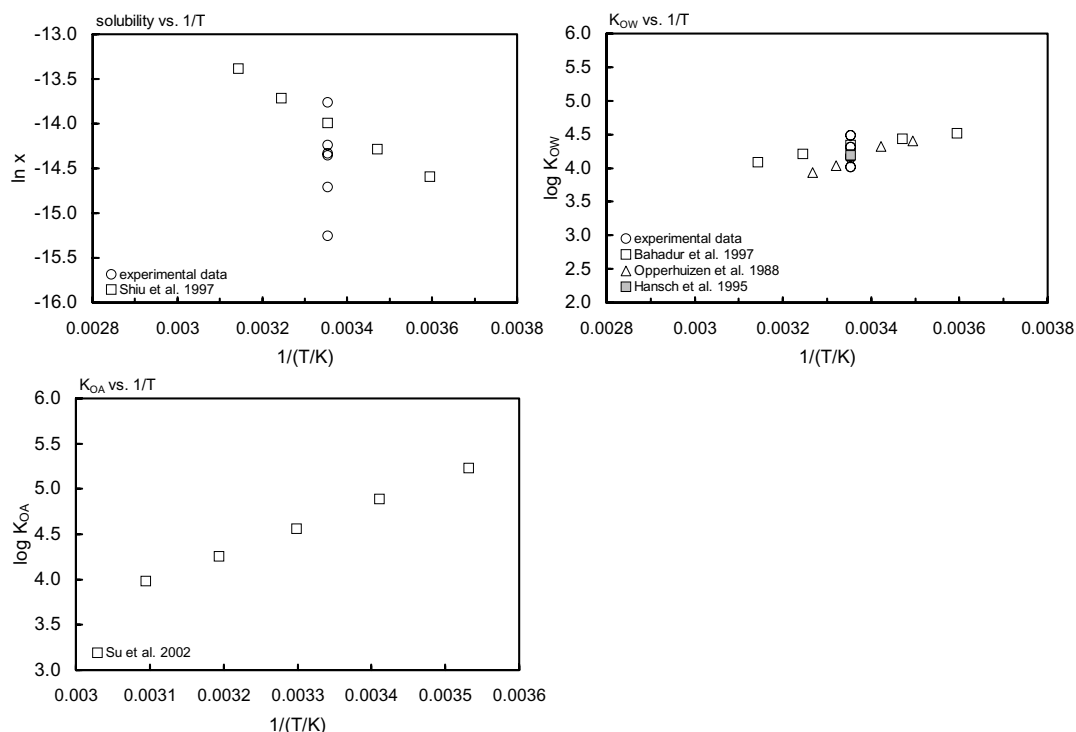


FIGURE 6.1.1.7.1 Logarithm of mole fraction solubility, K_{OW} and K_{OA} versus reciprocal temperature for 1,3,5-trichlorobenzene.

TABLE 6.1.1.7.2

Reported vapor pressures of 1,3,5-trichlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & \ln P = A - B/(C + T/K) & (3a) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Stull 1947		Sears & Hopke 1949		Poledniecek et al. 1996			
summary of lit. data		Rodebush gauge		pressure gauge			
t/ [°] C	P/Pa	t/ [°] C	P/Pa	t/ [°] C	P/Pa	t/ [°] C	P/Pa
63.8	666.6	measured between		0.29	solid	70.04	liquid
78.0	1333	9–28 [°] C	solid	0.29	1.493	70.05	760.47
93.7	2666			10.31	1.383	80.05	759.77
110.8	5333	eq. 1	P/μm	10.31	4.492	88.76	126.39
121.8	7999	A	12.176	20.25	4.556	88.77	1956.9
136.0	13332	B	2956.0	20.25	12.41	89.95	1954.0
157.7	26664			30.15	12.40	90.01	2007.8
183.0	53329	mp/ [°] C	63.45 to	30.15	34.58	99.25	2009.2
208.4	101325		63.50	40.09	34.56	108.75	3041.1
				40.09	83.96	118.8	4625.3
				40.09	83.89	128.8	6879.8
				50.09	193.4	138.89	9960.8
mp/ [°] C	63.5			60.13	442.4	148.98	14257
				25	20.44	159.03	19754
					interpolated	169.13	27045
						169.15	36475
					solid		36355
				eq. 3a	P/Pa		
				A	32.5109		
				B	8909 70		liquid
				C	3.94116	eq. 3a	P/Pa
						A	21.1215
						B	3939.56
						C	–71.2907

2.

Blok et al. 2001

torsion, mass-loss effusion		static-diaphragm manometer		static-diaphragm manometer	
t/ [°] C	P/Pa	t/ [°] C	P/Pa	t/ [°] C	P/Pa
	solid		solid	series I	liquid
–17.65	0.167	29.33	32.3	65.7	586
–15.65	0.218	29.34	32.3	68.1	669
–14.15	0.265	32.38	43.2	70.0	740
–12.15	0.343	32.38	43.6	72.17	828
–10.65	0.416	35.37	56.9	75.06	963
–9.15	0.502	38.38	74.0	77.84	1110
–7.15	0.643	38.39	74.4	79.57	1200

TABLE 6.1.1.7.2 (Continued)

Blok et al. 2001					
torsion, mass-loss effusion		static-diaphragm manometer		static-diaphragm manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-5.15	0.822	41.43	95.4	81.90	1350
-3.65	0.984	44.47	122	83.47	1460
-0.65	1.40	47.57	157	series II	
		50.51	197	76.43	1050
		53.61	254	84.40	1550
		57.47	253	91.37	2140
		57.48	338	98.34	2920
		57.48	344	105.31	3940
		57.48	342	112.28	5230
		57.48	341	119.25	6880
		57.49	340	123.23	7990
				127.21	9240
				131.18	10600
				135.16	12200
				139.14	13900
				142.12	15200
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 70.74$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 50.27$	
		at 298.15 K		at 375 K	

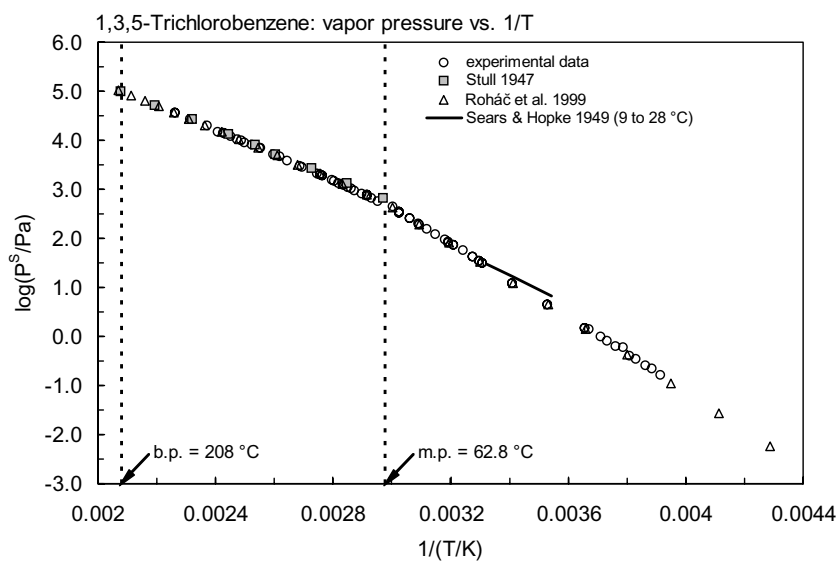
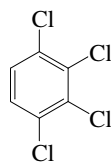


FIGURE 6.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trichlorobenzene.

6.1.1.8 1,2,3,4-Tetrachlorobenzene



Common Name: 1,2,3,4-Tetrachlorobenzene

Synonym:

Chemical Name: 1,2,3,4-tetrachlorobenzene

CAS Registry No: 634-66-2

Molecular Formula: $C_6H_2Cl_4$

Molecular Weight: 215.892

Melting Point ($^{\circ}C$):

47.5 (Weast 1972–73; Lide 2003)

Boiling Point ($^{\circ}C$):

254 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

142 (calculated-density, liquid molar volume, Chiou 1985)

179.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.0 (Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)

16.95 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

53.14 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 156\ J/mol\ K$), F: 0.602 (mp at $47.5^{\circ}C$)

0.608 ($25^{\circ}C$, Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.31 (shake flask-UV, Yalkowsky et al.)

3.42 (shake flask-GC, Könemann 1981)

4.32 (recommended, Horvath 1982)

3.50 ($22^{\circ}C$, Verschueren 1983)

12.2 (generator column-GC/ECD, Miller et al. 1984, 1985)

7.18 ($23^{\circ}C$, shake flask-GC, Chiou 1985)

5.92 (shake flask-HPLC, Banerjee et al. 1984)

4.33 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

12.2 (generator column-GC, Doucette & Andren 1988)

3.27 (shake flask-GC/ECD, Kim & Saleh 1990)

12.0 (shake flask-GC, Boyd et al. 1998)

1.40, 2.11, 2.80, 5.25 (5, 15, 25, $35^{\circ}C$, estimated- RP-HPLC- k' correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($68.5^{\circ}C$, summary of literature data, temp range 68.5 – $254.0^{\circ}C$, Stull 1947)

8.76 (extrapolated-Antoine eq., supercooled liquid P_L , Weast 1972–73)

5.21 (calculated-Antoine eq. from Weast 1972–73, converted to solid P_s ; Mackay & Shiu 1981)

$\log(P/mmHg) = [-0.2185 \times 12872.5/(T/K)] + 8.251056$; temp range 68.5 – $254^{\circ}C$ (Antoine eq., Weast 1972–73)

4.017, 3.49 (P_{GC} by GC-RT correlation with different GC columns, Bidleman 1984)

8.0 (supercooled liquid P_L , converted from literature P_s with ΔS_{fus} , Bidleman 1984)

6.285 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)

2.44 (supercooled liquid P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.7082 - 1517.2/(-117.384 + T/\text{K})$; temp range 331–527 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

5.60 (selected, supercooled liquid P_L , Suntio et al. 1988b; quoted, Ballschmiter & Wittlinger 1991)

8.0 (supercooled P_L , converted from literature P_S with ΔS_{fus} , Hinckley et al. 1990)

4.02 (P_{GC} by GC-RT correlation, Hinckley et al. 1990)

12.1 (supercooled liquid P_L , GC-Kovács retention indices correlation; Spijksma et al. 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

70 (gas stripping-GC, Oliver 1985)

62.0* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)

289 (modified EPICS method-GC, Ryu & Park 1999)

58.5 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 5.014 - 1945/(T/\text{K})$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section.:

4.72 (Leo et al. 1971)

4.46 (shake flask-GC, HPLC- k' correlation, Könemann et al. 1979)

4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)

4.37 (shake flask-GC, Watarai et al. 1982)

4.94 (TLC-RT correlation, Bruggeman et al. 1982)

4.75 (shake flask-GC, Bruggeman et al. 1982)

4.41 (HPLC- k' correlation, Hammers et al. 1982)

4.55 (generator column-GC, Miller et al. 1984)

4.60 (shake flask-GC, Chiou 1985)

4.65 (HPLC-RV/MS, Burkhard & Kuehl 1986)

4.61* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)

4.60 (shake flask-GC, Pereira et al. 1988)

4.635 (shake flask/slow stirring-GC, De Bruijn et al. 1989)

4.54 (recommended, Sangster 1993)

4.64 (recommended, Hansch et al. 1995)

$4.41 \pm 0.06^*$ (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)

$\log K_{\text{OW}} = 0.6978 - 21100/[2.303 \cdot R(T/\text{K})]$, temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)

4.30* (estimated RP-HPLC- k' correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

5.64*; 5.74 (generator column-GC; measured range –10 to 20°C, calculated, Harner & Mackay 1995)

$\log K_{\text{OA}} = -5.3 + 3254/(T/\text{K})$; $\Delta H_{\text{OA}} = 62.3 \text{ kJ/mol}$ (Harner & Mackay 1995)

5.64 (calculated- S_{oct} and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$ at 25°C or as indicated:

4.86 (guppy, lipid basis, Könemann & van Leeuwen 1980)

3.25 (Briggs 1981)

3.36–3.75 mean 3.72; 4.00–4.15 mean 4.08 (rainbow trout, 15°C, steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)

4.80–5.13 (rainbow trout, lipid basis, Oliver & Niimi 1983)

3.72–4.08 (fish, Oliver 1984)

3.70 (15°C, rainbow trout, Banerjee et al. 1984)

3.41–3.93 mean 3.80; 3.49–4.00 mean 3.91 (rainbow trout, wet wt. basis, 15°C, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)

3.72; .89 (rainbow trout, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)

3.38 (fathead minnow, Carlson & Kosian 1987)

4.9–5.4, 5.1; 4.1 (Niagara River plume, range, mean; calculated- K_{OW} , Oliver 1987b)

- 4.70, 4.74, 4.75, 4.84 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
 3.36 (guppy, Van Hoogan & Opperhuizen 1988)
 5.46, 5.70, 4.68, 5.30 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 3.68; 3.79 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption; purge desorption, Koelmans et al. 1993)
 3.40 (guppy, steady-state conditions, rate const. ratio k_1/k_2 , 96-h exposure, Sijm et al. 1993)
 4.70 (guppy, lipid normalized BCF, Sijm et al. 1993)
 3.72–4.08; 3.82 (*Oncorhynchus mykiss*; *Poecilia reticulata*, flow through conditions, Devillers et al. 1996)
 3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)
 4.28 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
 3.96; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 3.49 (soil, sorption isotherm, converted from reported log K_{OM} of 3.25, Briggs 1981)
 3.27 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
 3.16–4.42 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
 5.00; 4.90 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
 4.1–6.0, 5.2 (suspended sediment, average, Oliver 1987c)
 3.52, 3.91, 3.75, 3.48, 3.52 (five soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
 3.48–3.91 (soil, batch-equilibration, Kishi et al. 1990)
 4.28 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
 4.26 (sediment 3.86% OC, batch sorption equilibrium, Koelmans & Lijkelma 1992)
 4.39 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)
 3.70, 3.64, 3.84 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
 4.14 (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM} :

- 3.25 (soil, sorption isotherm, shake flask-GC, soil organic matter, Briggs 1981)
 4.90 (Niagara River-organic matter, Oliver & Charlton 1984)
 4.90–5.40; 5.10; 4.10; 4.50 (Niagara-River plume: range; average; calculated- K_{OW} , algae > 50 µm, Oliver 1987b)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: dechlorination pseudo-first order rate constant $k = 1.455 \text{ d}^{-1}$ with $t_{1/2} = 0.5 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 140 \text{ h}^{-1}$; $k_2 = 0.021 \text{ h}^{-1}$ (rainbow trout, 15°C, Banerjee et al. 1984)

$k_1 = 670 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.29 \text{ d}^{-1}$ (guppy, van Hoogan & Opperhuizen 1988)

$k_1 = 670 \pm 180 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.29 \pm 0.06 \text{ d}^{-1}$ (guppies, 96-h exposure, Sijm et al. 1993)

$k_1 = 1807.8 \text{ h}^{-1}$; $k_2 = 0.304 \text{ h}^{-1}$ (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)

$k_1 = 141 \text{ mL g}^{-1} \text{ d}^{-1}$, $k_2 = 1.5 \text{ d}^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air:

Surface Water:

Groundwater:

Sediment: dechlorination $t_{1/2} = 1.8$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota: biological half-lives, $t_{1/2} = 3$ d in sunfish and $t_{1/2} = 2$ d in guppy for tetrachlorobenzenes (Niimi 1987); $t_{1/2} < 5$ d in worms at 8°C (Oliver 1987a).

TABLE 6.1.1.8.1

Reported vapor pressures and Henry's law constants of 1,2,3,4-tetrachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
Vapor pressure		Henry's law constant	
Stull 1947		ten Hulscher et al. 1992	
summary of literature data		gas stripping-GC	
t/°C	P/Pa	t/°C	H/(Pa m³/mol)
68.5	133.3	14.8	48.5
99.6	666.6	20.0	62.0
114.7	1333	20.1	52.0
131.2	2666	22.1	68.1
149.2	5333	24.1	70.9
160.0	7999	34.8	129.9
175.7	13332	50.0	276.2
198.0	26664		
225.5	53329	temp dependence eq.	
254.0	101325	$\ln K_{\text{AW}} = A - B/(T/K)$	
		A	22.156
mp/°C	46.5	B	5532.84

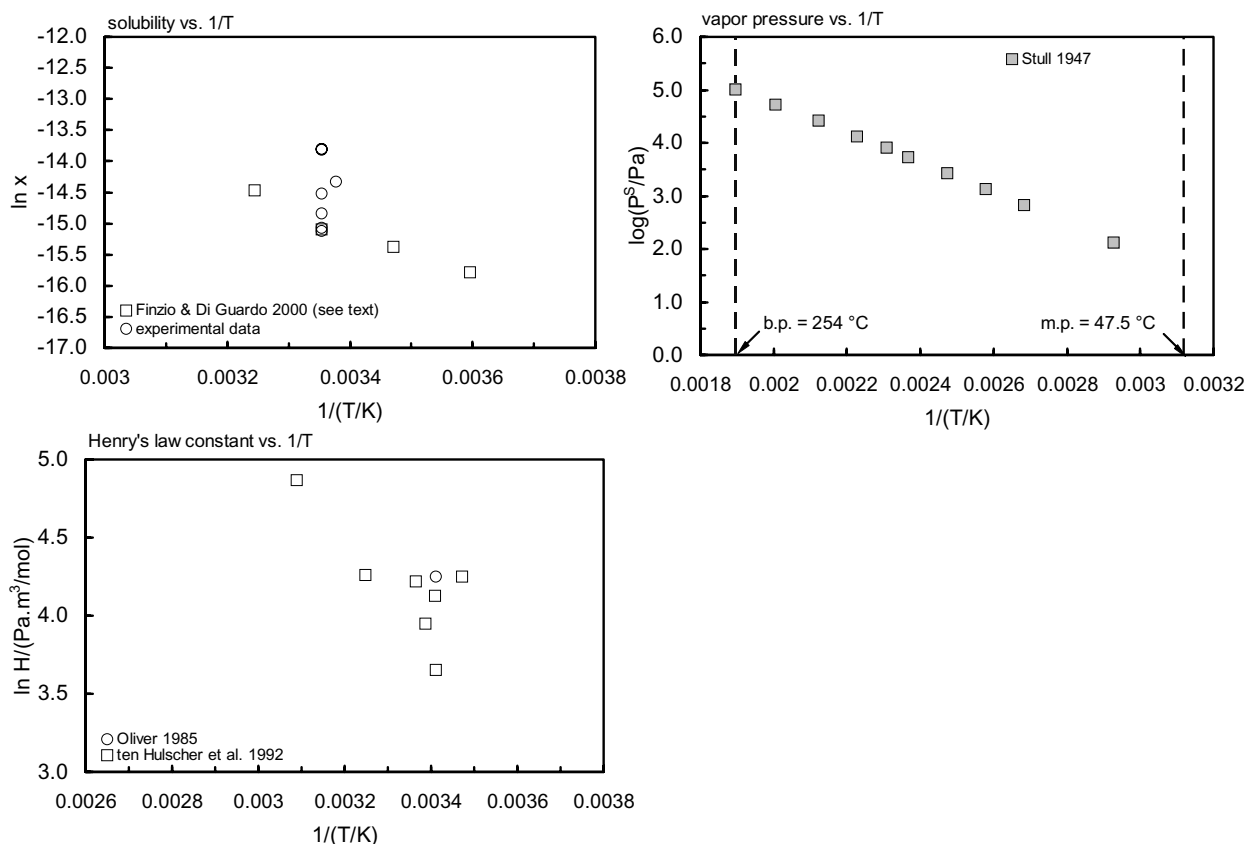


FIGURE 6.1.1.8.1 Logarithm of mole fraction solubility, vapor pressure and Henry's law constant versus reciprocal temperature for 1,2,3,4-tetrachlorobenzene.

TABLE 6.1.1.8.2

Reported octanol-water and octanol-air partition coefficients of 1,2,3,4-tetrachlorobenzene at various temperatures

log K _{OW}				log K _{OA}			
Opperhuizen et al. 1988		Bahadur et al. 1997		Finizio & Di Guardo 2001		Harner & Mackay 1995	
shake flask-GC/ECD		shake flask-GC/ECD		GC-RT correlation		generator column-GC	
t/°C	log K _{OW}	t/°C	log K _{OW}	t/°C	log K _{OW}	t/°C	log K _{OA}
13	4.83	5	4.65	5	4.52	25	5.64
19	4.61	15	4.53	15	4.4	-10	7.076
28	4.37	25	4.41	25	4.30	0	6.64
33	4.66	35	4.28	35	4.11	9.88	6.213
		45	4.15			19.85	5.818
$\Delta H/(\text{kJ mol}^{-1}) = -26.3$		enthalpy of transfer				$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 62.03$	
		$\Delta H/(\text{kJ mol}^{-1}) = -21.1$					
		$\log K_{\text{OW}} = A - \Delta H/2.303RT$				$\log K_{\text{OA}} = A + B/T$	
		A	0.6978			A	-5.3
		ΔH	-21100			B	3254

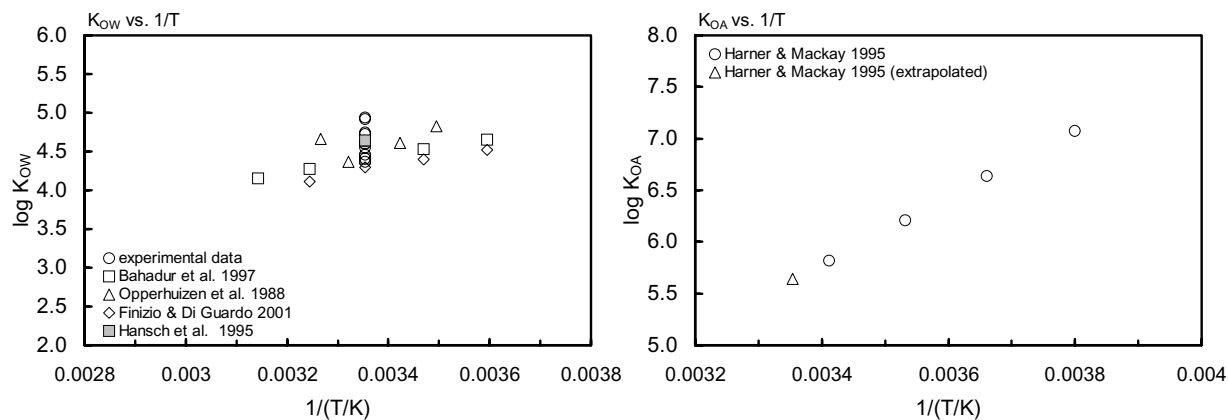
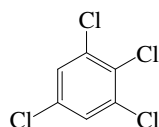


FIGURE 6.1.1.8.2 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for 1,2,3,4-tetrachlorobenzene.

6.1.1.9 1,2,3,5-Tetrachlorobenzene



Common Name: 1,2,3,5-Tetrachlorobenzene

Synonym:

Chemical Name: 1,2,3,5-tetrachlorobenzene

CAS Registry No: 634-90-2

Molecular Formula: $C_6H_2Cl_4$

Molecular Weight: 215.892

Melting Point ($^{\circ}C$):

54.5 (Weast 1972–73; 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

246 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

179.6 (calculated-Le Bas method at normal boiling point)

141.0 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.0 (Miller et al. 1984; Chickos et al. 1999)

19.32 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

58.576 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.514 (mp at $54.5^{\circ}C$)

0.556 (Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3.50 (shake flask-UV, Yalkowsky et al. 1979)

4.02 (shake flask-LSC, Banerjee et al. 1980)

4.11, 17.1 (LSC- ^{14}C , calculated- K_{ow} , Veith et al. 1980)

2.48 (shake flask-GC, Könnemann 1981)

3.51 (recommended, Horvath 1982)

2.40 ($22^{\circ}C$, Verschueren 1983)

5.10 (shake flask-HPLC, Banerjee 1984)

2.89 (generator column-GC/ECD, Miller et al. 1984, 1985)

3.23 (shake flask-GC, Chiou 1985)

3.46 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

4.32 (generator column-GC, Doucette & Andren 1988)

4.32 (shake flask-GC/ECD, Kim & Saleh 1990)

4.52 (shake flask-GC/ECD, Tam et al. 1996)

$3.44 \pm 0.15^*$, 3.79 ± 0.23 (generator column-GC/ECD, shake flask-GC at $27^{\circ}C$, Shiu et al. 1997)

$\ln x = -4.4222 - 3162.74/(T/K)$; temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* ($58.2^{\circ}C$, summary of literature data, temp range $58.2-246^{\circ}C$, Stull 1947)

18.6 (extrapolated-supercooled liquid P_L , Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 11982.1/(T/K)] + 7.925176$; temp range $58.2-246^{\circ}C$ (Antoine eq., Weast 1972–73)

9.80 (solid P_s , calculated from extrapolated vapor pressure P_L with a fugacity ratio correction, Mackay & Shiu 1981)

- 5.085 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
 17.2; 9.56 (extrapolated-Antoine eq., supercooled liquid P_L , converted to P_S , Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.7756 - 2394/(-17.85 + T/K)$; temp range 331–519 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
 15.1 (supercooled liquid P_L , GC-Kováš retention indices correlation; Spieksma et al. 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 159 (batch stripping-GC, Mackay & Shiu 1981)
 99 (20°C, gas stripping-GC, ten Hulscher et al. 1992)
 160 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section.:

- 4.50, 4.92 (shake flask-GC, HPLC-k' correlation, Könnemann et al. 1979)
 4.46 (HPLC-RT correlation, Veith et al. 1979b)
 4.46, 5.0 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
 4.52 (shake flask-LSC, Banerjee et al. 1980)
 5.05 (head-space GC, Hutchinson et al. 1980)
 4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)
 4.56 (shake flask-GC, Watarai et al. 1982)
 4.53 (HPLC-k' correlation, Hammers et al. 1982)
 4.51 (generator-column-GC/ECD, Miller et al. 1984; 1985)
 4.61–4.73 (HPLC-RV correlation, Garst 1984)
 4.59 (shake flask-GC, Chiou 1985)
 4.59 (shake flask-GC, Pereira et al. 1988)
 4.658 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 4.63 (recommended, Sangster 1993)
 4.66 (recommended, Hansch et al. 1995)
 4.55* \pm -0.02 (shake flask-GC/ECD, Bahadur et al. 1997)
 $\log K_{OW} = 1.0159 - 20200/[2.303 \cdot R(T/K)]$; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 5.55 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)
 5.78* (20°C, HPLC-k' correlation, measured range 10–50°C, Su et al. 2002)
 $\log K_{OA} = 66320/(2.303 \cdot RT) - 6.086$; temp range 10–50°C (HPLC-k' correlation, Su et al. 2002)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

- 3.26 (fathead minnow, Veith et al. 1979b)
 4.86 (guppy-lipid basis, Könnemann et al. 1979)
 4.15, 4.86 (guppy-lipid basis, Könnemann & van Leeuwen 1980)
 3.26 (bluegill sunfish, whole body, flow system, Barrows et al. 1980)
 4.80–5.13 (rainbow trout, lipid base, Oliver & Niimi 1983)
 3.46 (22°C, bluegill sunfish, Banerjee et al. 1984)
 3.59 (fish, calculated-concentration ratio C_A/C_W or k_1/k_2 , Connell & Hawker 1988; Hawker 1990)
 4.73 (guppy-lipid phase, 12 to 31-d exposure studies, Gobas et al. 1989)
 5.05, 5.20, 4.27, 4.90 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 3.64–4.89 (*Poecilia reticulata*, quoted lit., flow through conditions, Devillers et al. 1996)
 3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)
 4.27 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
 4.11; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.49 (soil, sorption isotherm, converted from reported $\log K_{OM}$ of 3.25, Briggs 1981)

- 3.20 (Koch 1983)
 4.25 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
 3.94 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)

Sorption Partition Coefficient, $\log K_{OM}$:

- 3.20, 2.98 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: dechlorination pseudo-first order rate constant $k = 0.639 \text{ d}^{-1}$ with $t_{1/2} = 1.1 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 15000 \text{ d}^{-1}$; $k_2 = 0.26 \text{ d}^{-1}$ (guppy, Könemann & van Leeuwen 1980)

$k_1 = 74 \text{ h}^{-1}$; $k_2 = 0.026 \text{ h}^{-1}$ (bluegill sunfish, Banerjee et al. 1984)

$k_1 = 33.8 \text{ h}^{-1}$; $1/k_2 = 92.0 \text{ h}$ (guppy, Hawker & Connell 1985)

$k_1 = 810 \text{ d}^{-1}$ (fish quoted, Opperhuizen 1986)

$\log k_1 = 2.91 \text{ d}^{-1}$; $\log 1/k_2 = -0.42 \text{ d}$ (guppy, quoted, Connell & Hawker 1988)

$\log k_1 = 3.00 \text{ d}^{-1}$; $\log k_2 = -0.59 \text{ d}^{-1}$ (guppy, 12 to 31-d exposure studies, Gobas et al. 1989)

$\log k_2 = -0.58 \text{ d}^{-1}$ (fish, calculated- K_{OW} , Thomann 1989)

$k_1 = 1807.8 \text{ h}^{-1}$; $k_2 = 0.304 \text{ h}^{-1}$ (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)

$k_1 = 131 \text{ mL g}^{-1} \text{ d}^{-1}$, $k_2 = 1.4 \text{ d}^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air:

Surface Water:

Groundwater:

Sediment: dechlorination $t_{1/2} = 1.8 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil:

Biota: $t_{1/2} = 2\text{--}4 \text{ d}$ in fish (Veith et al. 1980);

$2 < t_{1/2} < 4 \text{ d}$ in bluegill sunfish (Barrows et al. 1980).

TABLE 6.1.1.9.1

Reported aqueous solubilities, vapor pressures, octanol-water partition coefficients and octanol-air partition coefficients of 1,2,3,5-tetrachlorobenzene at various temperatures

Aqueous solubility		Vapor pressure		log K _{OW}		log K _{OA}	
Shiu et al. 1997		Stull 1947		Bahadur et al. 1997		Su et al. 2002	
shake flask-GC		summary of literature data		shake flask-GC/ECD		GC-RT correlation	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K _{OW}	t/°C	log K _{OA}
5	1.7	58.2	133.3	5	4.8	10	6.15.
15	2.43	89	666.6	15	4.67	20	5.78
25	3.44	104.1	1333	25	4.55	30	5.43
35	5.08	121.6	2666	35	4.42	40	5.11
45	7.03	140	5333	45	4.33	50	4.8
ΔH _{sol} = 26.3 kJ/mol		142	7999				
		168	13332	enthalpy of transfer		ΔH _{OA} /(kJ mol ⁻¹) = 66.32	
		193.7	26664	ΔH/(kJ mol ⁻¹) = -20.2			
		220	53329			log K _{OA} = A + B/2.303RT	
		246	101325	log K _{OW} = A - B/2.303RT		A	-6.086
				A		B	66320
		mp/°C	54.5	ΔH		-20200	

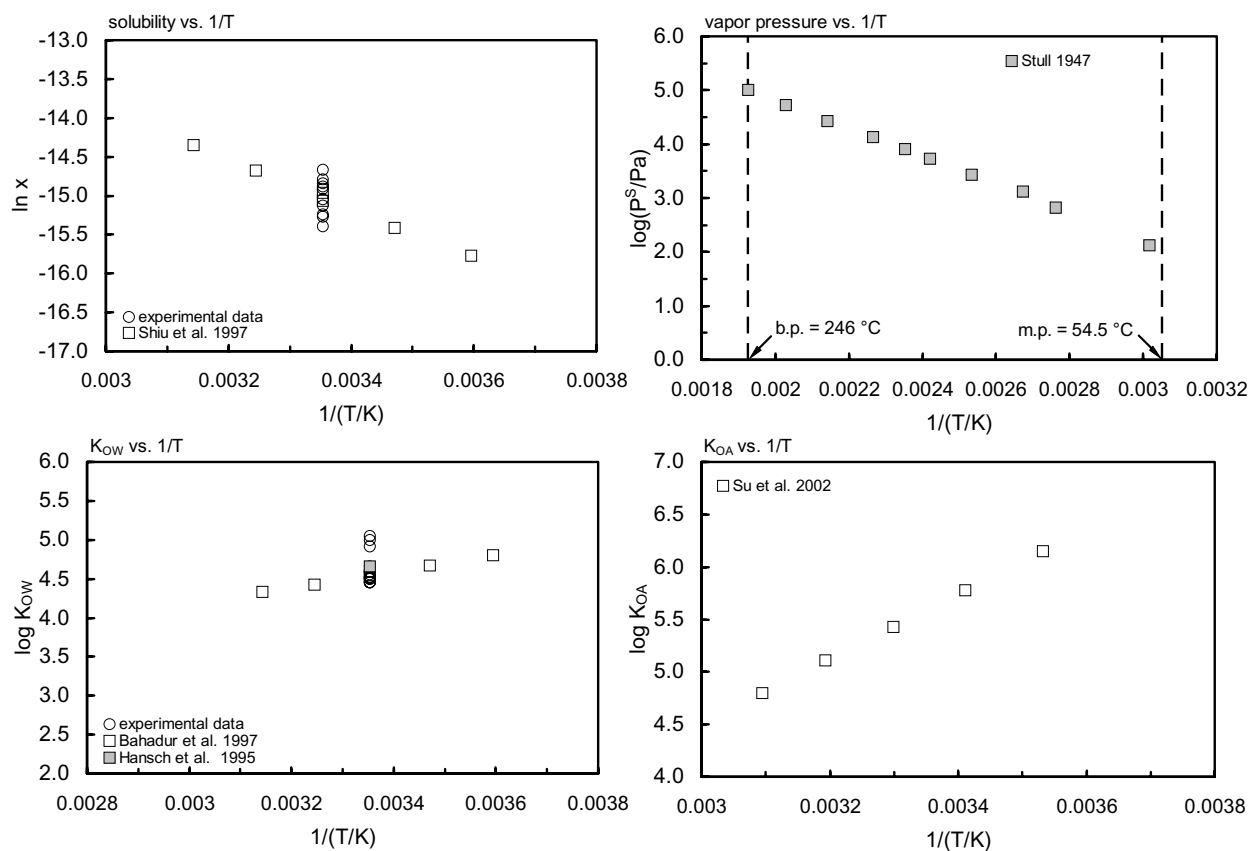
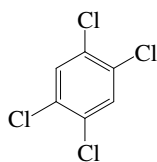


FIGURE 6.1.1.9.1 Logarithm of mole fraction solubility, vapor pressure, K_{OW} and K_{OA} versus reciprocal temperature for 1,2,3,5-tetrachlorobenzene.

6.1.1.10 1,2,4,5-Tetrachlorobenzene



Common Name: 1,2,4,5-Tetrachlorobenzene

Synonym:

Chemical Name: 1,2,4,5-tetrachlorobenzene

CAS Registry No: 95-94-3

Molecular Formula: $C_6H_2Cl_4$

Molecular Weight: 215.892

Melting Point ($^{\circ}C$):

139.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

244.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.858 ($22^{\circ}C$, Weast 1972–1973; Horvath 1982; Lide 2003)

Molar Volume (cm^3/mol):

116.2 ($22^{\circ}C$, calculated-density)

179.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.64 (Miller et al. 1984)

24.10 (Ruelle & Kesselring 1993; Chickos et al. 1999)

29.94 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

58.576 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.0753 (mp at $139.5^{\circ}C$)

0.073 (Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.595 (shake flask-UV, Yalkowsky et al. 1979)

0.29 (shake flask-GC, Könemann 1981)

0.596 (recommended, Horvath 1982)

0.30 ($22^{\circ}C$, quoted, Verschueren 1983)

2.35 (generator column-GC/ECD, Miller et al. 1984, 1985)

0.465 (shake flask-HPLC, Banerjee 1984)

0.606 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

0.56 (shake flask-GC/ECD, Kim & Saleh 1990)

$0.528^* \pm 0.018$, 0.543 ± 0.016 (generator column-GC/ECD, shake flask-GC at $27^{\circ}C$, Shiu et al. 1997)

2.20 (shake flask-GC, Boyd et al. 1998)

$\ln x = -4.529 - 3708.6/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5333^* ($146.0^{\circ}C$, summary of literature data, temp range 146.0 – $245^{\circ}C$, Stull 1947)

10.1 (extrapolated-Antoine eq., supercooled liquid P_L , Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 12828.8/(T/K)] + 8.282213$; temp range 146 – $245^{\circ}C$ (Antoine eq., Weast 1972–73)

0.72 (P_S converted from P_L of Weast 1972–73, Mackay & Shiu 1981)

0.20 (evaporation rate, Dobbs & Cull 1982)

2.163 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)

- 2.98, 0.22 (supercooled liquid P_L , solid P_S , Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 9.1357 - 4642.36/(132.952 + T/\text{K})$; temp range 419–518 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
 7.497 (GC-RT correlation, Watanabe & Tatsukawa 1989)
 0.615 (calculated-UNIFAC activity coefficients, Banerjee et al. 1990)
 15.1; 12.5 (supercooled liquid P_L , GC-Kovács retention indices correlation; quoted lit., Spieksma et al. 1994)
 0.392* (24.65°C, torsion, mass-loss effusion, measured range 17–32.5°C, Blok et al. 2001)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 101 (gas stripping-GC, Oliver 1985)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 4.72 (Leo et al. 1971)
 4.82, 4.56 (shake flask-GC, HPLC- k' correlation, Könemann et al. 1979)
 4.68 (20°C, shake flask-GC, isomer not specified, Briggs 1981)
 4.46 (shake flask-GC, Watarai et al. 1982)
 4.52 (HPLC- k' correlation, Hammers et al. 1982)
 4.51 (generator column-GC/ECD, Miller et al. 1984, 1985)
 4.70 (shake flask-GC, Chiou 1985)
 4.60 (HPLC- k' correlation, Mailhot 1987)
 5.16 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)
 4.604 (slow stirring-GC, De Bruijn et al. 1989)
 5.16 (calculated-fragment const., De Bruijn et al. 1989)
 4.70 (shake flask-GC, Pereira et al. 1988)
 4.63 (recommended, Sangster 1993)
 4.70 (recommended, Hansch et al. 1995)
 4.97–5.10 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1998)
 4.44* (estimated- RP-HPLC- k' correlation, measured range 5–35°C, Finizio & Di Guardo 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.:

- 5.63*; 5.81 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
 $\log K_{OA} = -5.0 + 3176/(T/\text{K})$; $\Delta H_{OA} = 60.8 \text{ kJ/mol}$ (Harner & Mackay 1995)
 5.62, 5.63 (calculated- S_{oct} and vapor pressure P , quoted lit., Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

- 0.20 (rats, adipose tissue, Geyer et al. 1980)
 3.65 (fish, flowing water, Kenaga & Goring 1980; Kenaga)
 3.36–3.79 mean 3.72; 4.04–4.18 mean 4.11 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
 4.80–5.13 (rainbow trout, lipid base, Oliver & Niimi 1983)
 3.72–4.11 (fish, Oliver 1984)
 2.80 (Tadokoro & Tomita 1987)
 3.89 (green algae, Mailhot 1987)
 4.08 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)
 5.05, 5.20, 4.27, 4.90 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 2.76 (*picea omorika*, Reischl et al. 1989)
 3.61, 4.70 (American flagfish: whole fish, fish lipid, Smith et al. 1990)
 3.20 (fish, calculated, Figueroa & Simmons 1991)
 3.72–4.11; 3.61 (*Oncorhynchus mykiss*; *Jordanella floridae*, quoted lit., flow through conditions, Devillers et al. 1996)
 3.89 (algae *Selenastrum capricornutum*, wet wt basis, isomer not specified, Wang et al. 1996)
 3.72, 4.80; 3.517, 3.417 (quoted: whole fish, lipid content; calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)

3.89; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

3.20 (Kenaga 1980a)
 3.49 (soil, sorption isotherm, converted from reported log K_{OM} of 3.25, Briggs 1981)
 3.36 (river sediment, 0.56% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
 3.24–4.50 (five soils, 0.04–0.73% OC, batch equilibrium-sorption isotherm, Schwarzenbach & Westall 1981)
 5.10; 4.70 (field data of sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
 2.79 (McLaurin sandy loam, OC 0.66%, pH 4.43, batch equilibrium-sorption isotherm, Walton et al. 1992)
 3.94 ± 0.33 (suspended particulates in coastal waters, Masunaga et al. 1996)
 3.48 (soil: organic carbon OC ≥ 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} = 763.1$ –7631 h, based on photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: base rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C with a calculated $t_{1/2} > 900$ yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)
 first order hydrolysis $t_{1/2} > 879$ yr (Howard et al. 1991)

Biodegradation: $t_{1/2}(\text{aerobic}) = 672$ –4320 h, based on unacclimated aerobic screening test data; $t_{1/2}(\text{anaerobic}) = 2880$ –17280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

dechlorination pseudo-first order $k = 0.037 \text{ d}^{-1}$ with $t_{1/2} = 18.7$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 1490 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.14 \text{ d}^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

$k_1 = 1630 \text{ d}^{-1}$, 171000 d^{-1} ; $k_2 = 0.4 \text{ d}^{-1}$, 0.34 d^{-1} (American flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 0.4 \text{ d}^{-1}$, 2.35 d^{-1} (American flagfish: bioconcentration data, toxicity data, Smith et al. 1990)

$k_1 = 1807.8 \text{ h}^{-1}$; $k_2 = 0.304 \text{ h}^{-1}$ (algae *Selenastrum capricornutum*, isomer not specified, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 763.1$ –7631 h, based on photooxidation half-life in air (Howard et al. 1991)

Surface Water: hydrolysis $t_{1/2} > 900$ yr at pH 7 and 25°C (Ellington et al. 1988)

$t_{1/2} = 672$ –4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Groundwater: $t_{1/2} = 1344$ –8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment: dechlorination $t_{1/2} = 18.7$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil: $t_{1/2} = 672$ –4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota: $t_{1/2} < 5$ d in worms at 8°C (Oliver 1987a);

biological $t_{1/2} = 3$ d in sunfish, $t_{1/2} = 2$ d in guppy for tetrachlorobenzenes (Niimi 1987);

$t_{1/2} = 33$ d in *Picea omorika* (Reischl et al. 1989);

$t_{1/2} = 1.72$ d clearance from American flagfish (Smith et al. 1990);

elimination $t_{1/2} = 2.01$ d from earthworm in water (Belfroid et al. 1993);

elimination $t_{1/2} = 0.204$ d and 2.63 d in a two-phase kinetics for earthworm in OECD soil (Belfroid et al. 1994).

TABLE 6.1.1.10.1

Reported aqueous solubilities and vapor pressures of 1,2,4,5-tetrachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Aqueous solubility		Vapor pressure					
Shiu et al. 1997	Stull 1947	Blok et al. 2001					
shake flask-GC	summary of literature data	torsion, mass loss effusion	static-diaphragm manometer				
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
5	0.298	146.0	5333	16.85	0.155	99.74	328
15	0.322	157.7	7999	19.45	0.212	104.82	461
25	0.528	173	13332	22.05	0.289	108.83	612
35	0.739	196	26664	24.65	0.392	113.82	844
45	1.127	220.5	53329	27.25	0.528	117.74	1100
		245	101325	29.85	0.707	121.82	1140
				32.45	0.943	125.84	1820
$\Delta H_{\text{sol}} = 30.8 \text{ kJ/mol}$						129.82	2310
						132.79	2770
						136.82	3500
				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 82.10$			
				at 353 K			

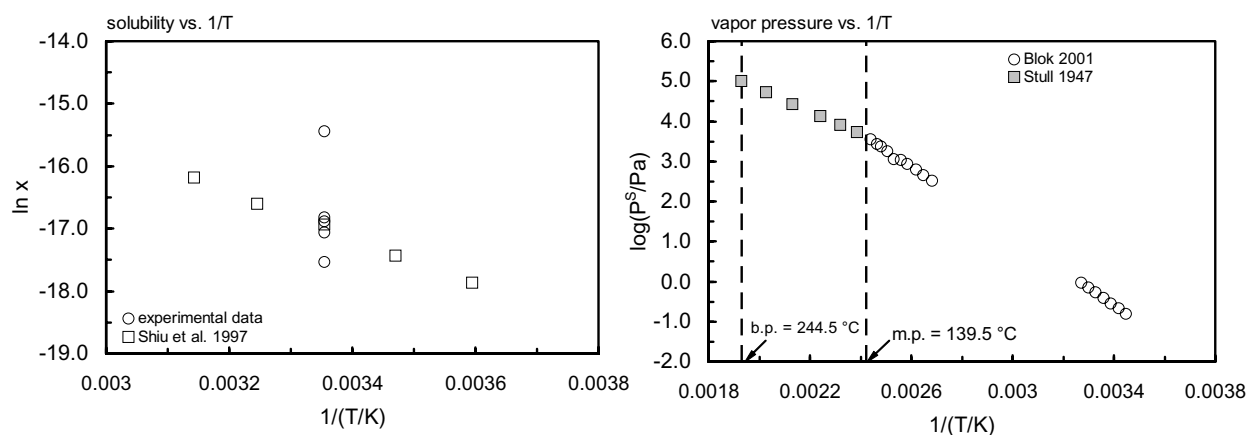


FIGURE 6.1.1.10.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,4,5-tetrachlorobenzene.

TABLE 6.1.1.10.2

Reported octanol-water partition coefficients and octanol-air partition coefficients of 1,2,4,5-tetrachlorobenzene at various temperatures

log K _{OW}		log K _{OA}	
Finizio & Di Guardo 2001		Harner & Mackay 1995	
GC-RT correlation		generator column-GC	
t/°C	log K _{OW}	t/°C	log K _{OA}
5	4.63	25	5.63
15	4.54	-10	7.056
25	4.44	0	6.622
35	4.26	9.88	6.204
		19.85	5.829
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 60.8$	
		$\log K_{OA} = A + B/T$	
		A	-5.0
		B	3176

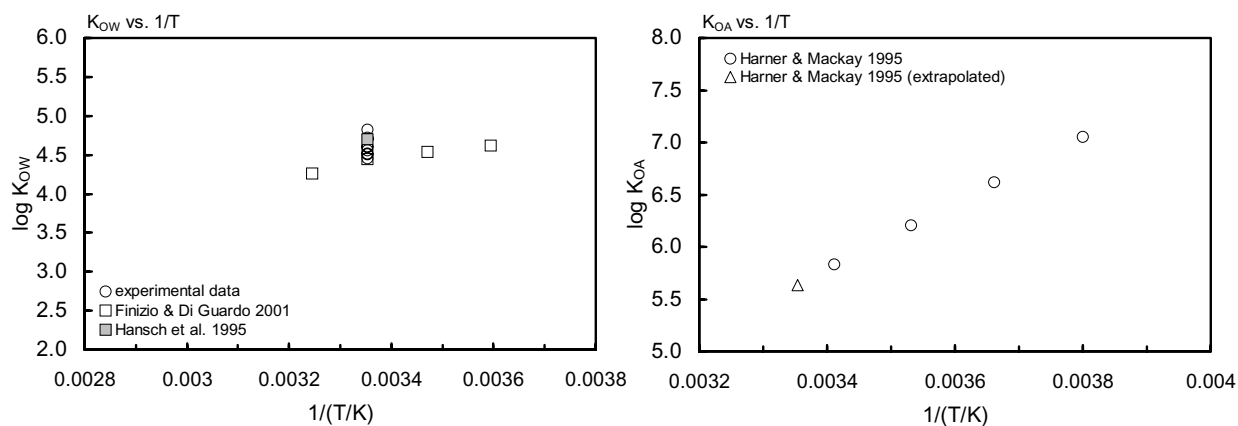
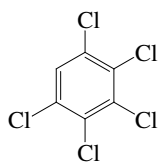


FIGURE 6.1.1.10.2 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for 1,2,4,5-tetrachlorobenzene.

6.1.1.11 Pentachlorobenzene



Common Name: Pentachlorobenzene

Synonym:

Chemical Name: Pentachlorobenzene

CAS Registry No: 608-93-5

Molecular Formula: C_6HCl_5

Molecular Weight: 250.337

Melting Point ($^{\circ}C$):

86 (Weast 1972–73; Lide 2003)

Boiling Point ($^{\circ}C$):

277 (Weast 1972–72; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.8342 (16.5 $^{\circ}C$, Weast 1972–73; Horvath 1982)

Molar Volume (cm^3/mol):

136.5 (16.5 $^{\circ}C$, calculated-density, Weast 1972–73; Horvath 1982)

166 (liquid molar volume, Chiou 1985)

200.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.585 (Miller et al. 1984)

20.60 (Ruelle et al. 1993; Chickos et al. 1999)

20.1 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

57.74 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K.), F: 0.252 (mp at $86^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.56 (shake flask-UV, Yalkowsky et al. 1979)

1.33 (shake flask-LSC, Banerjee et al. 1980)

0.135 (Kenaga & Goring 1980; Kenaga 1980a)

1.34 (shake flask-LSC- ^{14}C , Veith et al. 1980)

0.24 (shake flask-GC, Könnemann 1981)

0.562 (recommended, Horvath 1982)

0.831 (generator column-GC/ECD, Miller et al. 1984, 1985)

0.385 (23 $^{\circ}C$, shake flask-GC, Chiou 1985)

0.180 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.552 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

3.46 (calculated- K_{ow} and HPLC-RT correlation, Chin et al. 1986)

$0.419^* \pm 0.018$, 0.447 ± 0.014 (generator column-GC/ECD, shake flask-GC/ECD at $27^{\circ}C$, Shiu et al. 1997)

0.87 (shake flask-GC, Boyd et al. 1998)

$\ln x = -3.61482 - 4093.10/(T/K)$; temp range 5–50 $^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

2.75, 3.50 (supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133* (98.6 $^{\circ}C$, summary of literature data, temp range 98.6–276 $^{\circ}C$, Stull 1947)

- 0.889 (extrapolated-Antoine eq., supercooled liquid P_L , Weast 1972–73)
 0.219 (P_S calculated from P_L of Weast 1972–73; Mackay & Shiu 1981)
 $\log (P/\text{mmHg}) = [-0.2185 \times 15124.2/(T/K)] + 8.907497$; temp range 98.6–276°C (Antoine eq., Weast 1972–73)
 1.44 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
 1.08, 0.28 (supercooled liquid P_L , solid P_S , Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.00795 - 3325.33/(4.814 + T/K)$; temp range 371–549 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
 1.718 (GC-RT correlation, Watanabe & Tatsukawa 1989)
 2.49; 2.19 (supercooled liquid P_L , GC-Kovács retention indices correlation; quoted lit., Spijksma et al. 1994)
 0.212; 0.39* (25°C extrapolated; 30.3°C, static method-pressure gauge, measured range 30.3–179°C, Polednicek et al. 1996)
 $\ln (P_S/\text{Pa}) = 30.4445 - 8654.67/[(T/K) - 27.6534]$; temp range 303.45–353.17 K (solid, Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
 $\ln (P_L/\text{Pa}) = 23.4783 - 6188.33/[(T/K) - 34.6922]$; temp range 371.8–452.29 K (liquid, Antoine eq. from exptl data, pressure gauge measurement, Polednicek et al. 1996)
 0.11* (20°C, recommended, summary of literature data, temp range 233.15–503.15 K, Roháč et al. 1999)
 $\ln [(P_S/\text{Pa})/67.0] = [1 - (T/K)/357.0] \cdot \exp\{3.431590 - 1.8864070 \times 10^{-4} \cdot (T/K)\}$; temp range 300–353 K (Cox eq., solid, recommended, Roháč et al. 1999)
 $\ln [(P_L/\text{Pa})/67.0] = [1 - (T/K)/357.0] \cdot \exp\{3.419638 - 1.1673259 \times 10^{-3} \cdot (T/K) + 7.7842905 \times 10^{-7} \cdot (T/K)^2\}$; temp range 365–452 K (Cox eq., liquid recommended, Roháč et al. 1999)
 $\log (P/\text{kPa}) = 15.6174 - 4831.4/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 1.2, 1.0 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
 $\log (P_L/\text{Pa}) = -3220/(T/K) + 10.87$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 71.9 (gas stripping-GC, Oliver 1985)
 59.0* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)
 52.6 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 5.607 - 2132/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
 74, 70 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
 $\log K_{AW} = -2026/(T/K) + 5.27$ (LDV linear regression of literature data, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 5.79 (calculated-fragment const., Yalkowsky et al. 1979)
 4.88, 5.52 (shake flask-GC, HPLC- k' correlation, Könnemann et al. 1979)
 4.94 (shake flask-LSC, Banerjee et al. 1980)
 4.94, 5.29 (shake flask-LSC, HPLC-RT correlation, Veith et al. 1980)
 5.17 (shake flask-GC, Watarai et al. 1982)
 5.06 (HPLC- k' correlation, Hammers et al. 1982)
 5.69 (HPLC-RT correlation, Bruggeman et al. 1982)
 5.03 (generator column-GC/ECD, Miller et al. 1984; 1985)
 5.17 (shake flask-HPLC, Banerjee 1984)
 5.11–5.21 (HPLC-RV correlation, Garst 1984)
 5.20 (shake flask-GC, Chiou 1985)
 4.97 (calculated- K_{OW} and HPLC-RT correlation, Chin et al. 1986)
 6.12 (HPLC- k' correlation, De Kock & Lord 1987)
 5.47 (HPLC-RT correlation, Doucette & Andren 1988)
 5.20 (shake flask-GC, Pereira et al. 1988)
 5.05* (19°C, shake flask-GC, measured range 13–33°C, Opperhuizen et al. 1988)
 5.183 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 5.17 (recommended, Sangster 1993)
 5.18 (recommended, Hansch et al. 1995)
 4.94* ± 0.03 (shake flask-GC/ECD, Bahadur et al. 1997)

$\log K_{OW} = 0.9255 - 22800/[2.303 \cdot R(T/K)]$; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
 5.67–5.78 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1998)
 5.08, 5.19 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

6.27*; 6.46 (generator column-GC, measured range –10 to 20°C, calculated, Harner & Mackay 1995)
 7.93, 7.418, 6.931, 6.539 (–10, 0, 10, 18.7°C, generator column-GC, Harner & Mackay 1995)
 $\log K_{OA} = -6.2 + 3722.3/(T/K)$; temp range –10 to 20°C, $\Delta H_{OA} = 72.3$ kJ/mol (generator column-GC, Harner & Mackay 1995)
 6.50 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
 6.49, 6.27 (calculated- S_{oct} and vapor pressure P, quoted lit., Abraham et al. 2001)
 6.90, 6.73 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

3.89 (trout muscle, Neely et al. 1974)
 3.70 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980a)
 5.40 (guppy, lipid content, Könemann et al. 1979)
 3.53 (bluegill sunfish, Veith et al. 1980)
 3.53 (bluegill sunfish, whole body, flow system, Barrows 1980)
 5.41 (guppy, lipid basis, Könemann & van Leeuwen 1980)
 3.84 (fish, flowing water, Garten & Trabalka 1983)
 3.46–4.15 mean 4.11; 4.26–4.36 mean 4.30 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
 5.19–5.36 (rainbow trout, lipid basis, Oliver & Niimi 1983)
 4.11–4.30 (rainbow trout, Oliver 1984)
 3.71 (22°C, bluegill sunfish, 1.5% lipid, Banerjee et al. 1984)
 3.65; 3.86 (15°C, rainbow trout, 1.8% lipid; guppy, 2.8% lipid, Banerjee et al. 1984)
 3.60; 3.49 (algae: exptl.; calculated, Geyer et al. 1984)
 3.65 (algae, Freitag et al. 1984; Halfon & Reggiani 1986)
 3.48 (fish, Freitag et al. 1984; Halfon & Reggiani 1986)
 3.48, 3.65, 4.16 (fish, algae, activated sludge, Freitag et al. 1985)
 4.23 (guppy, calculated-rate constants ratio k_1/k_2 , Opperhuizen et al. 1985)
 3.92 (fathead minnow, Carlson & Kosian 1987)
 2.83, 2.65 (human fat, Geyer et al. 1987)
 4.28, 4.30 (worm, fish, Oliver 1987a)
 3.36–3.42 (fish, Tadokoro & Tomita 1987)
 5.46 (guppy, lipid weight base, 12 to 31-d exposure studies, Gobas et al. 1989)
 3.87 (*picea omorika*, Reischl et al. 1989)
 5.33 (fish, calculated- K_{OW} , Thomann 1989)
 4.14, 2.96, 4.23 (fish, Connell & Hawker 1988; Hawker 1990)
 5.11, 5.18, 5.20, 5.28 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
 3.67 (guppy, Van Hoogan & Opperhuizen 1988)
 5.93, 6.12, 4.96, 5.57 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 4.22 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption, Koelmans et al. 1993)
 3.70 (guppy, steady-state conditions, rate const. ratio k_1/k_2 , 96-h exposure, Sijm et al. 1993)
 5.00 (guppy, lipid normalized BCF, Sijm et al. 1993)
 4.11–4.30; 2.94–4.36; 3.53 (*Oncorhynchus mykiss*; *Poecilia reticulata*; *Lepomis macrochirus*, quoted lit., flow through conditions, Devillers et al. 1996)
 5.22–5.50 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
 4.11, 5.19; 3.797, 3.877 (quoted: whole fish, lipid content; calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)
 4.09; 3.96 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.11 (Kenaga 1980a)
- 5.30; 5.40 (field data of Lake Ontario sediment trap material; Niagara River-organic matter; Oliver & Charlton 1984)
- 4.60 (bottom sediment, Karickhoff & Morris 1985)
- 4.9–6.2, 5.8 (suspended sediment, average, Oliver 1987c)
- 5.7 (algae > 50 μm , Oliver 1987c)
- 5.50–5.90, 5.70 (Niagara River plume: range, average, Oliver 1987b)
- 4.49 (Ispra soil 1.87% OC, shake flask-GC, Paya-Perez et al. 1991)
- 4.68 (lake sediment 2.5% OC, batch sorption equilibrium, Schrap et al. 1994)
- 4.59 \pm 0.41 (suspended particulates in coastal waters, Masunaga et al. 1996)
- 4.91 (sediment: organic carbon OC \geq 0.1%, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} = 1088\text{--}10877$ h, based on estimated rate constant for the vapor phase reaction with OH radicals in air (Howard et al. 1991)Hydrolysis: base rate constant $k < 0.9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C with a calculated $t_{1/2} > 900$ yr at pH 7, based on assumed bases mediated 1% disappearance after 16 d at 85°C and pH 9.70 (Ellington et al. 1988)first order $t_{1/2} > 879$ yr (Howard et al. 1991)Biodegradation: $t_{1/2}(\text{aerobic}) = 4656\text{--}8280$ h, based on estimated unacclimated aerobic soil grab sample data; $t_{1/2}(\text{anaerobic}) = 18642\text{--}33120$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)dechlorination pseudo-first order rate constant $k = 0.557 \text{ d}^{-1}$ with $t_{1/2} = 1.2$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants: $k_1 = 18.76 \text{ h}^{-1}$; $k_2 = 0.00238 \text{ h}^{-1}$ (trout, Neely et al. 1974) $k_1 = 22000 \text{ d}^{-1}$; $k_2 = 0.14 \text{ d}^{-1}$ (guppy, Könemann & van Leeuwen 1980) $k_1 = 130 \text{ d}^{-1}$; $k_2 = 0.15 \text{ d}^{-1}$ (guppy, Bruggeman et al. 1984) $k_1 = 110 \text{ h}^{-1}$; $k_2 = 0.021 \text{ h}^{-1}$ (22°C, bluegill sunfish, Banerjee et al. 1984) $k_1 = 170 \text{ h}^{-1}$; $k_2 = 0.036 \text{ h}^{-1}$ (15°C, rainbow trout, Banerjee et al. 1984) $k_1 = 98 \text{ h}^{-1}$; $k_2 = 0.014 \text{ h}^{-1}$ (15°C, guppy, Banerjee et al. 1984) $k_1 = 5.4 \text{ h}^{-1}$; $1/k_2 = 160$ h (guppy, quoted, Hawker & Connell 1985) $k_1 = 1400 \text{ d}^{-1}$; $k_2 = 0.078 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1985) $k_1 = 1200 \text{ d}^{-1}$ (fish, quoted, Opperhuizen 1986) $k_2 = 0.00309, 0.00402 \text{ d}^{-1}$ (rainbow trout, calc-fish mean body weight, Barber et al. 1988) $\log k_1 = 3.08 \text{ d}^{-1}$; $\log 1/k_2 = 0.96 \text{ d}$ (fish, quoted, Connell & Hawker 1988) $k_1 = 710 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.15 \text{ d}^{-1}$ (guppy, Van Hoogan & Opperhuizen 1988) $\log k_1 = 3.24 \text{ d}^{-1}$; $\log k_2 = -0.96 \text{ d}^{-1}$ (guppy, 12 to 31-d exposure studies, Gobas et al. 1989a) $k_1 = 0.049 \text{ h}^{-1}$; $k_2 = 0.027 \text{ h}^{-1}$ (mayfly-sediment model II, Gobas et al. 1989b) $\log k_2 = -0.82 \text{ d}^{-1}$; -0.96 d^{-1} (fish, calculated- K_{OW} , Thomann 1989) $1/k_2 = 9.12, 12.9 \text{ d}$ (guppy, Clark et al. 1990) $k_1 = 710 \pm 290 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.15 \pm 0.04 \text{ d}^{-1}$ (guppies, 96-h exposure., Sijm et al. 1993) $k_2 = 0.00116 \text{ d}^{-1}$ (18°C earthworm in field-contaminated soil, Belfroid et al. 1995) $k_1 = (240\text{--}290) \text{ mL g}^{-1} \text{ d}^{-1}$, $k_2 = (0.3\text{--}0.19) \text{ d}^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

Half-Lives in the Environment:

Air: $t_{1/2} = 1088\text{--}10877$ h, based on estimated rate constant for the vapor phase reaction with OH radicals (Howard et al. 1991)Surface Water: $t_{1/2} = 4656\text{--}8280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)Groundwater: $t_{1/2} = 9312\text{--}16560$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment: dechlorination $t_{1/2} = 1.20$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Soil: $t_{1/2} = 4656\text{--}8280$ h, based on estimated unacclimated aerobic soil grab sample data (Howard et al. 1991)

Biota: $t_{1/2} > 7$ d in fish (Veith et al. 1980);

$t_{1/2} > 7$ d in bluegill sunfish (Barrows et al. 1980);

$t_{1/2} = 4.6$ d in guppy (Bruggeman et al. 1984);

$t_{1/2} = 8.9$ d in guppy (Opperhuizen et al. 1985);

$t_{1/2} < 5$ d in worms at 8°C (Oliver 1987a);

biological half-lives, $t_{1/2} > 7$ d in sunfish, $t_{1/2} = 4, 5$ and < 5 d in guppy (Niimi 1987);

$t_{1/2} = 27$ d in *picea omorika* (Reischl et al. 1989);

elimination $t_{1/2} = 5.46$ d from earthworm in water (Belfroid et al. 1993);

elimination $t_{1/2} = 0.53$ d and 5.9 d in a two-phase kinetics from earthworm in OECD soil (Belfroid et al. 1994);

elimination $t_{1/2} = 0.60$ d from earthworm in Volgermeerpolder soil (Belfroid et al. 1995).

TABLE 6.1.1.11.1

Reported aqueous solubilities of pentachlorobenzene at various temperatures

Shiu et al. 1997	
generator column-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
5	0.145
15	0.254
25	0.419
35	0.618
45	0.856
shake flask-GC	
27	0.447
$\Delta H_{\text{sol}} = 32.9$ kJ/mol	

TABLE 6.1.1.11.2

Reported vapor pressures of pentachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\log (P/\text{Pa}) = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^\circ\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^\circ\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3) \qquad \ln (P/\text{Pa}) = A - B/(C + T/K) \quad (3a)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

$$\ln (P/P_0) = (1 - T/T_0) \cdot \exp[\Sigma A_i T^i] \quad (5) - \text{Cox eq.}$$

1.

Stull 1947		Polednicek et al. 1996				Roháč et al. 1999	
summary of lit. data		pressure gauge				recommended	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	T/K	P/Pa
			solid		liquid		solid
98.6	133	30.3	0.385	98.65	167.99	233.15	0.00001
129.7	666.6	30.3	0.401	98.69	167.56	243.15	0.000066
144.3	1333	40.26	1.163	108.65	285.2	253.15	0.00037
160	2666	40.27	1.167	108.68	284.76	263.15	0.0019
178.5	5333	50.27	3.227	118.82	470.83	273.15	0.0081

(Continued)

TABLE 6.1.1.11.2 (Continued)

Stull 1947		Polednicek et al. 1996				Roháč et al. 1999	
summary of lit. data		pressure gauge				recommended	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
190.1	7999	50.27	3.209	118.84	471.55	283.15	0.032
205.5	13332	60.14	8.473	128.85	756.41	293.15	0.11
227	26664	60.16	8.480	128.85	755.7	303.15	0.37
251.5	53329	70.05	20.35	138.9	1189.2	313.15	1.10
276	101325	70.05	20.39	149.01	1820.6	232.15	3.20
		80.02	47.29	159.06	2731.2	333.15	8.40
mp/°C	85.5	25	0.212	169.11	4009.9	343.25	20.8
			extrapolated	179.14	5750.8	353.15	48.9
			solid		liquid	Cox eq.	
		eq. 3a	P/Pa	eq. 3a	P/Pa	eq. 5	P/Pa
		A	30.4445	A	22.4783	A ₀	3.431590
		B	8654.67	B	6188.33	10 ⁻⁴ A ₁	-1.8864070
		C	-27.6534	C	-34.6922	A ₂	0
						T ₀ /K	357.0
						P ₀ /Pa	67.0
						bp/K	558.42
for temp range 300–353 K							

2.

Roháč et al. 1999

recommended					
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
continued	liquid				
363.15	97.5	473.15	11440	Cox eq.	
373.15	173.9	483.15	15500	eq. 5	P/Pa
383.15	298.8	493.15	20700	A ₀	3.419638
393.15	486.4	503.15	27250	10 ⁻³ A ₁	-1.1673259
403.15	799.8	513.15	35430	10 ⁻⁷ A ₂	7.7842905
413.15	1253	523.15	45510	T ₀ /K	357.0
423.15	1912	533.15	57820	P ₀ /Pa	67.0
433.15	2848	543.15	72710	bp/K	558.42
443.15	4151	553.15	90570	for temp range 365–452 K	
453.15	5927	563.15	111800		
463.15	8306				

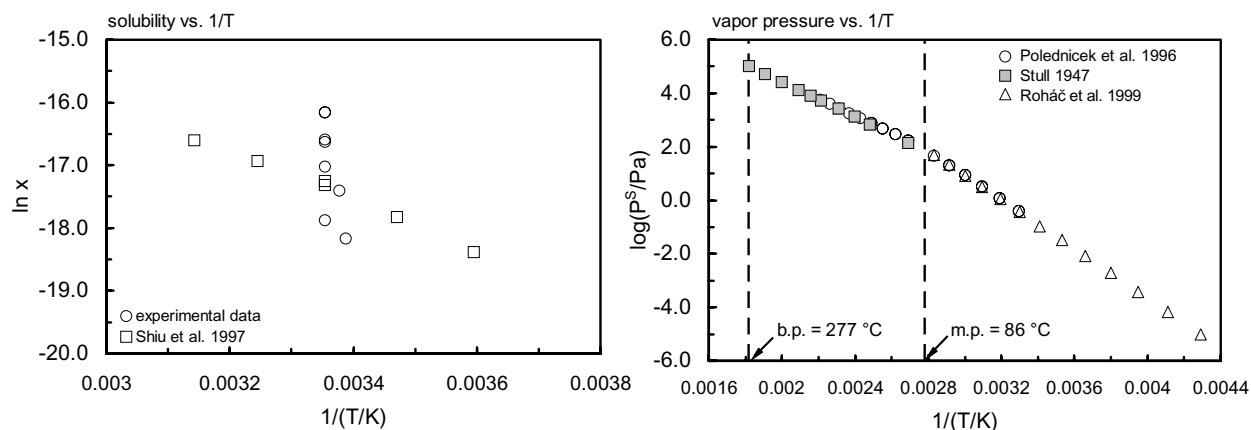


FIGURE 6.1.1.11.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for pentachlorobenzene.

TABLE 6.1.1.11.3

Reported Henry's law constants, octanol-water partition coefficients and octanol-air partition coefficients of pentachlorobenzene at various temperatures

Henry's law constant		log K _{OW}				log K _{OA}	
Ten Hulscher et al. 1992		Opperhuizen et al. 1988		Bahadur et al. 1997		Harner & Mackay 1995	
gas stripping-GC		shake flask-GC/ECD		shake flask-GC/ECD		generator column-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OW}	t/°C	log K _{OW}	t/°C	log K _{OA}
14.8	37.4	13	5.2	5	5.2	25	5.64
20	59.0	19	5.05	15	5.06	-10	7.93
20.1	49.4	28	4.70	25	4.94	0	7.418
22.1	68.1	33	4.66	35	4.79	10	6.931
24.1	66.7			45	4.66	18.7	6.539
34.8	124.1						
50.5	276.2	$\Delta H/(\text{kJ mol}^{-1}) = -30.8$		enthalpy of transfer $\Delta H/(\text{kJ mol}^{-1}) = -22.8$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 62.03$	
$\ln H = A - B/(T/K)$				$\log K_{OW} = A - \Delta H/2.303RT$		$\log K_{OA} = A + B/T$	
	H/(Pa m ³ /mol)			A	0.9255.	A	-6.2
A	21.4142			ΔH	-22800	B	3722.3
B	5108						

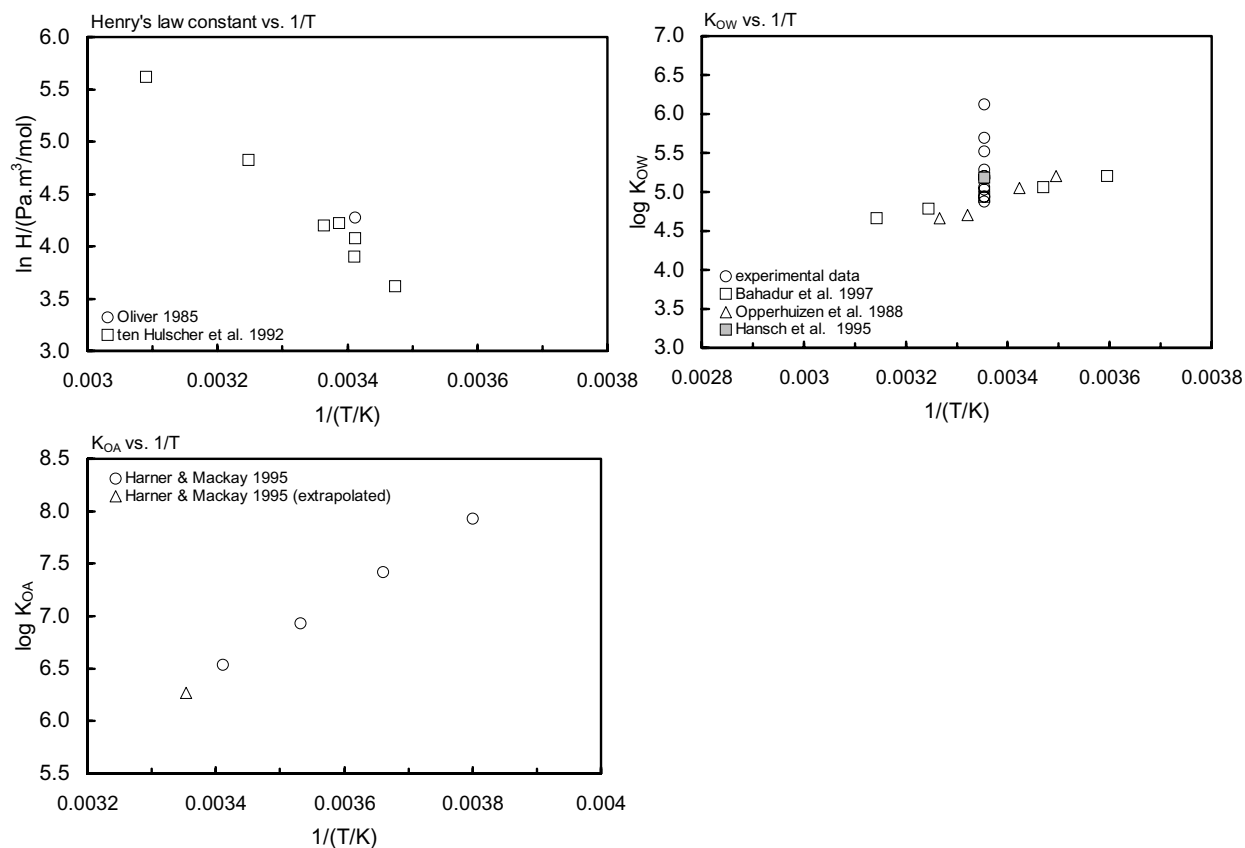
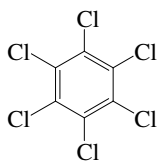


FIGURE 6.1.11.2 Logarithm of Henry's law constant, K_{OW} and K_{OA} versus reciprocal temperature for pentachlorobenzene.

6.1.1.12 Hexachlorobenzene



Common Name: Hexachlorobenzene

Synonym: HCB, perchlorobenzene, anticarie, Bunt-cure, Bunt-no-more, Julin's carbon chloride

Chemical Name: hexachlorobenzene

CAS Registry No: 118-74-1

Molecular Formula: C_6Cl_6

Molecular Weight: 284.782

Melting Point ($^{\circ}C$):

228.83 (Lide 2003)

Boiling Point ($^{\circ}C$):

325 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5691 ($23.6^{\circ}C$, Weast 1972–73; Horvath 1982)

2.004 ($23^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

181.5 ($23.6^{\circ}C$, calculated-density, Weast 1972–73; Horvath 1982)

221.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.85 (Plato & Glasgow 1969; Ruelle et al. 1993; Chickos et al. 1999)

28.74 (Tsonopoulos & Prausnitz 1971)

22.40 (Miller et al. 1984)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

57.32 (Tsonopoulos & Prausnitz 1971)

44.77 (Miller et al. 1984)

47.1 (Hinckley et al. 1990; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.01 (mp at $228.83^{\circ}C$)

0.009 (Miller et al. 1985; Suntio et al. 1988b)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.005 (generator column-GC/ECD, Weil et al. 1974)

0.006 (shake flask-LSC/ ^{14}C , Lu & Metcalf 1975)

0.11 (shake flask-nephelometric spectrophotofluorometry, Hollifield 1979)

0.005 (shake flask-UV, Yalkowsky et al. 1979)

0.0039 (shake flask-GC, Könemann 1981)

0.00921, 0.00996 (15, $25^{\circ}C$, generator column/elution method, average values of 6–7 labs., OECD 1981)

0.0054 (generator column-GC/ECD, Hashimoto et al. 1982)

0.0012–0.014 (shake flask-GC/ECD, Hashimoto et al. 1982)

0.005 (recommended, Horvath 1982)

0.047 (generator column-GC/ECD, Miller et al. 1984; 1985)

0.005 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

0.00544 ± 0.00018 (generator column-GC/ECD, measured range 5 – $45^{\circ}C$, Shiu et al. 1997)

0.38 (shake flask-GC, Boyd et al. 1998)

0.0050 ± 0.00002 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)

$\log [S_L/(mol/L)] = 0.450 - 1212/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -8.22956 - 4037.26/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.010* (generator column-GC/ECD, measured range 15 – $55^{\circ}C$, Oleszek-Kudlak et al. 2004)

0.0273, 0.398 (supercooled liquid: derivation of literature-derived value FAV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 133.3* (114.1°C, summary of literature data, temp range 114.1–309.4°C, Stull 1947)
 0.00028 (extrapolated from Antoine eq., Sears & Hopke 1949)
 $\log(P/\text{mmHg}) = 11.397 - 4197.3/(T/K)$; temp range 96–124°C (Rodebush gauge, Sears & Hopke 1949)
 $\log(P/\text{mmHg}) = [-0.2185 \times 15199.1/(T/K)] + 8.550497$; temp range 114.4–309.4°C (Antoine eq., Weast 1972–73)
 0.0015 (Callahan et al. 1979)
 0.0026 (OECD 1979)
 0.00145 (20°C, Kiltzer et al. 1979)
 0.0023* (gas saturation, measured range 15–45°C, Farmer et al. 1980)
 $\log P/\text{mmHg} = 12.94 - 5279/(T/K)$; temp range 15–45°C (gas saturation, Farmer et al. 1980)
 0.000453; 0.000167 (Klein et al. 1981)
 0.0019* (gas saturation, measured range 10–50°C, OECD 1981)
 $\log(P/\text{mmHg}) = 12.237 - 5152.1/(T/K)$; temp range 10–50°C (gas saturation, OECD 1981)
 0.00046 (evaporation rate, Dobbs & Cull 1982)
 0.00121 (extrapolated-Antoine eq., Gückel et al. 1982)
 0.0006 (20°C, evaporation rate and gravimetric method, Gückel et al. 1982)
 0.159, 0.122 (P_{GC} by GC-RT correlation with different GC columns, Bidleman 1984)
 0.303 (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} , Bidleman 1984)
 0.00332 (gas saturation-GC, interpolated from reported graph, Rordorf 1985)
 0.00205* (41.05°C, gas saturation-GC, measured range 41–100°C, Rordorf 1985)
 $\log(P/\text{Pa}) = 12.3243 - 4336.95/(T/K - 41.1905)$; temp range 41–100°C (gas saturation, Rordorf 1985)
 0.00147, 0.187 (20°C, quoted: solid P_S , supercooled liquid P_L , Bidleman & Foreman 1987)
 $\log(P_S/\text{kPa}) = 7.00706 - 2831.85/(-28.25 + T/K)$; temp range 387–502 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.35248 - 2786.78/(-61.33 + T/K)$; temp range 502–589 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 0.245 (supercooled liquid P_L , Suntio et al. 1988b)
 0.303, 0.127 (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 0.159, 0.119 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log(P_L/\text{Pa}) = 11.11 - 3582/(T/K)$ (supercooled liquid P_L , GC-RT correlation, Hinckley et al. 1990)
 0.00311* (gas saturation, measured range –15 to 40°C, Dickhut et al. 1994)
 0.001092* (20°C, gas saturation-GC/ECD, measured range –30 to 40°C, Wania et al. 1994)
 $\log(P_S/\text{Pa}) = 10.83 - 4044/(T/K)$; temp range –30 to 40°C (derived from gas saturation data, Wania et al. 1994)
 0.367; 0.344 (supercooled liquid P_L , GC-Kovács retention indices correlation; quoted lit., Spijksma et al. 1994)
 $\log(P/\text{mmHg}) = -134.3625 - 1.5459 \times 10^3/(T/K) + 61.748 \cdot \log(T/K) - 6.5123 \times 10^{-2} \cdot (T/K) + 2.0872 \times 10^{-5} \cdot (T/K)^2$;
 temp range 502–825 K (Yaws 1994)
 0.0339; 1.46×10^{-3} , 0.141 (liquid P_L from GC-RT correlation; quoted solid P_S , converted to P_L , Donovan 1996)
 $(4.6-26) \times 10^{-4}$, $(1.11-5.40) \times 10^{-3}$ (quoted exptl. solid P_S ranges: 20°C, Delle Site 1997)
 0.271; 0.00821 (P_L supercooled liquid, GC-RT correlation; solid P_S , Passivirta et al. 1999)
 $\log(P_L/\text{Pa}) = 8.42 - 2834/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 0.14, 0.094 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
 $\log(P_L/\text{Pa}) = -3530/(T/K) + 10.97$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 131.3 (gas stripping-GC, Atlas et al. 1982)
 48.6 (gas stripping-GC, Oliver 1985)
 172 (gas stripping-GC, Warner et al. 1987)
 41756 (computer value, Yaws et al. 1991)
 41.0* (gas stripping-GC/ECD, measured range 14.8–50.5°C, ten Hulscher et al. 1992)

$\ln [H/(\text{Pa m}^3/\text{mol})] = 22.7994 - 5630.6/(T/K)$, temp range 14–50°C (gas stripping-GC, ten Hulscher et al. 1992)
 26243, 29587 (26.0, 46.0°C, EPICS-GC, Hansen et al. 1993)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 7.97 - 1622/(T/K)$ (Passivirta et al. 1999)
 35.1 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 6.266 - 2377/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
 52, 65 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

6.18 (Neely et al. 1974)
 4.13 (radioisotope tracer- ^{14}C , Lu & Metcalf 1975)
 6.51 (calculated-fragment constant, Rekker 1977)
 4.13 (Hansch & Leo 1979)
 5.0, 6.27 (shake flask-GC, HPLC- k' correlation, Könemann et al. 1979)
 5.23 (HPLC-RT correlation, Veith et al. 1979b)
 6.18 (HPLC-RT correlation, Veith et al. 1979a)
 5.44 (shake flask-GC, Briggs 1981)
 6.22 (HPLC-RT correlation, McDuffie 1981)
 5.56, 5.04–5.92 (shake flask method: mean, range of mean values, OECD 1981)
 5.50 (shake flask-GC, Chiou et al. 1982; Chiou 1985)
 5.66 (HPLC-RT correlation, Hammers et al. 1982)
 5.40 (shake flask-GC, Watarai et al. 1982)
 6.13–6.27, 5.66 (range, mean, shake flask method, Eadsforth & Moser 1983)
 6.27–6.48, 6.38 (range, mean, HPLC method, Eadsforth & Moser 1983)
 5.46, 5.26; 5.47 (Review of HPLC methods; OECD/EEC shake-flask method, Harnisch et al. 1983)
 5.47 (generator column-GC/ECD, Miller et al. 1984; 1985)
 5.70–5.79 (HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)
 6.86 (HPLC/MS correlation, Burkhard et al. 1985)
 5.75; 5.60, 5.90 (selected OECD value; HPLC-RV correlation, Brooke et al. 1986)
 6.92 (HPLC- k' correlation, De Kock & Lord 1987)
 5.64 (HPLC- k' correlation, Mailhot 1987)
 6.22 (HPLC-RT correlation, Doucette & Andren 1988)
 5.7* (19°C, shake flask-GC/ECD, measured range 13–33°C, Opperhuizen et al. 1988)
 5.50 (shake flask-GC, Pereira et al. 1988)
 5.73 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 5.44 (recommended, Sangster 1993)
 5.73 (recommended, Hansch et al. 1995)
 5.46* \pm 0.02 (shake flask-GC/ECD, measured range 5–45°C, Bahadur et al. 1997)
 $\log K_{\text{OW}} = 1.1806 - 24.4/[2.303R(T/K)]$; temp range 5–45°C (van't Hoff eq., Bahadur et al. 1997)
 5.845 (solid-phase micro-extraction SPME-GC, Paschke et al. 1998)
 5.55 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
 5.52, 5.64 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

6.90*; 6.78 (generator column-GC, measured range –10 to 20°C; calculated, Harner & Mackay 1995)
 $\log K_{\text{OA}} = -6.30 + 3928/(T/K)$; temp range –10 to 20°C, $\Delta H_{\text{OA}} = 75.2 \text{ kJ/mol}$ (Harner & Mackay 1995)
 6.80 (calculated- $K_{\text{OW}}/K_{\text{AW}}$, Wania & Mackay 1996)
 7.17, 6.90 (calculated- S_{oct} and vapor pressure P , quoted lit., Abraham et al. 2001)
 7.384* (generator column-GC, measured range 5–25°C, Shoeib & Harner 2002)
 7.38, 7.21 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, $\log \text{BCF}$ at 25°C or as indicated:

3.89 (rainbow trout, calculated-rate constant ratio k_1/k_2 , Neely et al. 1974)
 3.09 (fish, Körte et al. 1978)

- 4.27, 3.73, 4.34 (fathead minnow, rainbow trout, green sunfish, Veith et al. 1979b)
 5.46 (guppy, lipid basis, Könnemann & van Leeuwen 1980;)
 4.27 (fish, Ciam et al. 1980)
 1.20 (rats, adipose tissue, Geyer et al. 1980)
 3.93, 2.46 (fish, flowing water, static water, Kenaga & Goring 1980; Kenaga 1980a)
 4.39 (algae, Geyer et al. 1981)
 3.38–4.08 mean 4.08; 3.88–4.30 mean 4.30 (rainbow trout, 15°C, wet wt., steady-state BCF on 8- to 119-d laboratory study in low exposure tank; 7- to 105-d high exposure water tank, Oliver & Niimi 1983)
 5.16–5.37 (15°C, rainbow trout, lipid basis, Oliver & Niimi 1983; quoted, Chiou 1985)
 4.39, 3.36, 4.54 (algae, fish, activated sludge, Klein et al. 1984)
 4.34 (sunfish; rainbow trout, 15°C, Davis & Dobbs 1984)
 4.54 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
 5.09 (green algae, dry wt basis, Geyer et al. 1985)
 4.39, 3.41, 4.54 (algae, fish, activated sludge, Freitag et al. 1985)
 2.62–2.97; 2.44–2.79 (human fat: lipid basis, wet weight, Geyer et al. 1987)
 4.41 (algae, Mailhot 1987)
 4.34 (fathead minnow, Carlson & Kosian 1987)
 4.38, 4.30 (worms, fish, Oliver 1987a)
 3.48 (fish-normalized, Tadokoro & Tomita 1987)
 5.57, 5.62, 5.66, 5.76 (13, 19, 28, 33°C, female guppy, Opperhuizen et al. 1988)
 6.42, 6.71, 5.96, 5.98 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 –1.35, –2.07, –0.32 (beef, milk, vegetable, reported as biotransfer factor log B_b , Travis & Arms 1988)
 5.46 (guppy-lipid base, 12 to 31-d exposure studies, Gobas et al. 1989)
 3.53 (*picea omorika*, Reischl et al. 1989)
 3.57 (fish, calculated, Figueroa & Simmons 1991)
 4.73; 4.76 (*Scenedesmus spp. Coenobia*, dry wt., batch adsorption; purge desorption, Koelmans et al. 1993)
 3.74–4.30; 4.21; 4.34; 4.16; (*Oncorhynchus mykiss*; *Poecilia reticulata*; *Lepomis cyanellus*; *Oryzias latipes*, quoted lit., flow through conditions, Devillers et al. 1996)
 5.62 (*Poecilia reticulata*, quoted lit., static and semi-static conditions, Devillers et al. 1996)
 3.18, 4.39 (macrophytes *Myriophyllum spicatum*, algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)
 5.55 (pond snail *Lymnaea stagnalis*, lipid wt basis, lipid content 0.5%, Legierse et al. 1998)
 4.38, 5.08 (algae *Chlorella*: wet wt basis, dry wt basis, Geyer et al.2000)
 3.98, 5.98 (*Daphnia*: wet wt basis, lipid wt basis, Geyer et al.2000)
 > 3.54, > 5.54 (mussel *Mytilus edulis* 21-d non-steady state: wet wt basis, lipid wt basis, Geyer et al.2000)
 3.69, 5.71 (golden orfe *Leuciscus idus melanotus*, 0.95% lipid: wet wt basis, lipid wt basis, Geyer et al.2000)
 2.65, 2.83 (human, fat: wet wt basis, lipid wt basis, Geyer et al.2000)
 3.74; 3.95 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 3.59 (Kenaga & Goring 1980; Kenaga 1980a)
 4.45 (Kenaga 1980a)
 4.49 (soil, sorption isotherm, converted from reported log K_{OM} of 4.25, Briggs 1981)
 2.56 (Speyer soil < 2.00 mm, Freundlich isotherm, Rippen et al. 1982)
 2.70 (Alfisol, Freundlich isotherm, Rippen et al. 1982)
 5.90; 5.50 (field data of Lake Ontario sediment trap material; Niagara River organic matter, Oliver & Charlton 1984)
 4.90, 5.2–6.0 (bottom sediment, range, Karickhoff & Morris 1985)
 5.2–6.7, 6.1; 5.80 (suspended sediment, average; algae > 50 μ m, Oliver 1987c)
 6.0–6.50, 6.30; 5.10 (Niagara River plume: range, mean; calculated- K_{OW} , Oliver 1987b)
 4.77 (HPLC- k' correlation, Hodson & Williams 1988)
 4.66, 3.08, 4.91 (soil/water, soil-dextran/water, humic acid/water, batch equilibrium-sorption isotherm, Enfield et al. 1989)

- 3.23, 4.73; 4.59 (Captina silt loam OC 1.49%, McLaurie sandy loam OC 0.66%; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 5.51 (organic matter, Koelmans et al. 1993)
- 4.89 ± 0.36 (suspended particulates in coastal waters, Masunaga et al. 1996)
- 4.70; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 4.23, 3.79 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
- 5.53, 5.48 (sediments: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log K_{OM} :

- 4.25 (soil-organic matter, sorption isotherm, shake flask-GC, Briggs 1981)
- 5.50 (Niagara River-organic matter, Oliver & Charlton 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 3.45 \times 10^{-10} \text{ mol m}^{-2} \text{ h}^{-1}$ (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant in air, $k = 1.44 \times 10^{-2} \text{ h}^{-1}$ (Brown et al. 1975; quoted, Mackay et al. 1985); photooxidation $t_{1/2} = 3753\text{--}37530 \text{ h}$, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987).

Hydrolysis: not expected to be important, based on $k_h = 0$ was observed after 13 d at pH 3, 7, 11, and 85°C (Ellington et al. 1987, 1988).

Biodegradation: $t_{1/2}$ (aq. aerobic) = 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974; Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 93024–200544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974; Howard et al. 1991);

degradation rate constant $k = 1.9 \times 10^{-5} \text{ h}^{-1}$ in soil (Beck & Hansen 1974; selected, Mackay et al. 1985; Mackay & Paterson 1991);

not significant in an aerobic environment, and no significant degradation rate (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2}$ (aerobic) = 970 d, $t_{1/2}$ (anaerobic) = 3900 d in natural waters (Capel & Larson 1995)

dechlorination pseudo-first order rate constant $k = 0.282 \text{ d}^{-1}$ with $t_{1/2} = 2.5 \text{ d}$ using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 18.76 \text{ h}^{-1}$; $k_2 = 0.00238 \text{ h}^{-1}$ (trout muscle, Neely et al. 1974)

$k_1 = 10000 \text{ d}^{-1}$ (guppy, Konemann & van Leeuwen 1980)

$k_1 = 22.5 \text{ h}^{-1}$ (guppy, quoted from Konemann & van Leeuwen 1980, Hawker & Connell 1985)

$\log k_1 = 1.35 \text{ d}^{-1}$ (fish, quoted from Konemann & Leeuwen 1980, Hawker & Connell 1985)

$k_1 = 18.8 \text{ h}^{-1}$ (trout, quoted from Bruggeman, Hawker & Connell 1985, Connell & Hawker 1988)

$\log k_1 = 1.27 \text{ d}^{-1}$ (trout, quoted from Bruggeman, Hawker & Connell 1985, Connell & Hawker 1988)

$1/k_2 = 420 \text{ h}$ (trout, quoted from Bruggeman et al. 1984, Hawker & Connell 1985)

$\log k_2 = 2.62 \text{ d}^{-1}$ (fish, quoted, Hawker & Connell 1985)

$k_1 = 540 \text{ d}^{-1}$ (fish, quoted, Opperhuizen 1986)

$k_2 = 0.00510, 0.00818, 0.00640, 0.0047 \text{ d}^{-1}$ (rainbow trout, calculated-fish mean body weight, Barber et al. 1988)

$\log k_1 = 2.73 \text{ d}^{-1}$ (fish, quoted from Konemann & Leeuwen 1980, Connell & Hawker 1988)

$\log k_1 = 2.65 \text{ d}^{-1}$; $\log 1/k_2 = 1.24 \text{ d}$ (fish, quoted from Bruggeman et al. 1984, Connell & Hawker 1988)

$\log k_2 = -1.24 \text{ d}^{-1}$ (fish, calculated- K_{OW} , Thomann 1989)

$k_1 = 0.049 \text{ h}^{-1}$; $k_2 = 0.023 \text{ h}^{-1}$ (mayfly-sediment model II, Gobas et al. 1989b)

$k_2 = 0.092 \text{ d}^{-1}$ with elimination $t_{1/2} = 7.5 \text{ d}$ (earthworm, Belfroid et al. 1995)

$k_1 = 6.558 \text{ h}^{-1}$, $k_2 = 0.00429 \text{ h}^{-1}$ (Macrophytes *Myrioophyllum spicatum*, Wang et al. 1996)

$k_1 = 10489 \text{ h}^{-1}$, $k_2 = 0.424 \text{ h}^{-1}$ (algae *Chlorella fusca*, Wang et al. 1996)

$k_2 = 0.016 \text{ d}^{-1}$ with $t_{1/2} = 43 \text{ d}$ and $k_2 = 0.017 \text{ d}^{-1}$ with $t_{1/2} = 42 \text{ d}$ for food concn of 14 ng/g and 103 ng/g respectively in a 30-d uptake followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_1 = 467 \text{ mL g}^{-1} \text{ d}^{-1}$, $k_2 = 0.26 \text{ d}^{-1}$ (pond snail *Lymnaea stagnalis*, Legierse et al. 1998)

$k_1 = 8 \text{ (food lipid mg)/(g worm lipid-d)}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

- Air: $t_{1/2} = 3753\text{--}37530$ h, based on estimated photooxidation half-life (Atkinson 1987, Howard et al. 1991)
 $t_{1/2} = 29 \pm 5.8$ yr at Eagle Harbor, $t_{1/2} = 15 \pm 1.9$ yr at Sleeping Bear Dunes and $t_{1/2} = 18 \pm 2.3$ yr in the Great Lakes = atmosphere at Sturgeon Point (Buehler et al. 2004).
- Surface Water: $t_{1/2} = 1.4\text{--}50$ d estimated, $t_{1/2} = 0.3\text{--}3$ d for river water and $t_{1/2} = 30\text{--}300$ d for lakes, estimated from persistence (Zoeteman et al. 1980)
 $t_{1/2} = 23256\text{--}50136$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974, Howard et al. 1991)
 $t_{1/2}(\text{aerobic}) = 970$ d, $t_{1/2}(\text{anaerobic}) = 3900$ d in natural waters (Capel & Larson 1995)
- Groundwater: $t_{1/2} = 30\text{--}300$ d, estimated from persistence (Zoeteman et al. 1980)
 $t_{1/2} = 46512\text{--}100272$ h, based on unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974, Howard et al. 1991)
- Sediment: dechlorination $t_{1/2} = 1.8$ d using a mixed enrichment culture derived from a contaminated estuarine sediment (Pavlostathis & Prytula 2000).
- Soil: $t_{1/2} > 50$ d (Ryan et al. 1988)
disappearance $t_{1/2} = 11.3$ d from testing soils (Anderson et al. 1991)
 $t_{1/2} = 23256\text{--}50136$ h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974; Howard et al. 1991)
 $t_{1/2} = 3\text{--}6$ yr in soil (Geyer et al. 2000)
 $t_{1/2} = 48.7$ and 11.7 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).
- Biota: $t_{1/2} = 163$ h, clearance from fish (Neely 1980)
 $t_{1/2} > 224$ d in rainbow trout (Niimi & Cho 1980);
 $t_{1/2} = 210$ d at 4°C , $t_{1/2} = 80$ d at 12°C , $t_{1/2} = 70$ d at 18°C in subadult rainbow trout (Niimi & Palazzo 1985)
 $t_{1/2} = 27$ d in worms at 8°C (Oliver 1987a)
biological $t_{1/2} = 12$ d in trout muscle, $t_{1/2} > 173$ d and > 224 d in trout, $t_{1/2} = 12$ d in guppy (Niimi 1987);
 $t_{1/2} = 30$ d in *picea omorika* (Reischl et al. 1989)
elimination $t_{1/2} = 1.44$ d and 12.3 d in a two-phase kinetics for earthworm in OECD soil (Belfroid et al. 1994)
elimination $t_{1/2} = 1.9\text{--}7.5$ d from earthworm in soil (Belfroid et al. 1995)
- Depuration $t_{1/2} = 42\text{--}43$ d in a 30-d dietary exposure and 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

TABLE 6.1.1.12.1

Reported aqueous solubilities and Henry's law constants of hexachlorobenzene at various temperatures

Solubility						Henry's law constant	
OECD 1981		Shiu et al. 1997		Oleszek-Kudlak et al. 2004		Ten Hulscher et al. 1992	
gen. col./elution method		generator column-GC/ECD		generator column-GC/ECD		gas stripping-GC	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{H}/(\text{Pa m}^3/\text{mol})$
15	0.00921 [†]	5	0.0022	15	0.007	14.8	23.6
25	0.00996 [‡]	15	0.0035	25	0.0096	20	41
		25	0.00544	25	0.010	20.1	30
[†] mean, 0.00206–0.0216 g/m ³		35	0.00853	35	0.018	22.1	46.6
[‡] mean, 0.00119–0.0231 g/m ³		45	0.014	45	0.024	24.1	52.5
				55	0.038	34.8	88.3
		$\Delta H_{\text{sol}} = 33.7$ kJ/mol		$\Delta H_{\text{sol}} = 33.5$ kJ/mol		50	217.2
						$\ln K_{\text{AW}} = A - B/(T/K)$	
						A	22.977
						B	5893.67

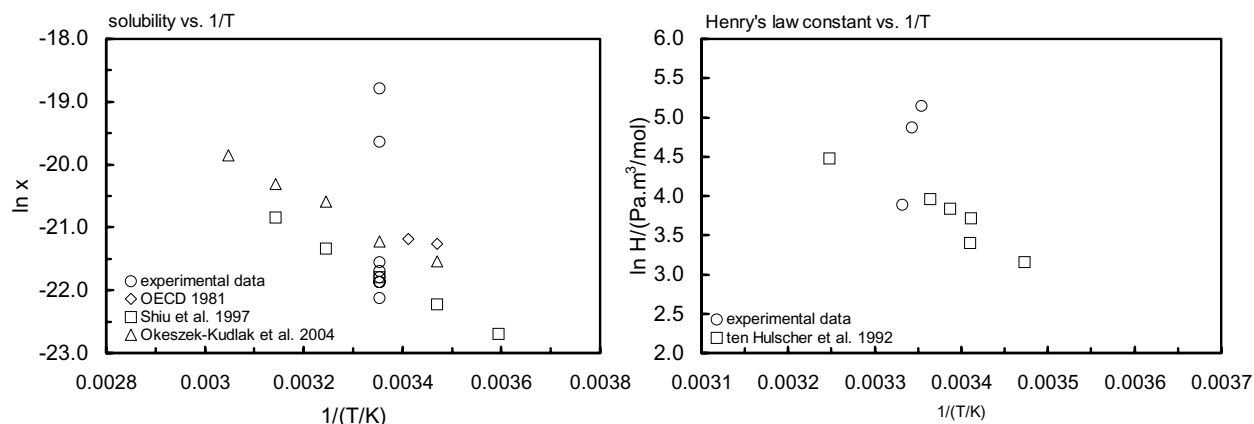


FIGURE 6.1.1.12.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for hexachlorobenzene.

TABLE 6.1.1.12.2

Reported vapor pressures of hexachlorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log (P/\text{Pa}) = A - B/(C + T/K) & (3) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \ln (P/\text{Pa}) = A - B/(C + T/K) & (3a) \end{array}$$

1.

Stull 1947		Sears & Hopke 1949		Farmer et al. 1980		OECD 1981	
summary of lit. data		Rodebush gauge		gas saturation-GC		gas saturation/balance	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
114.1	133	measured 96–124°C		15	0.000528	10	0.0008
149.3	667	eq. 1	P/mmHg	25	0.00255	20	0.0026
166.4	1333			35	0.00853	30	0.0081
185.7	2666			45	0.0279	40	0.023
206	5333	B	4793.6	25	0.0023	50	0.081
219	7999					10	0.00028
235.5	13332			eq. 1	P/mmHg	20	0.0011
258.8	26664			A	12.94	30	0.003
283.5	53329			B	5279	40	0.013
309.4	101325					50	0.039
						eq. 1	P/mmHg
mp/°C	230					A	12.237
						B	5152.1

TABLE 6.1.1.11.2 (Continued)

Rordorf 1985		Liu & Dickhut 1994		Wania et al. 1994	
gas saturation		gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70.3	0.452	25	3.11×10^{-3}	0	1.03×10^{-4}
80.3	1.155	40	0.121	10	3.556×10^{-4}
90.4	2.77			20	1.092×10^{-3}
100.25	6.29	$\Delta H_V/(\text{kJ mol}^{-1}) = 81.3$		30	3.276×10^{-3}
eq. 3	P/Pa	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 105$		eq. 1	P/Pa
A	12.3243			A	10.83
B	4336.95			B	4044
C	-41.1905			$\Delta H_V/(\text{kJ mol}^{-1}) = 77.4$	

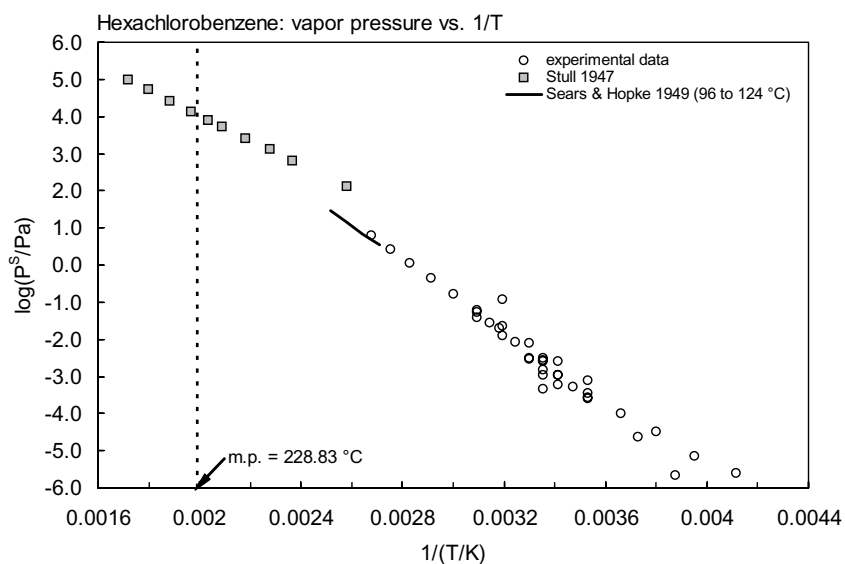


FIGURE 6.1.1.12.2 Logarithm of vapor pressure versus reciprocal temperature for hexachlorobenzene.

TABLE 6.1.1.12.3
Reported octanol-water partition coefficients and octanol-air partition coefficients of hexachlorobenzene at various temperatures

log K _{OW}				log K _{OA}			
Oppehuizen et al. 1988		Bahadur et al. 1997		Harner & Mackay 1995		Shoeib & Harner 2002	
shake flask-GC/ECD		shake flask-GC/ECD		generator column-GC			
t/°C	log K _{OW}	t/°C	log K _{OW}	t/°C	log K _{OA}	t/°C	log K _{OA}
13	5.68	5	5.74	25	6.9	5	8.1044
19	5.7	15	5.6	−10	8.653	10	7.887
28	5.58	25	5.46	0	8.105	15	7.7
33	4.66	35	5.3	10	6.213	20	7.5634
		45	5.17	18.5	7.185	25	7.3878
						25	7.384
ΔH/(kJ mol ^{−1}) = −24.4		enthalpy of transfer ΔH/(kJ mol ^{−1}) = −24.4 log K _{OW} = A − ΔH/2.303RT		ΔH _{OA} /(kJ mol ^{−1}) = 75.2		ΔH _{OA} /(kJ mol ^{−1}) = 55.8	
		A 1.1806		log K _{OA} = A + B/T		log K _{OA} = A + B/T	
		ΔH −24400		A −6.3		A −2.395	
				B 3928		B 2914	

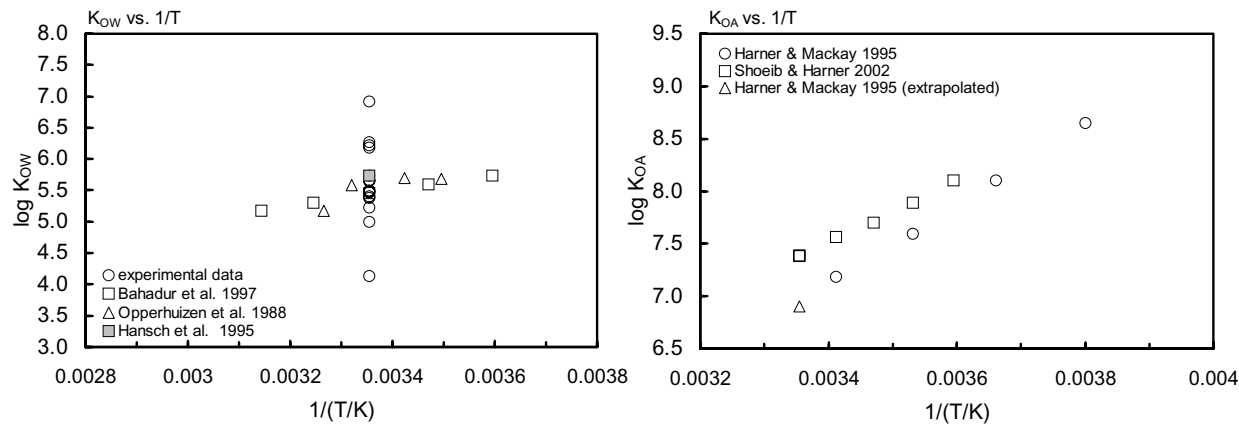
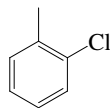


FIGURE 6.1.1.12.3 Logarithm of K_{OW} and K_{OA} versus reciprocal temperature for hexachlorobenzene.

6.1.2 CHLOROTOLUENES

6.1.2.1 2-Chlorotoluene



Common Name: 2-Chlorotoluene

Synonym: *o*-Tolylchloride, *o*-chlorotoluene, 2-chloro-1-methylbenzene

Chemical Name: 2-chlorotoluene

CAS Registry No: 95-49-8

Molecular Formula: C_7H_7Cl

Molecular Weight: 126.584

Melting Point ($^{\circ}C$):

−35.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

159.15 (Dreisbach 1955; Weast 1982–83)

159.0 (Dean 1985, 1992)

Density (g/cm^3 at $20^{\circ}C$):

1.08245, 1.07762 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm^3/mol):

116.9 ($20^{\circ}C$, calculated-density)

139.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.368 (Dreisbach 1955; Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

372 (Isnard & Lambert 1989)

252.0 (shake flask, Fredenlund et al. 1995)

$117^* \pm 5.1$ (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

487 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log P/mmHg = 7.29547 - 1701.60/(T/K - 45.42)$; temp range $4-75^{\circ}C$ (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)

133.3*, 666.6, 1333 (5.4, 30.6, $43.2^{\circ}C$, summary of lit. data, temp range $5.4-159^{\circ}C$, Stull 1947)

482.5 (calculated by formula, Dreisbach 1955; quoted, Riddick et al. 1986, Howard 1993)

$\log (P/mmHg) = 6.94763 - 1497.2/(209.0 + t/^{\circ}C)$; temp range $65-220^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

482.5 (extrapolated-Antoine eq., Weast 1972–73)

$\log (P/mmHg) = (-0.2185 \times 10279.3)/(T/K) + 8.091764$; temp range $5.4-159.3^{\circ}C$ (Antoine eq., Weast 1972–73)

5721* ($72.654^{\circ}C$, temp range $72.654-158.323^{\circ}C$, Cervenkova & Boublik 1982)

473 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.09563 - 1507.930/(t/^{\circ}C + 209.846)$; temp range $72.5-158.3^{\circ}C$ (Antoine eq., Boublik et al. 1984)

485 (interpolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 7.36797 - 1735.8/(t/^{\circ}C + 230.0)$; temp range $0-65^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 6.94763 - 1497.2/(t/^{\circ}C + 209.0)$; temp range: $65-220^{\circ}C$ (Antoine eq., Dean 1985, 1992)

472.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{Pa}) = 6.07253 - 1497.2/(T/\text{K} - 64.15)$; temp range 338–493K (liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 33.2792 - 3.4099 \times 10^3/(T/\text{K}) - 8.6743 \cdot \log (T/\text{K}) + 6.8174 \times 10^{-10} \cdot (T/\text{K}) + 1.8987 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 237–656 K (Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

370* (23°C, equilibrium cell-GC, measured range 1–23°C, Leighton & Calo 1981)

$\ln (k_H/\text{atm}) = 17.18 - 3545/(T/\text{K})$; temp range: 1.0–23.0°C (equilibrium cell-concn ratio, Leighton & Calo 1981)

295 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 3.890 - 1409/(T/\text{K})$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.42 (shake flask, Leo et al. 1971, Hansch & Leo 1979, Hansch et al. 1995)

3.52 (HPLC-RT correlation, Könnemann et al. 1979)

3.40 (HPLC- k' correlation, Hanai et al. 1981)

3.59 (RP-HPLC-RT correlation, Edsforth 1986)

3.52 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.2.1.1

Reported aqueous solubilities, vapor pressures and Henry's law constants of 2-chlorotoluene at various temperatures

Aqueous solubility		Vapor pressure				Henry's law constant	
Ma et al. 2001		Stull 1947		Cernenkova & Boublik 1982		Leighton & Calo 1981	
shake flask-GC		summary of lit. data				equilibrium cell-GC	
$t/^\circ\text{C}$	$\text{S/g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	$\text{Pa m}^3/\text{mol}$
5	89.4	5.4	133	72.654	5721	1	159.4
15	97.1	30.6	666.6	81.522	8325	3	112
25	117	43.2	1333	88.657	13911	12.4	178.5
35	128	56	2666	94.646	16792	12.5	216.1
45	132	72	5333	99.758	20277	17.9	243.5
		81.8	7999	105.05	24559	19.1	319.7
		94.7	13332	110.613	29367	22.7	3223
		115	26664	115.995	34778	23	369.7
		137.1	53329	121.252	40719	$\ln (H/\text{atm}) = A - B/(T/\text{K})$	
		159	101325	126.313	47579		
				139.532	60191		
		mp/°C	-	147.287	74587		
				155.689	93400		
				158.323	99991		
				bp/°C	158.849		
						A	17.18
						B	3545

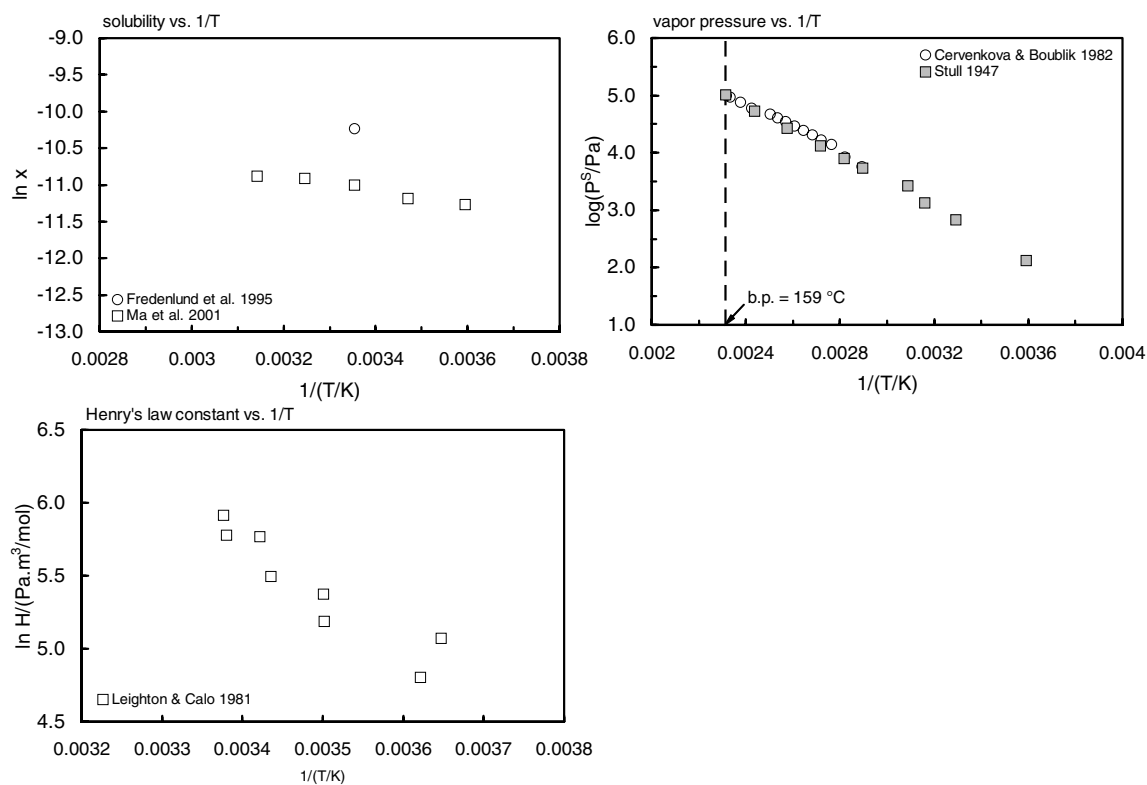
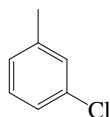


FIGURE 6.1.2.1.1 Logarithm of mole fraction solubility, vapor pressure and Henry's law constant versus reciprocal temperature for 2-chlorotoluene.

6.1.2.2 3-Chlorotoluene



Common Name: 3-Chlorotoluene

Synonym: *m*-Tolylchloride, 3-chloro-1-methylbenzene

Chemical Name: 3-chlorotoluene

CAS Registry No: 108-41-8

Molecular Formula: C_7H_7Cl

Molecular Weight: 126.584

Melting Point ($^{\circ}C$):

−47.8 (Weast 1982–83; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

161.8 (Dean 1985; 1992; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0722 (Weast 1982–83)

1.0728 ($20^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

118.1 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

139.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

43.76 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

372 (Isnard & Lambert 1989)

$117^* \pm 2.1$ (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

418 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log P/mmHg = 7.62515 - 1887.31/(T/K - 33.40)$; temp range $4-75^{\circ}C$ (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)

133.3^* , 666.6, 1333 (4.8, 30.3, $43.2^{\circ}C$, summary of lit. data, temp range $4.8-162.3^{\circ}C$, Stull 1947)

488.9 (extrapolated, Antoine eq., Weast 1972–73)

$\log (P/mmHg) = (-0.2185 \times 10081.1)/(T/K) + 7.952234$; temp range $4.8-162.3^{\circ}C$ (Antoine eq., Weast 1982–83)

403.0 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.09068 - 1511.858/(t/^{\circ}C + 208.119)$; temp range $64.8-159.8^{\circ}C$ (Antoine eq., Boublik et al. 1984)

670.0 (Riddick et al. 1986)

$\log (P/kPa) = 6.2794 - 1637.6/(223.3 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

512.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P/kPa) = 6.90317 - 2028.13/[(T/K) - 11.629]$; temp range $277-436\ K$ (liquid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.28 (shake flask, Leo et al. 1971, Hansch & Leo 1979)

3.40 (HPLC- k' correlation, Hanai et al. 1981)

- 3.28 (shake flask, Log P Database, Hansch & Leo 1987)
 3.17 (calculated-UNFIC activity coefficients, Dallos et al. 1993)
 3.28 (recommended, Sangster 1993)
 3.28 (recommended, 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.88 (activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.2.2.1
Reported aqueous solubilities and vapor pressures of 3-chlorotoluene at various temperatures

Aqueous solubility		Vapor pressure	
Ma et al. 2001		Stull 1947	
shake flask-GC		summary of literature data	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
5	101	4.8	133
15	99.3	30.3	666.6
25	117	43.2	1333
35	113	57.4	2666
45	128	73	5333
		83.7	7999
		96.3	13332
		116.6	26664
		139.7	53329
		162.3	101325
		mp/ $^{\circ}\text{C}$	–

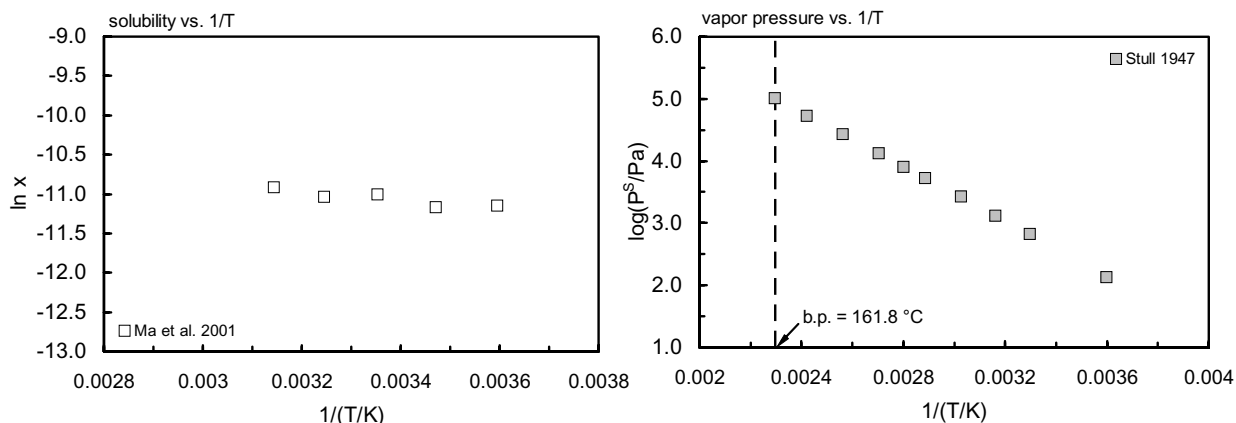
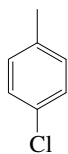


FIGURE 6.1.2.2.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 3-chlorotoluene.

6.1.2.3 4-Chlorotoluene



Common Name: 4-Chlorotoluene

Synonym: *p*-Tolylchloride, 4-chloro-1-methylbenzene

Chemical Name: 4-chlorotoluene

CAS Registry No: 106-43-4

Molecular Formula: C_7H_7Cl

Molecular Weight: 126.584

Melting Point ($^{\circ}C$):

7.5 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

162.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0697 (Weast 1982–83; Riddick et al. 1986; Dean 1985, 1992; Lide 2003)

Molar Volume (cm^3/mol):

118.3 (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

139.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

106.0 ($20^{\circ}C$, Yalkowsky 1987)

123 ± 6.1 (shake flask-GC/FID, Ma et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

422 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log P/mmHg = 23.07210 - 3041.02/(T/K) - 5 \cdot \log(T/K)$; temp range $4-75^{\circ}C$ (vapor pressure eq. based on exptl. data, Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)

133.3*, 666.6, 1333 ($5.5, 31.0, 43.8^{\circ}C$, temp range $5.5-162.3^{\circ}C$, summary of lit. data, Stull 1947)

471.6 (interpolated, Antoine eq., Weast 1982–83)

$\log(P/mmHg) = (-0.2185 \times 10151.7)/(T/K + 7.988366)$; temp range $5.5-162.3^{\circ}C$ (Antoine eq., Weast 1982–83)

$\log(P/kPa) = 6.09068 - 1511.858/(t/^{\circ}C + 208.199)$; temp range $65-160^{\circ}C$ (Antoine eq., Boublik et al. 1984)

670 ($30.3^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 6.75005 - 1887.31/(239.75 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

506.7 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.90317 - 2107.52/(T/K - 5.373)$; temp range $304-436\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 61.8901 - 4.3760 \times 10^3/(T/K) - 19.840 \cdot \log(T/K) + 7.991 \times 10^{-3} \cdot (T/K) + 1.0781 \times 10^{-13} \cdot (T/K)^2$, temp range $281-660\ K$ (Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

412.4 (calculated-P/C, Howard 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.33 (shake flask, Leo et al. 1971; Hansch & Leo 1979; 1985)
- 3.42 (HPLC-RT correlation, Könemann et al. 1979)
- 3.40 (HPLC- k' correlation, Hanai et al. 1981)
- 3.30 (shake flask, Wang et al. 1987)
- 3.33 (recommended, Sangster 1993)
- 3.33 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

- 1.65–2.30 (estimated from $\log K_{OW}$, Lyman et al. 1990; Howard 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.65–3.19 (estimated from $\log K_{OW}$, Lyman et al. 1990; Howard 1993)
- 4.10 (activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: based on the Henry's law constant, the volatilization $t_{1/2} \sim 3.5$ h from a model river 1 m deep, flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 8.4$ d in the atmosphere with rate constant $k = 1.9 \times 10^{-12}$ cm³/molecule·s at 25°C for the reaction with photochemically produced hydroxyl radicals (Atkinson 1987; quoted, Howard 1993).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 8.4$ d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Atkinson 1987; quoted, Howard 1993).

Surface water: $t_{1/2} = 1.2$ d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

TABLE 6.1.2.3.1

Reported aqueous solubilities and vapor pressures of 4-chlorotoluene at various temperatures

Aqueous solubility		Vapor pressure			
Ma et al. 2001		Stull 1947		Cervenkova & Boublik 1982	
shake flask-GC		summary of lit. data			
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
5	99	5.50	133	64.855	3584
15	103	31.0	666.6	75.304	5727
25	123	43.8	1333	84.258	8333
35	136	57.8	2666	91.408	11078
45	153	73.5	5333	97.416	13924
		83.2	7999	102.574	16819
		96.6	13332	107.91	20322
		117.1	26664	113.464	24580
		139.8	53329	118.857	29380
		162.3	101325	124.14	34794
				129.212	40761
		mp/°C	7.3	134.395	47661
				142.507	60218
				150.285	74704
				158.718	93384
				159.801	96011
				bp/°C	161.904

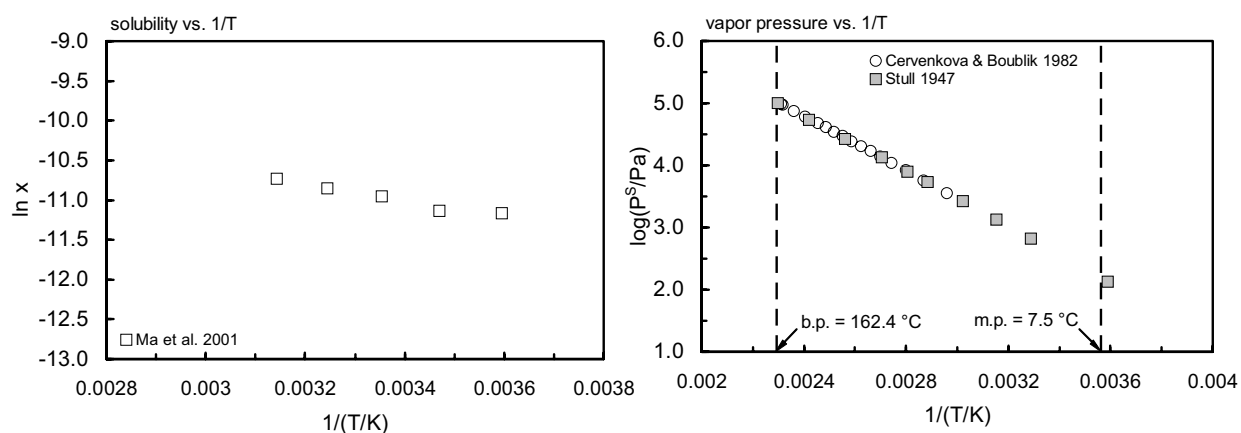
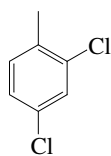


FIGURE 6.1.2.3.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 4-chlorotoluene.

6.1.2.4 2,4-Dichlorotoluene



Common Name: 2, 4-Dichlorotoluene

Synonym: 2, 4-dichloro-1-methylbenzene

Chemical Name: 2, 4-dichlorotoluene

CAS Registry No: 95-73-8

Molecular Formula: $C_7H_6Cl_2$

Molecular Weight: 161.029

Melting Point ($^{\circ}C$):

-13.5 (Weast 1982–83, Lide 2003)

Boiling Point ($^{\circ}C$):

201 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2498 (Weast 1982–83)

1.2476 (Riddick et al. 1986, Lide 2003)

1.246 (Dean 1985, 1992)

Molar Volume (cm^3/mol):

128.6 (calculated-density, Stephenson & Malanowski 1987)

160.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

26.20 ± 2.1 (shake flask-GC/FID, Ma et al. 2001)

18.9, 26.2, 30.7, 37 (15, 25, 35, $45^{\circ}C$, shake flask-GC, Ma et al. 2001)

25.9 ± 2.2 (generator column-GC/FID, Ma et al. 2001)

22.3, 23.1, 25.9, 32, 36.6 (5, 15, 25, 35, $45^{\circ}C$, generator column-GC, Ma et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

55.5 (Riddick et al. 1986)

$\log(P/kPa) = 5.6199 - 1330.4/(t/^{\circ}C + 168.5)$ (Antoine eq., Riddick et al. 1986)

55.51 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.6199 - 1330.4/(T/K - 104.65)$; temp range 346–475 K (Antoine eq., Stephenson & Malanowski 1987)

61.06 (Daubert & Danner 1989)

$\log(P/mmHg) = 31.9325 - 3.7438 \times 10^3/(T/K) - 8.0123 \cdot \log(T/K) - 7.5077 \times 10^{-11} \cdot (T/K) + 1.250 \times 10^{-6} \cdot (T/K)^2$, temp range 260–705 K (Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

350.6 (calculated, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.24 (HPLC-RT correlation, Könemann et al. 1979)

4.24 (recommended, Sangster 1993)

4.24 (shake flask, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.99 (estimated from $\log K_{OW}$, Howard 1997)

Sorption Partition Coefficient, $\log K_{OC}$:

3.68 (estimated from $\log K_{OW}$, Howard 1997)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 4.0$ h in a model river 1-m deep with a 1 m/s current and a 3 m/s wind, $t_{1/2} = 1$ d in the Rhine River in the Netherlands (Howard 1997)

Photolysis:

Oxidation: photooxidation $t_{1/2} = 11.6$ d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

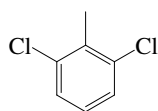
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 11.6$ d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

Surface water: $t_{1/2} = 1.0$ d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

volatilization $t_{1/2} = 4$ h in a model river, $t_{1/2} = 1$ d in Rhine River in the Netherlands (Howard 1993)

6.1.2.5 2,6-Dichlorotoluene

Common Name: 2, 6-Dichlorotoluene

Synonym:

Chemical Name: 2, 6-dichlorotoluene

CAS Registry No: 118-69-4

Molecular Formula: $C_7H_6Cl_2$

Molecular Weight: 161.029

Melting Point ($^{\circ}C$): liquid

25.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

198 (Weast 1982–83, Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.254 (Dean 1992)

1.2686 (Lide 2003)

Molar Volume (cm^3/mol):

126.9 ($20^{\circ}C$, calculated-density)

160.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

23.3 ± 0.81 (shake flask-GC/FID, Ma et al. 2001)

16.7, 19.8, 23.3, 30.1, 33 (5, 15, 25, 35, $45^{\circ}C$, shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

53.19 (estimated, Lyman et al. 1990, Howard 1997)

Henry's Law Constant ($Pa \cdot m^3/mol$):

350.6 (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.29 (HPLC- k' correlation, Könnemann et al. 1979)

4.29 (recommended, Sangster 1983)

4.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.03 (estimated from $\log K_{ow}$, Howard 1997)

Sorption Partition Coefficient, $\log K_{OC}$:

3.71 (estimated from $\log K_{ow}$, Howard 1997)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: based on Henry's law constant, an estimated $t_{1/2} = 4.0$ h of volatilization from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Howard 1997).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 11.6$ d in the atmosphere for reaction with photochemically produced hydroxyl radical (Howard 1997).

Hydrolysis:

Biodegradation:

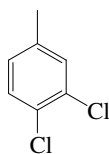
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 11.6$ d in the atmosphere for the reaction with photochemically produced hydroxyl radical (Howard 1997).

6.1.2.6 3,4-Dichlorotoluene



Common Name: 3, 4-Dichlorotoluene

Synonym: 3, 4-dichloro-1-methylbenzene

Chemical Name:

CAS Registry No: 95-75-0

Molecular Formula: $C_7H_6Cl_2$

Molecular Weight: 161.029

Melting Point ($^{\circ}C$):

-15.2 (Weast 1982-83; Lide 2003)

Boiling Point ($^{\circ}C$):

208.9 (Weast 1982-83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.25256, 1.24751 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955; Riddick et al. 1986)

1.2564 (Weast 1982-83; Lide 2003)

Molar Volume (cm^3/mol):

127.9 (calculated-density, Stephenson & Malanowski 1987)

160.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

13.33, 10.13 ($25^{\circ}C$, bp, Dreisbach 1955; Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.544 (Dreisbach 1955)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

26 ($30^{\circ}C$, Dreisbach 1955; IUPAC Solubility Data Series, Horvath & Getzen 1985; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

42 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.97925 - 1655.4/(195.0 + t/^{\circ}C)$; temp range $105-270^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = 6.91048 - 946.35/(246.68 + t/^{\circ}C)$; temp range -87 to $7^{\circ}C$ (Antoine eq., Dean 1985, 1992)

42.0 (Riddick et al. 1986)

$\log(P/kPa) = 6.10415 - 1655.44/(195.0 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.10415 - 1655.4/(T/K - 78.15)$; temp range $378-543 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.067 (Verhaar et al. 1992)

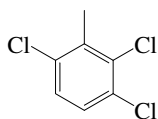
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.2.7 2,3,6-Trichlorotoluene

Common Name: 2, 3, 6-Trichlorotoluene

Synonym:

Chemical Name: 2, 3, 6-trichlorotoluene

CAS Registry No: 2077-46-5

Molecular Formula: $C_7H_5Cl_3$

Molecular Weight: 195.474

Melting Point ($^{\circ}C$):

45–46 (Weast 1982–83)

Boiling Point ($^{\circ}C$):

229.5 (Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

180.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.629 (mp at $45.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.08 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.6249 - 1323/(T/K - 144.15)$; temp range 384–509 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

152 (gas stripping-GC, Oliver 1985)

245 (calculated-bond contribution method, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.80 (calculated as per Hansch & Leo 1979, Oliver 1987b)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

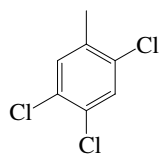
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: elimination $t_{1/2} < 5$ d, observed and corrected for growth dilution in oligochaete worms (Oliver 1987b)

6.1.2.8 2,4,5-Trichlorotoluene

Common Name: 2, 4, 5-Trichlorotoluene

Synonym: 2, 4, 5-TCT

Chemical Name: 2, 4, 5-trichlorotoluene

CAS Registry No: 6639-30-1

Molecular Formula: $C_7H_5Cl_3$

Molecular Weight: 195.474

Melting Point ($^{\circ}C$):

82.4 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

231 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1004 (Lide 2003)

Molar Volume (cm^3/mol):

115.0 ($20^{\circ}C$, calculated-density)

180.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.273 (mp at $82.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2.33 ± 0.22 (shake flask-GC/FID, Ma et al. 2001)

1.10, 1.38, 2.33, 3.33, 5.64 (5, 15, 25, 35, $45^{\circ}C$, shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

152 (gas stripping-GC, Oliver 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.82 (calculated- π method of Hansch & Leo 1979, Oliver & Niimi 1984, 1985)

4.80 (Oliver & Niimi 1985)

4.780 (Verhaar et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.68 (rainbow trout, Oliver & Niimi 1984; Oliver 1987)

3.54–3.99 with mean value of 3.88; 3.52–4.04 with mean value of 3.93 (rainbow trout, wet wt., $15^{\circ}C$, steady-state BCF on 7- to 96-d laboratory study on two tanks of different water concn, Oliver & Niimi 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air:

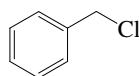
Surface water: $t_{1/2} = 1.8$ d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} < 5$ d, observed and corrected for growth dilution in oligochaete worms (Oliver 1987b).

6.1.2.9 α -Chlorotoluene

Common Name: α -Chlorotoluene

Synonym: chloromethylbenzene, benzyl chloride

Chemical Name:

CAS Registry No: 100-44-7

Molecular Formula: C_7H_7Cl , $C_6H_5CH_2Cl$

Molecular Weight: 126.584

Melting Point ($^{\circ}C$):

−45 (Lide 2003)

Boiling Point ($^{\circ}C$):

179 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

118.0 (calculated-density, Stephenson & Malanowski 1987)

139.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

493 ($20^{\circ}C$, Riddick et al. 1986)

579 (calculated-fragment const., Wakita et al. 1986)

236 (calculated-group contribution, Kühne et al. 1995)

409 ($20^{\circ}C$, limiting activity coeff. by equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($22.0^{\circ}C$, summary of lit. data, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11158.7/(T/K)] + 8.290189$; temp range $22-179.4^{\circ}C$ (Antoine eq., Weast 1972–73)

641* ($47.84^{\circ}C$, isoteniscope method, measured range $47.84-117.08^{\circ}C$, Ashcroft 1976)

$\log(P/mmHg) = 6.801 - 1477/(216.9 + t/^{\circ}C)$; temp range $48-117^{\circ}C$ (isoteniscope method, Ashdroft 1976)

641 (Riddick et al. 1986)

$\log(P/kPa) = 5.926 - 1477/(193.7 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

170 (interpolated-Anotine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.7176 - 1954.13/(T/K - 38.02)$; temp range $295-453$ K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 7.73903 - 2642.08/(T/K + 12.819)$; temp range $320-390$ K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 12.1503 - 2.9139 \times 10^3/(T/K) - 0.3712 \cdot \log(T/K) - 5.2889 \times 10^{-3} \cdot (T/K) + 2.6296 \times 10^{-6} \cdot (T/K)^2$, temp range $234-686$ K (Yaws 1994)

133.05* ($24.05^{\circ}C$, transpiration method, measured range $276-309$ K, Krasnykh et al. 2002)

$\ln(P/Pa) = 281.417/R - 71588.799/R(T/K) - (72.0/R) \cdot \ln[(T/K)/298.15]$; temp range $276-309$ K (transpiration method, Krasnykh et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

159.4, 122, 178, 216, 243.5, 320, 322, 370 (1.0, 3.0, 12.4, 12.5, 17.9, 19.1, 22.7, $23.0^{\circ}C$, equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)

$\ln(k_H/atm) = 17.18 - 3545/(T/K)$; temp range $1.0-23.0^{\circ}C$ (equilibrium cell-concn ratio, Leighton & Calo 1981)

36.07 ($20^{\circ}C$, equilibrium air stripping-GC, Hovorka & Dohnal 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} < 0.04 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K with a tropospheric lifetimes $\tau > 290 \text{ d}$ and $\tau \sim 3 \text{ d}$ due to reactions with O_3 and OH radical at room temp. (Atkinson et al. 1982)

$k_{OH} = (2.95 \pm 0.15) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a atmospheric lifetime $\tau = 3.9 \text{ d}$ at room temp. (relative rate method, Edney et al. 1986)

$k_{OH}(\text{calc}) = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs}) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = 2.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$t_{1/2} = 22\text{--}218 \text{ h}$, based on photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: rate constant $k = 1.28 \times 10^{-5} \text{ s}^{-1}$ and $t_{1/2} = 15 \text{ h}$ at 25°C and pH 7 (Mabey & Mill 1978)

neutral rate constant $k = 8.5 \pm 0.5 \text{ min}^{-1}$ at 25°C (Ellington et al. 1988)

$t_{1/2} = 25\text{--}290 \text{ h}$ based on overall hydrolysis rate constant (Howard et al. 1991)

Biodegradation: $t_{1/2}(\text{aerobic}) = 168\text{--}672 \text{ h}$, based on unacclimated aqueous screening test data; $t_{1/2}(\text{anaerobic}) = 672\text{--}2688 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetimes $\tau > 290 \text{ d}$ and $\tau \sim 3 \text{ d}$ due to reactions with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982);

calculated atmospheric lifetime $\tau = 3.9 \text{ d}$ due to reaction with OH radical at room temp. (Edney et al. 1986)

$t_{1/2} = 22\text{--}218 \text{ h}$, based on photooxidation half-life in air (Howard et al. 1991)

Surface water: $t_{1/2} = 15\text{--}290 \text{ h}$, based on estimated hydrolysis half-lives (Howard et al. 1991)

Groundwater: $t_{1/2} = 15\text{--}290 \text{ h}$, based on estimated hydrolysis half-lives (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 15\text{--}290 \text{ h}$, based on estimated hydrolysis half-lives (Howard et al. 1991)

Biota:

TABLE 6.1.2.9.1

Reported vapor pressures of a-chlorotoluene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

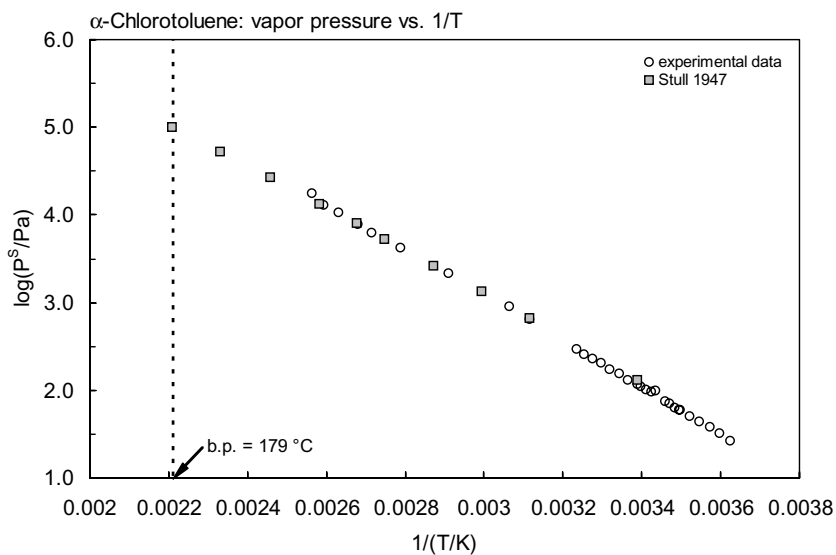
$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

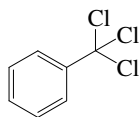
Stull 1947		Ashcroft 1976		Krasnykh et al. 2002	
summary of lit. data		isoteniscope method		transpiration method	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
22.0	133	47.84	641.3	2.85	26.95
47.8	666.6	53.37	905.3	4.85	32.31
60.8	1333	70.60	2177	6.85	38.60

(Continued)

TABLE 6.1.2.9.1 (Continued)

Stull 1947		Ashcroft 1976		Krasnykh et al. 2002	
summary of lit. data		isoteniscope method		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
75.0	2666	85.63	4246	8.85	43.78
90.7	5333	95.35	6330	10.85	51.48
100.5	7999	100.2	7905	12.85	60.14
114.2	13332	106.95	10566	12.95	60.61
134.0	26664	122.67	12883	13.95	64.27
1558	53329	117.08	17857	14.95	70.50
179.4	101325			15.95	75.36
		eq. 2	P/mmHg	17.95	98.72
mp/°C	-39	A	6.801	18.95	97.84
		B	1477	20.05	101.6
		C	193.7	21.15	111.0
				22.05	117.44
				24.05	133.06
				26.05	153.53
				28.15	175.98
				30.15	204.90
				32.15	232.87
				34.15	257.42
				36.15	295.82
				$\Delta H_V(\text{kJ mol}^{-1}) = 50.12$	
				at 25°C	

FIGURE 6.1.2.9.1 Logarithm of vapor pressure versus reciprocal temperature for α -chlorotoluene.

6.1.2.10 α, α, α -Trichlorotoluene

Common Name: α, α, α -Trichlorotoluene

Synonym: trichloromethylbenzene, benzotrichloride

Chemical Name: α, α, α -Trichlorotoluene

CAS Registry No: 98-07-7

Molecular Formula: $C_7H_5Cl_3$, $C_6H_5CCl_3$

Molecular Weight: 195.474

Melting Point ($^{\circ}C$):

−4.42 (Lide 2003)

Boiling Point ($^{\circ}C$):

221 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.3723 ($20^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

142.4 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

180.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

5.30 ($5^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (45.8, summary of lit. data, Stull 1947)

$\log (P/mmHg) = [-0.2185 \times 8869.7/(T/K)] + 8.071972$, temp range $32-102.2^{\circ}C$ (Antoine eq., Weast 1972–73)

34.67 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.95923 - 2268.82/(T/K - 28.669)$; temp range $318-487 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 0.4912 - 2.7285 \times 10^3/(T/K) + 4.4706 \cdot \log (T/K) - 1.058 \times 10^{-2} \cdot (T/K) + 4.7621 \times 10^{-6} \cdot (T/K)^2$; temp range $268-737 K$ (Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.92 (shake flask, Leo et al. 1979, Hansch & Leo 1979, Hansch et al. 1995; quoted, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} = 173.7-1737 h$, based on photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: rate constant $k = 6.3 \times 10^{-2} s^{-1}$ and $t_{1/2} = 19 s$ at $25^{\circ}C$ and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 11 s - 3 min$, based on overall hydrolysis rate constants (Howard et al. 1991)

Biodegradation: $t_{1/2}$ (aerobic) = 24–168 h, based on limited aqueous screening test data; $t_{1/2}$ = 96–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 173.7–1737 h, based on photooxidation half-life in air (Howard et al. 1991)

Surface water: $t_{1/2}$ = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

Groundwater: $t_{1/2}$ = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

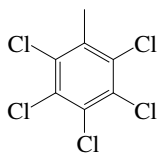
Sediment:

Soil: $t_{1/2}$ = 11 s – 3.0 min, based on measured hydrolysis rate constants (Howard et al. 1991)

Biota:

TABLE 6.1.2.10.1
Reported vapor pressures of α , α , α -chlorotoluene at various temperatures

Stull 1947	
summary of literature data	
$t/^{\circ}\text{C}$	P/Pa
45.8	133.3
73.7	666.6
87.6	1333
102.7	2666
119.8	5333
130.0	7999
144.3	13332
165.6	26664
189.2	53329
213.5	101325
mp/ $^{\circ}\text{C}$	–21.2

6.1.2.11 Pentachlorotoluene

Common Name: Pentachlorotoluene

Synonym:

Chemical Name: pentachlorotoluene

CAS Registry No: 877-11-1

Molecular Formula: $C_7H_3Cl_5$

Molecular Weight: 264.364

Melting Point ($^{\circ}C$):

224.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

301 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

222.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.011 (mp at $224.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.028 ± 0.001 , 0.047 ± 0.004 (25, $35^{\circ}C$, shake flask-GC, Ma et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.20 (calculated as per Hansch & Leo 1979, Oliver & Niimi 1985; Oliver 1987b)

5.50 (assumed to have approx. the same K_{ow} of HCB, Oliver & Charlton 1984)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ at $25^{\circ}C$ or as indicated:

3.38–3.86 mean 3.83 (rainbow trout, wet wt., $15^{\circ}C$, steady-state BCF, 7- to 96-d laboratory study, Oliver & Niimi 1985)

3.83; 4.36 (rainbow trout, laboratory data; Lake Ontario field data, Oliver & Niimi 1985)

4.45; 3.83 (oligochaete worm; fish, Oliver 1987b)

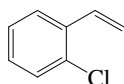
Sorption Partition Coefficient, $\log K_{OC}$:

5.30 (field data of sediment trap material; Oliver & Charlton 1984)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 22$ and 26 d, observed and corrected for growth dilution, respectively, in oligochaete worms (Oliver 1987b)

6.1.2.12 *o*-Chlorostyrene

Common Name: *o*-Chlorostyrene

Synonym: *o*-chlorovinylbenzene, 2-chlorostyrene

Chemical Name: *o*-chlorostyrene

CAS Registry No: 2039-87-4

Molecular Formula: C₈H₇Cl

Molecular Weight: 138.595

Melting Point (°C):

−63.1 (Lide 2003)

Boiling Point (°C):

188.7 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm³):

1.10001, 1.09532 (20°C, 25°C, Dreisbach 1955)

Molar Volume (cm³/mol):

126.0 (20°C, calculated-density, Stephenson & Malanowski 1987)

153.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

51.03, 40.01 (25°C, bp, Dreisbach 1955)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

127.5 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.86644 − 1542.1/(198 + t/°C); temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/kPa) = 6.11856 − 1627.284/(207.112 + t/°C); temp range 98.5–154.9°C (Antoine eq. derived from experimental data of Dreisbach & Shrader 1949, Boublik et al. 1984)

log (P_L/kPa) = 5.99134 − 1541.1/(−75.15 + T/K); temp range 363–543 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{ow}:

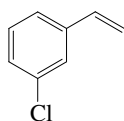
Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

6.1.2.13 *m*-Chlorostyrene

Common Name: *m*-Chlorostyrene

Synonym: *m*-chlorovinylbenzene, 3-chlorostyrene

Chemical Name: *m*-chlorostyrene

CAS Registry No: 2039-85-2

Molecular Formula: C₈H₇Cl

Molecular Weight: 138.595

Melting Point (°C):

Boiling Point (°C):

Density (g/cm³):

1.1033 (20°C, Lide 2003)

Molar Volume (cm³/mol):

124.1 (20°C, calculated-density, Stephenson & Malanowski 1987)

153.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* (25.3°C, summary of literature data, Stull 1947)

148.06 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.83847 – 2156.77/(–16.882 + T/K); temp range 298–463 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{ow}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

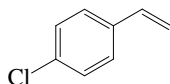
Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constant, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

TABLE 6.1.2.13.1**Reported vapor pressures of m-chlorostyrene at various temperatures****Stull 1947****summary of literature data**

t/°C	P/Pa
25.3	133.3
51.3	666.6
65.2	1333
80.0	2666
96.5	5333
107.2	7999
121.1	13332
142	26664
165.7	53329
190	101325

6.1.2.14 *p*-Chlorostyrene

Common Name: *p*-Chlorostyrene

Synonym: *p*-chlorovinylbenzene, 4-chlorostyrene

Chemical Name: *p*-chlorostyrene

CAS Registry No: 1073-67-2

Molecular Formula: C₈H₇Cl

Molecular Weight: 138.595

Melting Point (°C):

−15.9 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

192.0 (Dreisbach 1955, Lide 2003)

Density (g/cm³):

1.08682, 1.08214 (20°C, 25°C, Dreisbach 1955)

1.0868 (20°C, Lide 2003)

Molar Volume (cm³/mol):

127.5 (20°C, calculated-density, Stephenson & Malanowski 1987)

153.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

51.11, 40.07 (25°C, bp, Dreisbach 1955)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* (28.0°C, summary of literature data, temp range 28.0–191.0°C, Stull 1947)

6287* (100.91°C, ebulliometry, measured range 100.91–127.27°C, Dreisbach & Shrader 1949)

116.3 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.84248 – 1545.0/(198 + t/°C); temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/kPa) = 9.18404 – 4186.871/(398.256 + t/°C); temp range 100.9–127.27°C (Antoine eq. derived from experimental data of Dreisbach & Shrader 1949, Boublik et al. 1984)

log (P_L/kPa) = 5.96738 – 1545.0/(−75.15 + T/K); temp range 363–523 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{ow}:

3.66 (estimated, Kaiser 1987)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

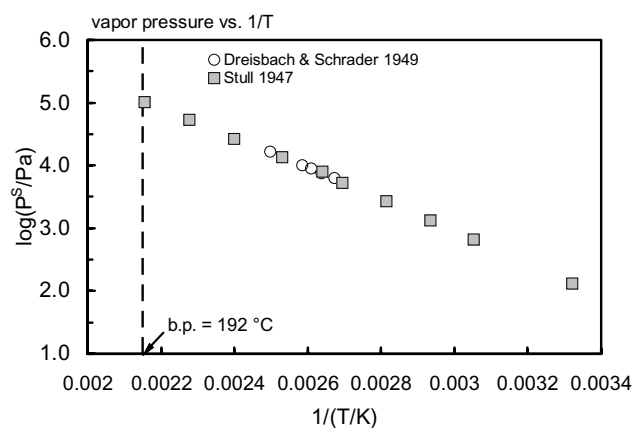
Environmental Fate Rate Constant, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

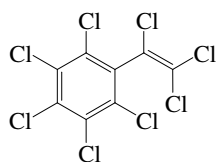
TABLE 6.1.2.14.1

Reported vapor pressures of *p*-chlorostyrene at various temperatures

Stull 1947		Dreisbach & Shrader 1949	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
28.0	133.3	100.91	6287
54.5	666.6	106.09	7605
67.5	1333	109.97	8851
82.0	2666	113.76	10114
98.0	5333	127.27	16500
105.8	7999		
122.0	13332		
143.5	26664		
166.0	53329		
191.0	101325		

FIGURE 6.1.2.14.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-chlorostyrene.

6.1.2.15 Octochlorostyrene



Common Name: Octochlorostyrene

Synonym:

Chemical Name: octachlorostyrene

CAS Registry No: 29082-74-4

Molecular Formula: C_8Cl_8

Molecular Weight: 379.710

Melting Point ($^{\circ}C$):

99 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

300.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.188 (mp at $99^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

22.9($20^{\circ}C$, calculated-bond contribution method, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.29 (HPLC-RT correlation, Veith et al.1979b)

6.20 (HPLC-RT correlation, Veith et al. 1979a)

Bioconcentration Factor, $\log BCF$:

4.52 (fathead minnow, 32-d exposure, Veith et al. 1979b)

2.91–3.91, mean 3.91 (rainbow trout, $15^{\circ}C$, wet wt., steady-state BCF on 7- to 96-d laboratory study; Oliver & Niimi 1985)

5.38; 6.15 (rainbow trout, calculated- K_{ow} , Lake Ontario field BCF, Oliver & Niimi 1985)

4.49; 3.91 (oligochaete worms; fish, Oliver 1987b)

Sorption Partition Coefficient, $\log K_{oc}$:

6.10 (field data of sediment trap material, Oliver & Charlton 1984)

5.90–7.30; 6.60 (suspended sediment: range; mean, Oliver 1987a)

6.30 (algae $> 50 \mu m$, mean, Oliver 1987a)

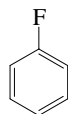
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 71$ d, observed and $t_{1/2} = 100$ d, corrected for growth dilution in worms ($8^{\circ}C$, Oliver 1987).

6.1.3 FLUOROBENZENES

6.1.3.1 Fluorobenzene



Common Name: Fluorobenzene

Synonym: phenyl fluoride

Chemical Name: fluorobenzene, phenyl fluoride

CAS Registry No: 462-06-6

Molecular Formula: C_6H_5F

Molecular Weight: 96.102

Melting Point ($^{\circ}C$):

−42.18 (Lide 2003)

Boiling Point ($^{\circ}C$):

84.73 (Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0225 (Horvath 1982; Lide 2003)

1.0131 ($30^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

94.4 (Stephenson & Malanowski 1987; Wang et al. 1992)

101.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.305 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1540 ($30^{\circ}C$, shake flask-IR, Gross et al. 1933)

1550 (shake flask-UV spectrophotometer, Andrews & Keefer 1950)

1296 (Deno & Berkheimer 1960)

922 (shake flask-GC, Jones et al. 1977/1978)

189.3* (shake flask-GC, measured range $5-45^{\circ}C$, Nelson & Smit 1978)

1559 (Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

1540 ($27.5^{\circ}C$, recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

1530 ($30^{\circ}C$, Riddick et al. 1986)

1700*, 1550 ($19.2^{\circ}C$, $29.7^{\circ}C$, shake flask-GC/TC, measured range $0-80^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

10246* ($24.9^{\circ}C$, Ramsay-Young method, measured range -17.85 to $83.85^{\circ}C$, Young 1889)

7999* ($19.6^{\circ}C$, summary of literature data, temp range -43.4 to $84.7^{\circ}C$, Stull 1947)

19920* ($39.4^{\circ}C$, comparative ebulliometry, measured range $39.4-120.5^{\circ}C$, Scott et al. 1956)

$\log(P/mmHg) = 6.95208 - 1248.083/(221.827 + t/^{\circ}C)$; temp range $34.5-120.5^{\circ}C$ (Antoine eq., comparative ebulliometry, Scott et al. 1956)

$\log(P/mmHg) = [-0.2185 \times 7980.4/(T/K)] + 7.699237$; temp range $-43.4-279.3^{\circ}C$ (Antoine eq., Weast 1972-73)

10200 (interpolated-Antoine eq., Boublik et al. 1973, 1984)

$\log(P/mmHg) = 7.18703 - 1381.828/(235.563 + t/^{\circ}C)$; temp range -17.85 to $83.85^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log(P/kPa) = 6.31155 - 1381.646/(235.548 + t/^{\circ}C)$; temp range -17.85 to $83.85^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.1870 - 1381.8/(235.6 + t/^{\circ}\text{C})$; temp range -18 to 84°C (Antoine eq., Dean 1985, 1992)
10480 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.07698 - 1248.083/(221.827 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.07234 - 1245.564/(-51.587 + T/\text{K})$; temp range 312–394 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.4113 - 1398.61/(-31.295 + T/\text{K})$; temp range 358–530 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14135 - 1291.116/(-45.664 + T/\text{K})$; temp range 373–419 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.37857 - 1478.807/(-18.847 + T/\text{K})$; temp range 414–501 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.59182 - 2876.741/(171.093 + T/\text{K})$; temp range 497–561 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -5.4849 - 1.8597 \times 10^3/(T/\text{K}) + 7.1515 \cdot \log (T/\text{K}) - 1.6467 \times 10^{-2} \cdot (T/\text{K}) + 9.2622 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 231–560 K (Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

632 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.27 (shake flask-AS, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971)

2.28 (calculated-fragment const., Rekker 1977)

2.27 (recommended, Sangster 1989, 1993)

2.26 (centrifugal partition chromatography, El Tayar et al. 1991)

2.27 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}(\text{calc}) = 2.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs}) = 0.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (6.31 \pm 0.84) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{OH} = 6.31 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{OH} = 6.90 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range 234–303 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 1.08 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 6.1.3.1.1

Reported aqueous solubilities of fluorobenzene at various temperatures

Gross et al. 1933		Nelson & Smit 1978		Stephenson 1992	
shake flask-interferometer		shake flask-GC		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
30	1540	5	118.4	0	1620
		25	189.3	9.5	1660
		35	336	29.7	1700
		45	512	39.6	1530
				47.7	1730
Andrews & Keefer 1950				60.1	1900
shake flask-UV				70	1901
t/°C	S/g·m ⁻³			80	1880
25	1550				

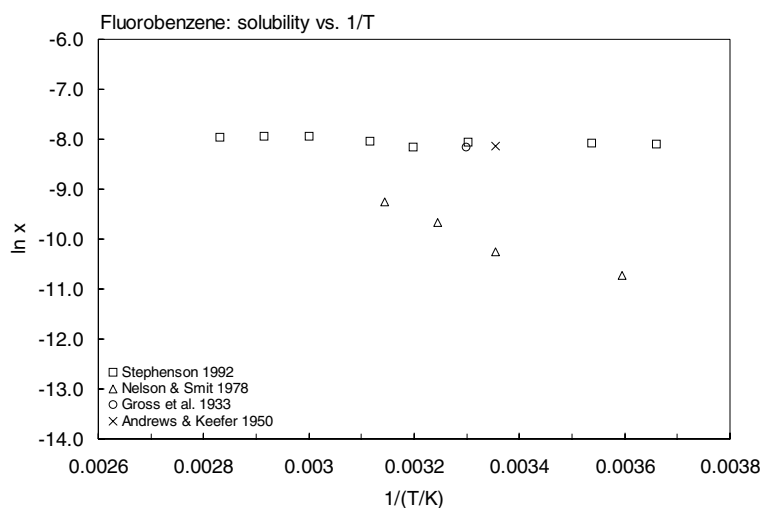
FIGURE 6.1.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for fluorobenzene.

TABLE 6.1.3.1.2

Reported vapor pressures of fluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Young 1889		Stull 1947		Scott et al. 1956	
Ramsay-Young method		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-17.85	927	-43.4	133.3	39.404	19920
-5.95	1980	-22.8	666.6	44.920	25007
0.15	2806	-12.4	1333	50.480	31160
4.7	3613	-1.20	2666	56.081	38567
10.65	5000	11.5	5333	61.726	47359
16.75	6873	19.6	7999	67.412	57803
19.5	7866	30.4	13332	73.141	70109
24.9	10246	47.2	26664	78.916	84525
30.35	12999	65.7	53329	84.734	101325
36.05	16759	84.7	101325	90.590	120798
42.05	21558			96.497	143268
49.6	29317	mp/°C	-42.1	102.438	169-53
56.2	37610			108.431	198530
62.75	47889			114.462	232088
71	63995			120.538	270111
78.75	82473				
83.85	97378				

complete set of data see [ref.](#)

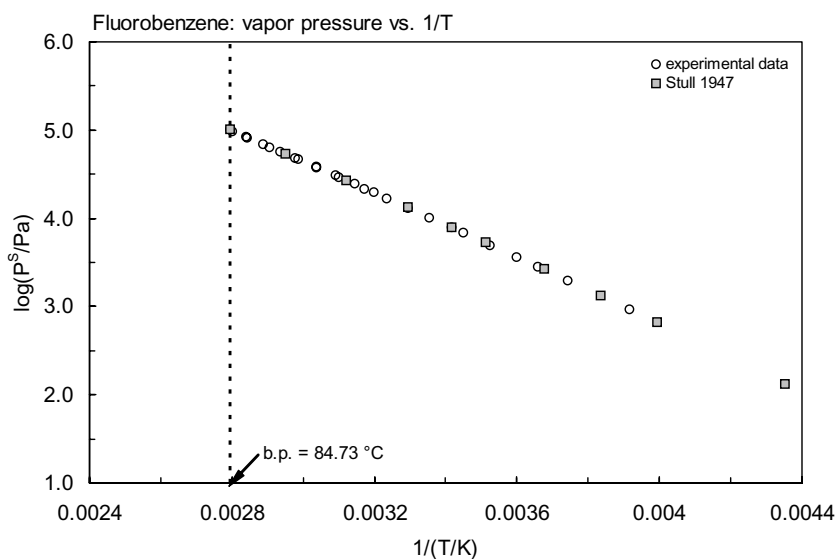
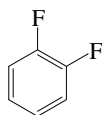


FIGURE 6.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for fluorobenzene.

6.1.3.2 1,2-Difluorobenzene



Common Name: 1,2-Difluorobenzene

Synonym: *o*-difluorobenzene

Chemical Name: 1,2-Difluorobenzene

CAS Registry No: 367-11-3

Molecular Formula: C₆H₄F₂

Molecular Weight: 114.093

Melting Point (°C):

−47.1 (Lide 2003)

Boiling Point (°C):

94 (Lide 2003)

Density (g/cm³ at 20°C):

1.158 (Dean 1992)

Molar Volume (cm³/mol):

99.2 (calculated-density, Stephenson & Malanowski 1987)

106.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

1141 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980; Yalkowsky et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9582* (31.17°C, comparative ebulliometry, measured range 31–130°C, Scott et al. 1963)

log (P/kPa) = 6.12360 – 1297.243/(211.103 + t/°C); temp range 31.2–130°C (Antoine eq. derived from experimental data of Scott et al. 1963, Boublik et al. 1984)

Henry's Law Constant (Pa·m³/mol at 25°C):

713 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow}:

2.59 (calculated-fragment const., Valvani & Yalkowsky 1980)

2.58 (calculated-fragment const., Yalkowsky et al. 1983)

2.56 (calculated-molar volume correlation, Wang et al. 1992)

2.43 (calculated, Müller & Klein 1992)

2.37 (recommended, Hansch et al. 1995)

2.25; 2.33 (predicted; calc-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:

Half-Lives in the Environment:

TABLE 6.1.3.2.1

Reported vapor pressures of 1,2-difluorobenzene at various temperatures

Scott et al. 1963					
comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa		
31.168	9582	111.903	169053		
33.916	10884	117.980	198530	data also fitted to Cox eq.	
36.668	12335	124.099	232088	Cox eq. P/mmHg	
39.436	13950	130.256	270111	$\log (P/760)=A[1-B/(T/K)]$	
42.210	15740			$\log A = a - b(T/K) + c(T/K)^2$	
44.996	17725	mp/K	226.0148	a	0.841936
47.803	19920	bp/K	367.07	$10^{-4} \cdot b$	6.77698
53.423	25007	$\Delta H_{\text{fus}} = 11.045 \text{ kJ/mol}$		$10^{-7} \cdot c$	6.52099
59.084	31160	$\Delta H_{\text{v}} = 36.11 \text{ kJ/mol}$		B	367.072
64.787	38547	Antoine eq.			
70.530	47359	$\log P = A - B/(C + t/^{\circ}\text{C})$			
76.314	57803		P/mmHg		
82.142	70109	A	7.00003		
88.009	84525	B	1298.053		
93.921	101325	C	221.197		
99.874	120798				
105.869	143268				

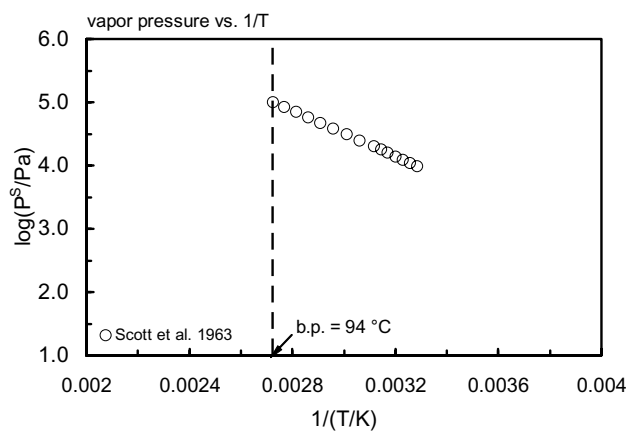
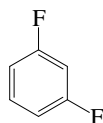


FIGURE 6.1.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2-difluorobenzene.

6.1.3.3 1,3-Difluorobenzene

Common Name: 1,3-Difluorobenzene

Synonym: *m*-difluorobenzene

Chemical Name: 1,3-Difluorobenzene

CAS Registry No: 372-18-9

Molecular Formula: C₆H₄F₂

Molecular Weight: 114.093

Melting Point (°C):

−69.12 (Lide 2003)

Boiling Point (°C):

82.6 (Lide 2003)

Density (g/cm³ at 20°C):

1.1552 (18°C, Horvath 1982)

1.1572 (Lide 2003)

Molar Volume (cm³/mol):

98.6 (20°C, calculated-density, Stephenson & Malanowski 1987, Ruelle & Kesselring 1997)

106.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

1141 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19924* (38.284°C, comparative ebulliometry, measured range 311.334–391.523 K, Osborn & Scott 1980)

Henry's Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:

2.58 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)

2.56 (calculated-molar volume correlation, Wang et al. 1992)

2.43 (calculated, Müller & Klein 1992)

2.26; 2.33 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

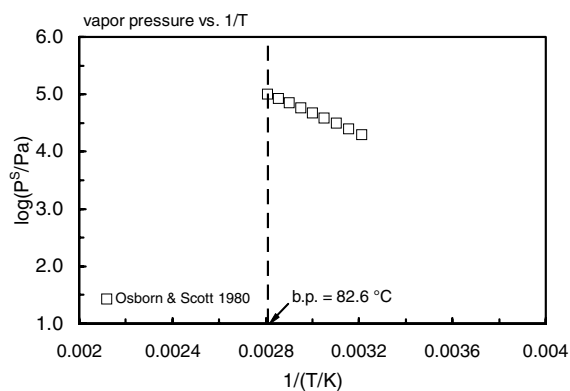
Sorption Partition Coefficient, log K_{oc}:

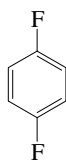
Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:

Half-Lives in the Environment:

TABLE 6.1.3.3.1**Reported vapor pressures of 1,3-difluorobenzene at various temperatures**

Osborn & Scott 1980			
ebulliometry			
t/°C	P/Pa	t/°C	P/Pa
38.184	19924	88.808	120800
43.646	25014	94.641	143270
49.148	31167	100.511	169050
54.692	38553	106.425	198540
60.273	47363	112.378	232090
65.898	57806	118.373	270120
71.564	70112		
77.272	84528	data fitted to a 4-constant vapor pressure eq.	
83.02	101325		

**FIGURE 6.1.3.3.1** Logarithm of vapor pressure versus reciprocal temperature for 1,3-difluorobenzene.

6.1.3.4 1,4-Difluorobenzene

Common Name: 1,4-Difluorobenzene

Synonym: *p*-difluorobenzene

Chemical Name: 1,4-Difluorobenzene

CAS Registry No: 540-36-3

Molecular Formula: C₆H₄F₂

Molecular Weight: 114.093

Melting Point (°C):

−23.55 (Lide 2003)

Boiling Point (°C):

89 (Lide 2003)

Density (g/cm³ at 20°C):

1.1701 (20°C, Horvath 1982, Dean 1992; Lide 2003)

Molar Volume (cm³/mol):

97.4 (20°C, calculated-density, Stephenson & Malanowski 1987)

106.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

1222 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980; Yalkowsky et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9577* (27.25°C, comparative ebulliometry, measured temp range 300.4–397.7 K, Osborn & Scott 1980)

Henry's Law Constant (Pa m³/mol at 25°C):

776 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

2.58 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)

2.43 (calculated, Müller & Klein 1992)

2.84 (calculated-molar volume, Wang et al. 1992)

2.24; 2.33 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Half-Lives in the Environment:

TABLE 6.1.3.4.1

Reported vapor pressures of 1,4-difluorobenzene at various temperatures

Osborn & Scott 1980			
ebulliometry			
t/°C	P/Pa	t/°C	P/Pa
28.248	9577	84.078	84528
30.95	10879	89.886	101325
33.658	12331	95.727	120800
36.376	13944	101.611	143270
39.101	15736	107.535	169050
41.837	17721	113.503	198540
44.588	19924	119.507	232090
50.109	25104	125.552	270120
55.671	31167		
61.273	38553	data fitted to a 4-constant vapor pressure eq.	
66.910	47363		
72.593	57806		
78.319	70112		

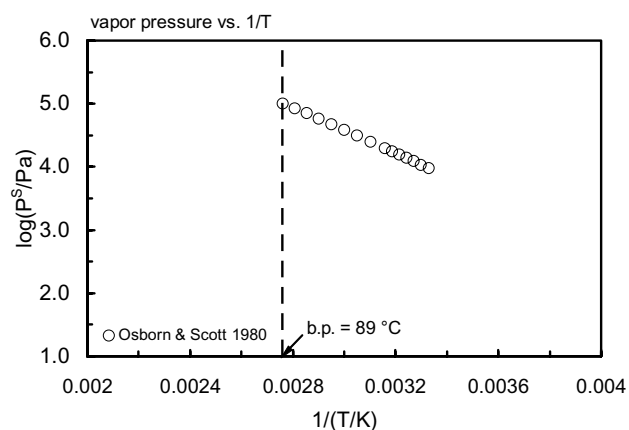
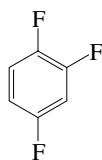


FIGURE 6.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for 1,4-difluorobenzene.

6.1.3.5 1,2,4-Trifluorobenzene



Common Name: 1,2,4-Trifluorobenzene

Synonym:

Chemical Name: 1,2,4-trifluorobenzene

CAS Registry No: 367-23-7

Molecular Formula: $C_6H_3F_3$

Molecular Weight: 132.083

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

90 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.52 (HPLC-RT correlation, Garst 1984, quoted, Sangster 1993)

2.41 (recommended, Hansch et al. 1995)

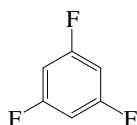
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.3.6 1,3,5-Trifluorobenzene

Common Name: 1,3,5-Trifluorobenzene

Synonym:

Chemical Name: 1,3,5-trifluorobenzene

CAS Registry No: 372-38-3

Molecular Formula: $C_6H_3F_3$

Molecular Weight: 132.083

Melting Point ($^{\circ}C$):

-5.5 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

75.4 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

103.4 (calculated-density, Stephenson & Malanowski 1987)

111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

139.68* ($25.21^{\circ}C$, static system-Hg manometer, measured range 6.18 – $50^{\circ}C$, Findlay 1969)

$\log(P/mmHg) = 6.91873 - 1196.385/(219.01 + t/^{\circ}C)$; temp range 6.18 – $50^{\circ}C$ (Hg manometer, Findlay 1969)

$\log(P_L/kPa) = 6.04363 - 1198.385/(-54.131 + T/K)$; temp range 279 – 350 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.3.6.1

Reported vapor pressures of 1,3,5-trifluorobenzene at various temperatures

Findlay 1969					
Hg manometer					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
6.18	5385	25.24	13965	46.97	35156
6.19	5389	29.98	17331	46.97	35168
10.03	6615	29.98	17339	49.98	39.453
15.01	8530	35.15	21679	49.99	39.462
15.01	8534	35.25	21806		
19.99	10915	35.39	21846	log P = A - B/(C + t/°C)	
19.99	10911	40.05	26654		
20.49	11.202	40.11	26704	A	P/mmHg
20.53	11210	43.85	31019	B	6.91873
22.79	12468	43.94	31188	C	1196.385
25.21	13968	44.2	31463		219.019

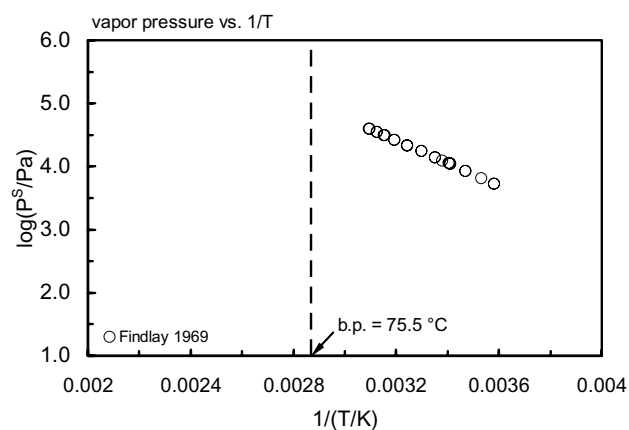
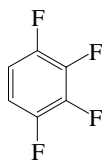


FIGURE 6.1.3.6.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trifluorobenzene.

6.1.3.7 1,2,3,4-Tetrafluorobenzene



Common Name: 1,2,3,4-Tetrafluorobenzene

Synonym:

Chemical Name: 1,2,3,4-tetrafluorobenzene

CAS Registry No: 551-62-2

Molecular Formula: $C_6H_2F_4$

Molecular Weight: 150.074

Melting Point ($^{\circ}C$):

−42 (Stephenson & Malanowski 1987)

Boiling Point ($^{\circ}C$):

94.3 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

105.5 (calculated-density, Stephenson & Malanowski 1987)

116.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

33.0 (Ambrose et al. 1975)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6545* (24.82 $^{\circ}C$, static-system-Hg manometer, Findlay 1969)

$\log(P/mmHg) = 7.19386 - 1396.067/(228.837 + t/^{\circ}C)$; temp range 6.05–49.87 $^{\circ}C$ (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)

6509* (extrapolated from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.15854 - 1291.080/(-50.617 + T/K)$; temperature range 300.8–367.51(normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.16107 - 1292.550/(-56.453 + T/K)$; temperature range 300.8–391.65 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.21410 - 1341.655/(223.721 + t/^{\circ}C)$; temp range 24.78–84.98 $^{\circ}C$ (Antoine eq. derived from Findlay 1969 data, Boublik et al. 1984)

$\log(P/kPa) = 6.15932 - 1291.522/(216.58 + t/^{\circ}C)$; temp range 27.65–118.5 $^{\circ}C$ (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.31876 - 1396.067/(-44.277 + T/K)$; temp range 279–323 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.16042 - 1292.174/(-56.495 + T/K)$; temp range 300–392 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.3.7.1

Reported vapor pressures of 1,2,3,4-tetrafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log(T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Findlay 1969				Ambrose et al. 1975			
Hg manometer				ebulliometry			
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	T/K	P/Pa	T/K	P/Pa
6.05	2385	44.01	15919	27.65	7437	90.123	88.788
6.06	2377	46.91	18024	31.417	8945	94.228	100917
10.36	3041	46.91	18024	35.073	10646	95.082	103593
15.21	3970	48.82	19620	38.868	12.688	99.87	119685
20.64	5277	48.83	19621	42.74	15095	104.196	135850
24.82	6545	49.84	20380	46.466	17757		
24.82	6547	49.87	20.428	51.321	21794	Antoine eq. for temp. range 300–367 K	
29.98	8433			55.476	25823		
29.99	8433	eq. 2	P/mmHg	60.207	31137	eq. 3	P/kPa
35.05	10722	A	7.19386	64.859	37177	A	6.15854
35.06	10722	B	1396.067	69.749	44535	B	129.08
40.07	13438	C	228.984	75.125	53942	C	–56.617
40.07	13439			79.797	63.331		
43.99	15904			83.34	71.305		

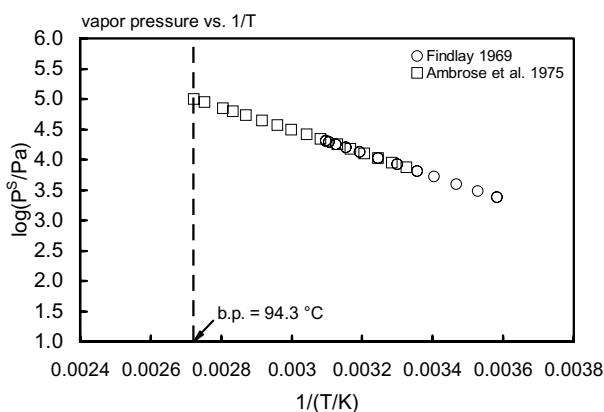
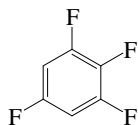


FIGURE 6.1.3.7.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,4-tetrafluorobenzene.

6.1.3.8 1,2,3,5-Tetrafluorobenzene

Common Name: 1,2,3,5-Tetrafluorobenzene

Synonym:

Chemical Name: 1,2,3,5-tetrafluorobenzene

CAS Registry No: 2367-82-0

Molecular Formula: $C_6H_2F_4$

Molecular Weight: 150.074

Melting Point ($^{\circ}C$):

−46.25 (Lide 2003)

Boiling Point ($^{\circ}C$):

84.4 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

107.7 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

116.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.1 (Ambrose et al. 1975)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

9770* ($24.81^{\circ}C$, static method-Hg manometer, measured range 6.08 – $50^{\circ}C$, Findlay 1969)

$\log(P/mmHg) = 7.07758 - 1290.984/(222.855 + t/^{\circ}C)$; temp range 6.08 – $49.83^{\circ}C$ (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)

9801* (interpolated from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.15414 - 1255.781/(-54.898 + T/K)$; temperature range 287.6 – 357.61 (normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.15507 - 1255.981/(-54.919 + T/K)$; temperature range 287.6 – 381.5 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.12070 - 1250.027/(218.829 + t/^{\circ}C)$; temp range 6.08 – $49.83^{\circ}C$ (Antoine eq. derived from Findlay 1969 data, Boublik et al. 1984)

$\log(P/kPa) = 6.1500 - 1253.079/(217.903 + t/^{\circ}C)$; temp range 14.44 – $108.37^{\circ}C$ (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.20248 - 1290.984/(-50.295 + T/K)$; temp range 279 – 323 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.15119 - 1253.771/(-55.168 + T/K)$; temp range 287 – 382 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.24644 - 1317.349/(-46.898 + T/K)$; temp range 385 – 416 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.3.8.1

Reported vapor pressures of 1,2,3,5-tetrafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Findlay 1969				Ambrose et al. 1975			
Hg manometer				ebulliometry			
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	T/K	P/Pa	T/K	P/Pa
6.05	2385	48.82	19620	287.593	5719	357.291	100305
6.06	2377	48.83	19621	291.414	6987	357.743	101755
10.36	3041	49.84	20380	295.169	8457	362.582	118237
15.21	3970	49.87	20428	298.091	9773	366.716	133926
20.64	5277			303.399	12598	371.603	154528
24.82	6545	eq. 2	P/mmHg	307.963	15541	376.423	177795
24.82	6547	A	7.07758	312.406	18930	381.524	203.907
29.98	8433	B	1290.984	314.635	20846		
29.99	8433	C	223.855	317.751	24802	Antoine eq. for temp range 287–356 K	
35.05	10722			324.852	31779		
35.06	10722			329.202	37666		
40.07	13438			334.506	46007	eq. 2	P/kPa
40.07	13439			338.643	53501	A	6.15414
43.99	15904			343.224	62911	B	1255.781
44.01	15919			347.715	73374	C	–54.898
46.91	18024			352.951	87269		
46.91	18024			356.719	98504		

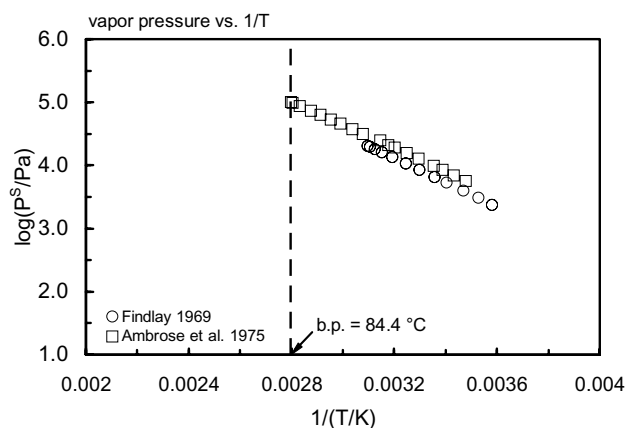
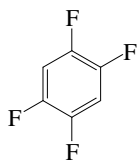


FIGURE 6.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,5-tetrafluorobenzene.

6.1.3.9 1,2,4,5-Tetrafluorobenzene



Common Name: 1,2,4,5-Tetrafluorobenzene

Synonym:

Chemical Name: 1,2,4,5-tetrafluorobenzene

CAS Registry No: 327-54-8

Molecular Formula: $C_6H_2F_4$

Molecular Weight: 150.074

Melting Point ($^{\circ}C$):

3.88 (Lide 2003)

Boiling Point ($^{\circ}C$):

90.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4255 (Lide 2003)

Molar Volume (cm^3/mol):

105.3 ($20^{\circ}C$, calculated-density)

105.4 (calculated-density, Stephenson & Malanowski 1987)

116.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.9 (Ambrose et al. 1975)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7556* (interpolated from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.17340 - 1277.452/(-56.889 + T/K)$; temp range 293.2–363.413 (normal bp) K (Antoine eq.-I from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.17788 - 1279.904/(-56.642 + T/K)$; temp range 293.2–387.6 K (Antoine eq.-II from ebulliometric measurements, Ambrose et al. 1975)

$\log(P/kPa) = 6.17439 - 1277.918/(216.289 + t/^{\circ}C)$; temp range 20.05 – $114.42^{\circ}C$ (Antoine eq. derived from Ambrose et al. 1975 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.17614 - 1278.93/(-56.748 + T/K)$; temp range 293–390 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.42009 - 1454.406/(-33.675 + T/K)$; temp range 390–488 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.88521 - 3090.851/(174.387 + T/K)$; temp range 488–543 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.3.9.1

Reported vapor pressures of 1,2,4,5-tetrafluorobenzene at various temperatures:

Ambrose et al. 1975			
ebulliometry			
T/K	P/Pa	T/K	P/Pa
293.198	5855	363.049	100177
296.489	6944	363.591	101.896
300.519	8505	368.237	117566
303.459	9822	372.427	133286
308.374	12399	377.572	154790
313.302	15524	382.398	177330
315.839	17370	387.568	204254
320.056	20841		
324.073	24655	Antoine eq. for temp	
330.275	31652	range 293–363 K	
334.497	37286	$\log P = A - B/(C + T/K)$	
339.931	45699	P/kPa	
344.142	53227	A	6.1734
348.439	61895	B	1277.452
353.384	73237	C	–56.889
358.929	87873		
362.593	98750		

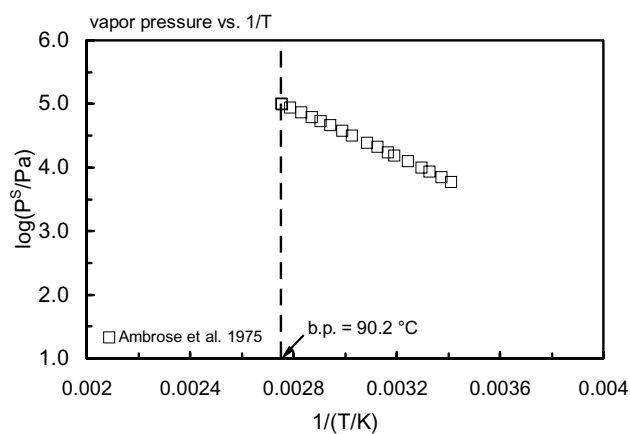
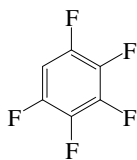


FIGURE 6.1.3.9.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4,5-tetrafluorobenzene.

6.1.3.10 Pentafluorobenzene



Common Name: Pentafluorobenzene

Synonym:

Chemical Name: pentafluorobenzene

CAS Registry No: 363-72-4

Molecular Formula: C_6HF_5

Molecular Weight: 168.064

Melting Point ($^{\circ}C$):

−47.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

85.74 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

111.0 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

121.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.38 (Ambrose 1968)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

9015* ($24.78^{\circ}C$, static method, measured range 24.78 – $84.98^{\circ}C$, Patrick & Prosser 1964)

$\log(P/mmHg) = 6.94904 - 1218.91/(213.313 + t/^{\circ}C)$; temp range 24.98 – $84.98^{\circ}C$, Patrick & Prosser 1964)

26584* ($48.729^{\circ}C$, ebulliometry, measured range 49 – $94^{\circ}C$, Ambrose et al. 1975)

$\log(P/mmHg) = 7.03348 - 1253.043/(215.897 + t/^{\circ}C)$; temp range 48.7 – $94.3^{\circ}C$ (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/kPa) = 6.07634 - 1220.72/(213.425 + t/^{\circ}C)$; temp range 24.78 – $84.98^{\circ}C$ (Antoine eq. derived from Patrick & Prosser 1946 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.15571 - 1250.946/(-57.457 + T/K)$; temp range 322 – $368\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.20712 - 1282.574/(-53.619 + T/K)$; temp range 358 – $397\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.47368 - 1477.401/(-27.81 + T/K)$; temp range 393 – $479\ K$ (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.3.10.1

Reported vapor pressures of pentafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Patrick & Prosser 1964		Ambrose 1968	
static method-Hg manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
24.78	9015	48.729	26584
29.85	11492	54.355	33360
34.85	14540	59.041	40023
39.85	18206	63.033	46499
44.85	22507	66.698	53178
49.85	27527	69.91	59642
54.87	33877	72.828	66050
59.92	41071	75.604	72643
64.95	49217	78.158	79163
69.95	59052	80.643	85953
74.95	70191	82.998	92792
79.95	82728	85.123	99333
84.98	97125	85.496	100521
		87.212	106123
bp/°C	86.3	89.093	112557
Antoine eq.		91.014	119417
eq. 2	P/mmHg	92.509	124989
A	6.94904	94.296	131878
B	1218.91		
C	213.313	eq. 2	P/mmHg
$\Delta H_v/(\text{kJ mol}^{-1}) =$		A	7.03488
at 25°C	36.67	B	1253.043
at bp	32.07	C	215.987

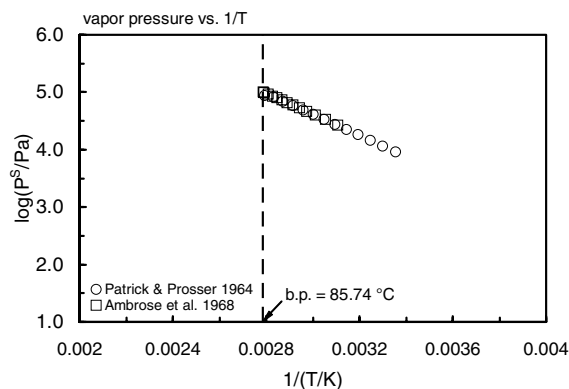
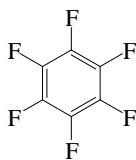


FIGURE 6.1.3.10.1 Logarithm of vapor pressure versus reciprocal temperature for pentafluorobenzene.

6.1.3.11 Hexafluorobenzene



Common Name: Hexafluorobenzene

Synonym: perfluorobenzene

Chemical Name: hexafluorobenzene

CAS Registry No: 392-56-3

Molecular Formula: C_6F_6

Molecular Weight 180.054

Melting Point ($^{\circ}C$):

5.0.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

80.26 (Lide 2003)

Density (g/cm^3):

1.61866, 1.60732 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

1.6184 ($20^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

115.8 (calculated-density, Stephenson & Malanowski 1987)

126.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.47 ($25^{\circ}C$, Findlay 1969)

35.69, 31.67 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.585 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11196* ($24.78^{\circ}C$, static method, measured range 19.75 – $84.98^{\circ}C$, Patrick & Prosser 1964)

$\log(P/mmHg) = 7.39075 - 1432.91/(237.470 + t/^{\circ}C)$; temp range 19.76 – $84.98^{\circ}C$, Patrick & Prosser 1964)

19957* ($37.303^{\circ}C$, gas saturation/manometer, measured range 37.303 – $88.79^{\circ}C$, Counsell et al. 1965)

11402* ($25.1^{\circ}C$, Hg manometer, measured range 4.74 – $47.85^{\circ}C$, Findlay 1969)

$\log(P/mmHg) = 6.86088 - 1152.442/(208.663 + t/^{\circ}C)$; temp range 4.74 – 47.85 (Antoine eq. derived from Hg U-tube manometer measurements, Findlay 1969)

10733* ($24.005^{\circ}C$, ebulliometry, measured range 290 – $377 K$, Ambrose 1981)

$\log(P/kPa) = 6.05252 - 1177.973/(210.677 + t/^{\circ}C)$; temp range 19.75 – $84.98^{\circ}C$ (Antoine eq. derived from Patrick & Prosser 1964 data, Boublik et al. 1984)

$\log(P/kPa) = 6.14363 - 1220.148/(214.610 + t/^{\circ}C)$; temp range 37.3 – $88.8^{\circ}C$ (Antoine eq. derived from Counsell et al. 1965 data, Boublik et al. 1984)

$\log(P/kPa) = 6.15013 - 1223.989/(215.084 + t/^{\circ}C)$; temp range 17 – $104^{\circ}C$ (Antoine eq. derived from Ambrose 1981 data, Boublik et al. 1984)

10733 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.14213 - 1219.41/(214.55 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_s/kPa) = 11.49514 - 3518.13/(44.44 + T/K)$; temp range 215 – $278 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15233 - 1224.974/(-57.984 + T/\text{K})$; temp range 278–354 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.19544 - 1251.177/(-54.775 + T/\text{K})$; temp range 348–389 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -38.8085 - 1.3422 \times 10^3/(T/\text{K}) + 22.204 \cdot \log (T/\text{K}) - 3.8813 \times 10^{-221} \cdot (T/\text{K}) + 2.10 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 278–517 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.22 (shake flask, Log P Database, Hansch & Leo 1987)

2.22 (recommended, Sangster 1993)

2.54 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 1.7 \times 10^{-5} \text{ h}^{-1}$, $1.32 \times 10^{-4} \text{ h}^{-1}$, with H_2O_2 under photolysis at 25°C in F-113 solution and with HO in the gas (Dilling et al. 1988).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = 2.19 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{\text{OH}}(\text{obs}) = 2.19 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{calc}) = 1.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}}^* = (1.61 \pm 0.24) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{\text{OH}}^* = 1.72 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Half-Lives in the Environment:

TABLE 6.1.3.11.1

Reported vapor pressures of hexafluorobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Patrick & Prosser 1964	Counsell et al. 1965	Findlay 1969	Ambrose 1981				
static method-Hg manometer	gas saturation/manometer	Hg manometer	comparative ebulliometry				
t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	T/K	P/Pa
19.75	8714	37.303	19957	4.74	3849	290.029	7747
24.78	11196	43.536	26124	5.7	4065	293.503	8940
29.85	14289	49.109	32880	7.07	4426	297.155	10733
34.85	17966	53.82	39638	7.14	4429	300.564	12667
39.85	22461	57.848	46271	9.77	5118	304.801	15466
44.85	27687	61.585	53199	17.23	7646	309.383	19,045

TABLE 6.1.3.11.1 (Continued)

Patrick & Prosser 1964		Counsell et al. 1965		Findlay 1969		Ambrose 1981	
static method-Hg manometer		gas saturation/manometer		Hg manometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
49.85	33860	64.655	59496	17.23	7650	313.187	22511
54.87	41446	67.63	66152	19.68	8757	316.417	25904
59.92	50169	70.172	72295	24.28	10915	321.165	31474
64.95	59860	72.666	78764	24.4	10988	325.511	37460
69.95	71569	75.337	86190	25.1	11402	330.676	45736
74.95	84741	77.535	92707	27.08	12511	335.031	53811
80.05	100199	79.632	99284	29.92	14296	339.642	63567
84.98	117109	81.446	105264	29.92	14300	343.774	73469
		83.445	112211	29.92	14303	349.246	88.428
Antoine eq.		85.353	119111	35.92	18822	352.884	88642
eq. 2	P/mmHg	87.027	125463	41.81	24289	353.038	100.13
A	7.39075	88.79	132447	47.32	30456	353.849	102794
B	1432, 91			47.85	31064	358.125	117749
C	237.470	bp/°C	80.261			362.14	133296
		Antoine eq.		eq. 2	P/mmHg	366.773	153.186
bp/°C	80.3	eq. 2	P/mmHg	A	6.86088	371.657	176.601
ΔH_v /(kJ mol ⁻¹) =		A	7.01741	B	1152.442	377.323	207.154
at 25°C	35.75	B	1219.410	C	208.663		
at bp	32.70	C	214.525			eq. 2	P/mmHg
		Kirchhoff eq.				A	
		eq. 4	P/mmHg			B	
		A	22.85552			C	
		B	2524.92				
		C	5.03484				

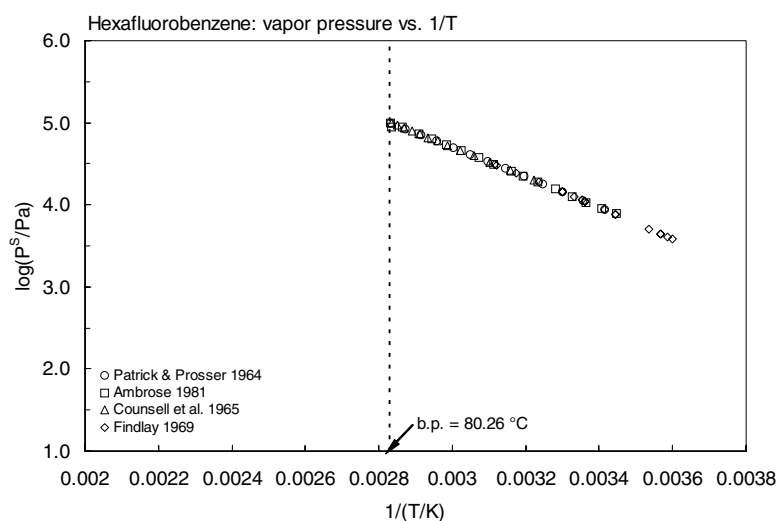
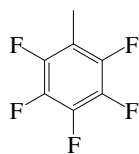


FIGURE 6.1.3.11.1 Logarithm of vapor pressure versus reciprocal temperature for hexafluorobenzene.

6.1.3.12 Pentafluorotoluene



Common Name: Pentafluorotoluene

Synonym: 2, 3, 4, 5, 6-pentafluorotoluene

Chemical Name: 2, 3, 4, 5, 6-pentafluorotoluene

CAS Registry No: 771-56-2

Molecular Formula: $C_7H_3F_5$, $C_6(CH_3)F_5$

Molecular Weight: 182.091

Melting Point ($^{\circ}C$):

-29.78 (Lide 2003)

Boiling Point ($^{\circ}C$):

117.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.440 (Lide 2003)

Molar Volume (cm^3/mol):

126.5 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

143.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.19 (Ambrose 1968)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5056* ($39.164^{\circ}C$, ebulliometry, measured range 39 – $138^{\circ}C$ or pressure range 30 – 1500 mmHg, Ambrose 1968)

$\log(P/\text{mmHg}) = 7.07209 - 1384.062/(212.731 + t/^{\circ}C)$; temp range ~ 76 – $127^{\circ}C$ or pressure range 200 – 1000 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/\text{mmHg}) = 7.09119 - 1388.288/(213.646 + t/^{\circ}C)$; temp range 39 – $138^{\circ}C$ or pressure range 30 – 1500 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/\text{mmHg}) = 13.68523 - 2813.814/(T/K) - 1.2691 \times 10^{-2} \cdot (T/K) + 0.8888 \cdot 10^{-5} \cdot (T/K)^2$; temp range 39 – $138^{\circ}C$ (Cragoe eq., ebulliometry, Ambrose 1968)

$\log(P_L/\text{kPa}) = 6.19445 - 1382.934/(-60.494 + T/K)$; temp range 312 – 416 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.21241 - 1394.345/(-59.194 + T/K)$; temp range 348 – 401 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

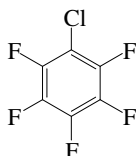
Half-Lives in the Environment:

TABLE 6.1.3.12.1

Reported vapor pressures of pentafluorotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot (T/K)^2$	(5)		
Ambrose 1968			
ebulliometry			
$t/^{\circ}\text{C}$	P/Pa		
39.164	5056	Antoine eq.	
50.578	8787	eq. 2	P/mmHg
58.357	12354	A	7.09119
62.734	14885	B	1396.198
66.375	17308	C	214.112
72.174	21831	for full range 30–1000 mmHg	
76.551	25854	or temp range 39–138°C	
81.824	31492		
85.651	36176	eq. 2	P/mmHg
92.625	46172	A	7.07209
97.287	54019	B	1384.062
102.370	63757	C	212.731
107.382	66700	for range 200–1000 mmHg	
112.608	87655	or temp range ~76–127°C	
116.158	97433		
117.884	102509	Cragoe eq.	
118.979	105812	eq. 5	P/mmHg
123.337	119831	A	13.68523
127.924	136155	B	2813.814
133.176	156948	C	1.2691×10^{-2}
138.226	179191	D	0.8888×10^{-5}
bp/ $^{\circ}\text{C}$	117.493		
$\Delta H_v = 35.18 \text{ kJ mol}^{-1}$			

6.1.3.13 Chloropentafluorobenzene



Common Name: Chloropentafluorobenzene

Synonym:

Chemical Name: chloropentafluorobenzene

CAS Registry No: 344-07-0

Molecular Formula: C_6ClF_5

Molecular Weight: 202.509

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

117.96 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

129.2 (calculated-density, Stephenson & Malanowski 1987)

141.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.15 (Ambrose 1968)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4186* ($35.576^{\circ}C$, ebulliometry, measured range 36 – $144^{\circ}C$ or pressure range 30 – 1500 mmHg, Ambrose 1968)

$\log(P/\text{mmHg}) = 7.06976 - 1389.841/(213.833 + t/^{\circ}C)$; temp range ~ 80 – $127^{\circ}C$ or pressure range 100 – 1000 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/\text{mmHg}) = 7.06747 - 1388.288/(213.646 + t/^{\circ}C)$; temp range 36 – $144^{\circ}C$ or pressure range 30 – 1500 mmHg (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P/\text{mmHg}) = 14.36999 - 2894.645/(T/K) - 1.4603 \times 10^{-2} \cdot (T/K) + 1.0612 \cdot 10^{-5} \cdot (T/K)^2$; temp range 36 – $144^{\circ}C$ (Cragoe eq., ebulliometry, Ambrose 1968)

$\log(P_L/\text{kPa}) = 6.19201 - 1388.701/(-59.393 + T/K)$; temp range 348 – 402 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.18873 - 1386.456/(-59.659 + T/K)$, temp range 307 – 417 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.3.13.1

Reported vapor pressures of chloropentafluorotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C \cdot (T/K)^2$	(5)		

Ambrose 1968

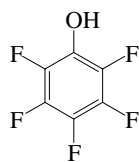
ebulliometry

$t/^{\circ}C$	P/Pa		
35.576	4186	Antoine eq.	
44.790	6614	eq. 2	P/mmHg
55.927	11028	A	7.06747
61.852	14216	B	1388.288
65.865	16811	C	213.646
70.085	19929	full range 30–1000 mmHg	
75.343	24459	or temp range 35.6–144°C	
81.691	31024		
86.763	37244	eq. 2	P/mmHg
92.135	44900	A	7.06976
97.254	53331	B	1389.841
102.357	62963	C	213.833
107.155	73251	for range 200–1000 mmHg	
112.764	86927	or temp range ~80–128°C	
116.436	96926		
117.448	99832	Cragoe eq.	
118.893	104118	eq. 5	P/mmHg
125.580	118997	A	14.36999
127.992	134517	B	2894.645
133.467	155905	C	1.4603×10^{-2}
138.689	178705	D	1.0612×10^{-5}
144.131	205189		

bp/ $^{\circ}C$ 117.954

$\Delta H_v = 35.15 \text{ kJ mol}^{-1}$

6.1.3.14 Pentafluorophenol



Common Name: Pentafluorophenol

Synonym:

Chemical Name: pentafluorophenol

CAS Registry No: 771-61-9

Molecular Formula: $C_6(OH)F_5$

Molecular Weight: 184.063

Melting Point ($^{\circ}C$):

37.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

145.6 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

128.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.59 (Ambrose 1968)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.754 (mp at $37.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

26578* ($105.448^{\circ}C$, ebulliometry, measured range 105.5 – $155^{\circ}C$, Ambrose 1968)

$\log(P/mmHg) = 7.06296 - 1377.185/(183.680 + t/^{\circ}C)$; temp range 105 – $155^{\circ}C$ (Antoine eq. from ebulliometric measurements, Ambrose 1968)

$\log(P_S/kPa) = 11.291 - 3523/(T/K)$; temp range 273 – $296 K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.18665 - 1377.011/(-89.435 + T/K)$; temp range 378 – $428 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

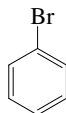
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.3.14.1**Reported vapor pressures of pentafluorophenol at various temperatures**

Ambrose 1968			
ebulliometry			
t/°C	P/Pa	t/°C	P/Pa
105.448	26578	153.041	125269
111.328	32076	154.963	132153
116.192	39393		
120.720	46087	bp/°C	145.621
124.827	52940	$\Delta H_v = 41.59 \text{ kJ mol}^{-1}$	
128.292	59367	Antoine eq.	
131.565	65904	$\log P = A - B/(C + t/^\circ\text{C})$	
134.647	72670	P/mmHg	
137.240	78804	A	7.03488
140.302	86489	B	1253.043
142.507	92412	C	215.897
145.002	99506	full range 200–1000 mmHg	
147.069	105684	or temp range 105–155°C	
149.090	112009		
151.190	118917		

6.1.4 BROMOBENZENES AND BROMOTOLUENES**6.1.4.1 Bromobenzene**

Common Name: Bromobenzene

Synonym: phenyl bromide

Chemical Name: bromobenzene

CAS Registry No: 108-86-1

Molecular Formula: C_6H_5Br

Molecular Weight: 157.008

Melting Point ($^{\circ}C$):

-30.72 (Dean 1985; Lide 2003)

Boiling Point ($^{\circ}C$):

156.06 (Dreisbach & Martin 1949; Dreisbach 1955; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):1.4950, 1.48824 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.4950 (Weast 1982-83; Lide 2003)

1.4952 (Dean 1985)

Molar Volume (cm^3/mol):105.0 ($20^{\circ}C$, calculated-density, Chiou 1985)

119.3 (Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.63 (Dreisbach 1955)

10.70 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

446 ($30^{\circ}C$, shake flask-IR, Gross & Saylor 1931)

410 (shake flask-UV, Andrews & Keefer 1950)

462 (shake flask-interferometry, Donahue & Bartell 1952)

328 (Deno & Berkheimer 1960)

458.5 ($35^{\circ}C$, shake flask-UV spectrophotometry, Hine et al. 1963)457* (shake flask-spectrophotometry, measured range $10-35^{\circ}C$, Vesala 1973)

446 (shake flask-UV, Vesala 1974)

148* (shake flask-GC, measured range $5-45.5^{\circ}C$, Nelson & Smit 1978)

360 (shake flask-UV, Yalkowsky et al. 1979)

274* (summary of literature data, temp range $25-40^{\circ}C$, Horvath 1982)

411 (generator column-HPLC/UV, Wasik et al. 1983)

330 (headspace-GC, McNally & Grob 1984)

445* (recommended, temp range $10-40^{\circ}C$, IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(g/kg) = 1.8293 - 1.35675 \times 10^{-2} \cdot (T/K) + 2.99322 \times 10^{-5} \cdot (T/K)^2$; temp range 288-308 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

384* ($20^{\circ}C$, limiting activity coeff. by equilibrium air stripping-GC, temp range $10-50^{\circ}C$, Hovorka & Dohnal 1997)

384* (estimated- RP-HPLC- k' correlation, measured range $5-35^{\circ}C$, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 666.6* (29.8°C, static method-pressure gauge, Kahlbaum 1898)
 666.6* (27.8°C, summary of literature data, Stull 1947)
 $\log(P/\text{mmHg}) = 7.25422 - 1688.4/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)
 6287* (71.86°C, ebulliometry, measured range 71.86–158.06°C, Dreisbach & Shrader 1949)
 3066* (56.07°C, temp range 56.07–154.24°C, Dreyer et al. 1954)
 558 (calculated by formula, Dreisbach 1955)
 $\log(P/\text{mmHg}) = 6.91444 - 1474.06/(209.4 + t/^\circ\text{C})$; temp range 60–190°C (Antoine eq. for liquid state, Dreisbach 1955)
 997 (35°C, gas saturation-gravitational or UV, Hine et al. 1963)
 697 (ebulliometry, extrapolated-Antoine eq., measured range 49–131°C, Hammaker & Kerlinger 1969)
 $\log(P/\text{mmHg}) = 7.7807 - 2105.4/(T/\text{K})$; temp range 49–131°C (ebulliometry, Hammaker & Kerlinger 1969)
 570 (extrapolated-Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 10157.7/(T/\text{K})] + 8.07500$; temp range –26 to –15°C (Antoine eq., Weast 1972–73)
 552 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 5.86064 - 1438.817/(205.441 + t/^\circ\text{C})$; temp range 56.07–154°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 553, 555 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.99238 - 1443.265/(205.94 + t/^\circ\text{C})$; temp range 56.07–154°C (Antoine eq. from reported exptl. data of Dreyer et al. 1954/55, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 5.98225 - 1433.858/(204.562 + t/^\circ\text{C})$; (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = 6.86064 - 1438.817/(205.441 + t/^\circ\text{C})$; temp range 56–154°C (Antoine eq., Dean 1985, 1992)
 557.6 (Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.37912 - 1688.4/(230 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P_L/\text{kPa}) = 6.03934 - 1474.03/(-63.75 + T/\text{K})$; temp range 333–463 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.40524 - 1776.58/(-25.639 + T/\text{K})$; temp range 429–633 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = -9.4583 - 2.5177 \times 10^3/(T/\text{K}) + 9.2584 \cdot \log(T/\text{K}) - 1.9386 \times 10^{-2} \cdot (T/\text{K}) + 9.6324 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 242–670 K (vapor pressure eq., Yaw et al. 1994)
 $\log(P/\text{kPa}) = 5.99238 - 1443.265/(T/\text{K})$ (database of CDATA 1991, Hovorka & Dohnal 1997)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

- 211 (1/K_{AW} or C_w/C_A, Hine & Mookerjee 1975;)
 247 (gas stripping-GC, Mackay & Shiu 1981, 1990)
 210 (recommended, Mackay & Shiu 1981)
 211 (computer value, Yaws et al. 1991)
 256, 332, 579 (30.0, 35, 44.8°C, EPICS-GC, Hansen et al. 1993)
 $\ln[H/(\text{kPa} \cdot \text{m}^3/\text{mol})] = -5341/(T/\text{K}) + 16.0$; temp range 30–45°C (EPICS measurements, Hansen et al. 1993)
 92.0, 167, 280, 430, 610 (10, 20, 30, 40, 50°C, equilibrium air stripping-GC, Hovorka & Dohnal 1997)
 139 (20°C, selected from literature of experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 6.375 - 2233/(T/\text{K})$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} (at 25°C or as indicated):

- 2.99 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)
 3.03 (calculated-fragment const.; Rekker 1977)
 3.16 (HPLC-k' correlation, McDuffie 1981)
 2.98 (generator column-HPLC, Wasik et al. 1983)
 3.02 (HPLC-RT correlation, D'Amboise & Hanai 1982)
 3.01 (shake flask-GC, Watarai et al. 1982)
 3.02 (HPLC-RT correlation, Eadsforth & Moser 1983)

- 3.01 (HPLC-RT correlation, Garst & Wilson 1984)
- 3.15 (HPLC correlation, Eadsforth 1986)
- 2.99 (recommended, Sangster 1989, 1993)
- 2.75, 2.94 (shake flask-UV/VIS spec. 25, 60°C; Kramer & Henze 1990)
- 2.99 (recommended, Hansch et al. 1995)
- 3.29, 3.25, 3.14, 3.12 (5, 15, 25, 35°C, estimated- RP-HPLC- k' correlation, Finizio & Di Guardo 2001)

Bioconcentration Factor, log BCF:

- 3.18 (activated sludge, Freitag et al. 1984)
- 2.28 (algae, Freitag et al. 1984)
- 1.68 (fish, Freitag et al. 1984)
- 1.68, 2.28, 3.18 (fish, algae, activated sludge, Halfon & Reggiani 1986)
- 1.70 (Freitag et al. 1985)
- 1.899, 1.928 (calculated- K_{OW} , calculated- MCI χ , Lu et al. 1999)

Sorption Partition Coefficient, log K_{OC} :

- 2.18 (soil, selected lit., Kenaga & Goring 1980)
- 2.18 (calculated-S. Kenaga 1980)
- 2.80 (calculated-MCI χ , Koch 1983)
- 2.56 (calculated-MCI. Sabjic 1984)
- 2.65 (calculated-MCI, Bahnick & Doucette 1988)
- 2.65 (HPLC-RT correlation, cyanopropy column, Hodson & Williams 1988)
- 3.37 (activated carbon, Blum et al. 1994)
- 2.49 (soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}^* = 7.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 245–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{OH}(\text{calc}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs}) = 0.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (9.15 \pm 0.97) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 234–438 K ((flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{OH} = 7.70 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range 234–362 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 0.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: relative rate from activated sludge approximately of 34.8% CO_2 (Freitag et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 6.1.4.1.1

Reported aqueous solubilities of bromobenzene at various temperatures

$$S(\text{wt}\%) = 1.09002 \times 10^{-2} + 4.43314 \times 10^{-4} \cdot (t/^{\circ}\text{C}) + 1.20007 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 - 1.33342 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3 \quad (1)$$

$$S(\text{g/kg}) = 1.8293 - 1.35675 \times 10^{-2} \cdot (T/\text{K}) + 2.99322 \times 10^{-5} \cdot (T/\text{K})^2 \quad (2)$$

1.

Vesala 1973		Nelson & Smit 1978		Horvath 1982		Horvath & Getzen 1985	
shake flask-UV		shake flask-GC		summary of literature data		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	389.57	5	1168	25	274	10	387
15.2	406.05	25	148	30	314	15	405
19.6	411.07	39	244	40	393	20	424
25.0	457.19	45.5	314			25	445
30.0	464.56			eq. 1	S/wt%	30	467
35.0	489.19					35	491
						40	516
						eq. 2	S/(g/kg)

2.

Hovorka & Dohnal 1997		Finizio & Di Guardo 2001	
γ [∞] by air stripping-GC		RP-HPLC-k' correlation	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	354.6	5	278
20	384.3	15	274.5
30	427.6	25	384
40	499.0	35	368
50	598.7		

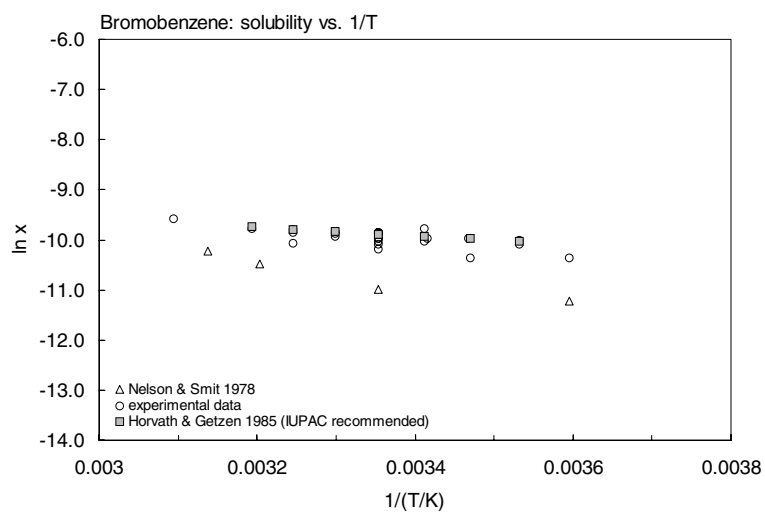


FIGURE 6.1.4.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for bromobenzene.

TABLE 6.1.4.1.2

Reported vapor pressures of bromobenzene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Dreyer et al. 1954	
static method*		summary of lit. data		ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
29.8	666.6	2.9	133.3	71.86	6287	56.07	3066
40.6	1333.2	27.8	666.6	76.39	7605	63.52	4400
47.7	1999.8	40	1333	80.08	8851	69.7	5706
52.8	2666.4	53.8	2666	83.99	10114	74.88	7119
57.3	3333	68.6	5333	96.32	16500	78.25	8213
61.2	3999.7	78.1	7999	127.47	42066	81.9	9546
67.7	4666	90.8	13332	140.69	67661	85.55	10986
70.4	5333	110.1	26664	158.06	101325	88.53	12332
73.0	6666.1	132.3	53329			90.82	13426
82.8	9999.2	156.2	101325	bp/°C	156.06	93.49	14839
90.0	13332			mp/°C	−30.82	97.09	16932
109.5	26664	mp/°C	−30.7			99.41	18465
122.0	39997			eq. 2	P/mmHg	101.26	19705
131.6	53329			A	7.25422	105	22425
139.4	66661			B	1688.4	109.5	26118
145.9	79993			C	230	115.59	31877
152.5	93326					122.79	39970
155.5	101325					129.61	49156
						135.48	58275
						139.94	66128
						144.73	75527
						149.51	85433
						151.95	91046
						154.24	96685
						bp/°C	156.083

*complete list see [ref.](#)

*complete list see [ref.](#)

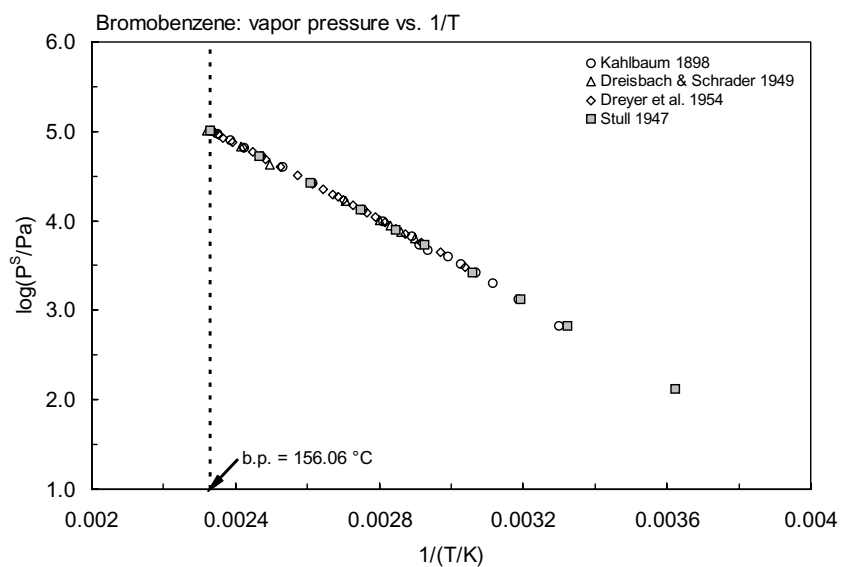
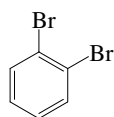


FIGURE 6.1.4.1.2 Logarithm of vapor pressure versus reciprocal temperature for bromobenzene.

6.1.4.2 1,2-Dibromobenzene



Common Name: 1,2-Dibromobenzene

Synonym: *o*-dibromobenzene

Chemical Name: 1,2-Dibromobenzene

CAS Registry No: 583-53-9

Molecular Formula: $C_6H_4Br_2$

Molecular Weight: 235.904

Melting Point ($^{\circ}C$):

7.1 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

225 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.98429, 1.9767 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.9843 ($20^{\circ}C$, Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

120.2 (calculated-density, Stephenson & Malanowski 1987)

142.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

59.31, 42.594 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.279 (Dreisbach 1955)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

74.55 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

74.8 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 7.44451 - 2050.3/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

25.7 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.10265 - 1825.77/(207.0 + t/^{\circ}C)$; temp range 115 – $295^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

26.0 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.50128 - 2093.1/(t/^{\circ}C + 230)$; temp range 28 – $117^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.10265 - 1825.77/(t/^{\circ}C + 207)$; temp range 117 – $300^{\circ}C$ (Antoine eq., Dean 1985, 1992)

22.80 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 6.22755 - 1825.77/(T/K - 66.15)$; temp range 388 – $588\ K$ (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.64 (shake flask, Hansch & Leo 1979; Hansch et al. 1995)

3.68 (HPLC-RT correlation, Garst & Wilson 1984)

3.64 (recommended, Sangster 1993)

3.64 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

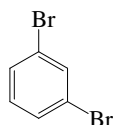
2.70; 3.50 (*Pimephales promelas*; *Poecilia reticulata*, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.4.3 1,3-Dibromobenzene



Common Name: 1,3-Dibromobenzene

Synonym: *m*-dibromobenzene

Chemical Name: 1,3-Dibromobenzene

CAS Registry No: 108-36-1

Molecular Formula: $C_6H_4Br_2$

Molecular Weight: 235.904

Melting Point ($^{\circ}C$):

−7.0 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

218 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.9523 ($20^{\circ}C$, Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

120.8 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

142.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

67.4 ($30^{\circ}C$, shake flask-UV, Hine et al. 1963)

98.45 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

64.0 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

57.06 ($35^{\circ}C$, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)

22.78 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 5.971 - 1603.4/(T/K - 87.55)$; temp range 417–500 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

157, 61.05 (calculated- ΔS_v , mp and bp, Antoine eq., Yalkowsky & Mishra 1990, Mishra & Yalkowsky 1991)

$\log(P/mmHg) = 59.2974 - 4.6960 \times 10^3/(T/K) - 18.444 \cdot \log(T/K) + 6.7598 \times 10^{-3} \cdot (T/K) - 2.5567 \times 10^{-13} \cdot (T/K)^2$; temp range 226–761 K (vapor pressure eq., Yaw et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.75 (shake flask, Hansch & Leo 1979; Hansch et al. 1995)

3.79 (shake flask-GC, Watarai et al. 1982)

3.78 (Oliver & Niimi 1984)

3.74 (HPLC- k' correlation, Haky & Yeung 1984)

3.75 (recommended, Sangster 1993)

3.75 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.78 (mean value, rainbow trout, Oliver & Niimi 1984)

2.82 (rainbow trout, Oliver 1987)

2.82 (*Oncorhynchus mykiss*, under flow-through conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: pseudo-first order reaction rate constant for direct photolysis $k = 0.009 \text{ min}^{-1}$ with $t_{1/2} = 76.8 \text{ min.}$ in dilute aqueous solution (Peijnenburg et al. 1992).

Half-Lives in the Environment:

Air:

Surface water: pseudo-first order reaction rate constant for direct photolysis $k = 0.009 \text{ min}^{-1}$ with $t_{1/2} = 76.8 \text{ min.}$ in dilute aqueous solution (Peijnenburg et al. 1992).

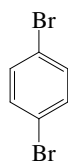
Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 3 \text{ d}$ (guppy, Niimi 1987)

6.1.4.4 1,4-Dibromobenzene



Common Name: 1,4-Dibromobenzene

Synonym: *p*-dibromobenzene

Chemical Name: 1,4-Dibromobenzene

CAS Registry No: 106-37-6

Molecular Formula: C₆H₄Br₂

Molecular Weight: 235.904

Melting Point (°C):

87.43 (Lide 2003)

Boiling Point (°C):

218.5 (Lide 2003)

Density (g/cm³ at 20°C):

1.5742 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):

121 (calculated-density, Lande & Banerjee 1981)

142.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.837 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.244 (mp at 87.43°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

20.0 (shake flask-UV, Andrews & Keefer 1950)

26.42 (35°C, shake flask-UV spectrophotometry, Hine et al. 1963)

20.08 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

20.0 (recommended-tentative, IUPAC Solubility Data Series, Horvath & Getzen 1985)

17.0* (shake flask-HPLC, measured range 10–35°C, Kuramochi et al. 2004)

ln [S/(mol/L)] = −3151.3.7/(T/K) + 1.06; temp range 10–35°C (shake flask-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (61°C, summary of literature data, Stull 1947)

log (P/mmHg) = 7.44830 − 2057.2/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

9.33* (25.8°C, manometer, temp range 25.8–80.5°C, Walsh & Smith 1961)

log (P/mmHg) = 11.592 − 3826.2/(T/K); temp range 25.8–80.5°C (manometer, Walsh & Smith 1961)

17.87 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)

log (P/mmHg) = [−0.2185 × 13047.8/(T/K)] + 8.769771; temp range 61–218.6°C (Antoine eq., Weast 1972–73)

3.96* (18.13°C, capacitance manometer; De Kruif et al. 1981)

7.65 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

log P/kPa = 10.717 − 3826.2/(T/K); temp range 298–354 K (Antoine eq., solid, Stephenson & Malanowski 1987)

log P/kPa = 6.5732 − 2047.2/(T/K − 43.15); temp range 373–493 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

35.95, 53.18 (calculated-bp, Antoine eq., Yalkowsky & Mishra 1990)

Henry's Law Constant (Pa·m³/mol at 25°C):

106 (derived from γ_w, infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, log K_{ow} :

3.75	(shake flask, Hansch & Leo 1979)
4.07	(calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980)
4.13	(calculated-fragment const., Yalkowsky et al. 1983)
3.79	(shake flask-GC, Watarai et al. 1982)
3.89	(Gobas et al. 1989)
3.79	(recommended, Sangster 1993)
3.79	(recommended, Hansch et al. 1995)
3.62	(GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C:

5.21	(calculated- S_{oct} and vapor pressure, Abraham et al. 2001)
------	---

Bioconcentration Factor, log BCF:

3.15	(guppy, lipid-weight based, Gobas et al. 1989)
1.96	(<i>Poecilia reticulata</i> , under flow-through conditions, Devillers et al. 1996)
2.70; 3.40	(<i>Poecilia reticulata</i> ; <i>Pimephales promelas</i> , under static and semi-static conditions, Devillers et al. 1996)
3.15	(Gobas et al. 1989)

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
 log $k_1 = 2.11 \text{ d}^{-1}$; log $k_2 = 0.15 \text{ d}^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

TABLE 6.1.4.4.1

Reported aqueous solubilities and vapor pressures of 1,4-dibromobenzene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log (P/mmHg) = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log (P/Pa) = A – B/(C + T/K)		(3)					
log (P/mmHg) = A – B/(T/K) – C·log (T/K)		(4)					
Aqueous solubility		Vapor pressure					
Kuramochi et al.2004		Stull 1947		Walsh & Smith 1961		de Kruif et al. 1981	
shake flask-GC		summary of literature data		manometry		diaphragm gauge	
t/°C	S/(g m ⁻³)	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
10	9.91	61.0	133.3	25.8	9.33	1.54	0.617
25	17.0	79.3	666.6	26.8	9.33	3.93	0.829
35	24.6	87.7	1333	27.5	10.67	3.95	0.832
mp/°C	84.55	103.6	2666	31.9	14.67	7.62	1.253
		120.8	5333	38.1	26.66	10.54	1.736
		131.6	7999	42.6	38.66	14.02	2.544
ΔH _{sol} /(kJ mol ⁻¹) = 26.2		146.5	13332	42.6	40.0	18.13	3.960
ΔH _{fusl} /(kJ mol ⁻¹) = 18.6		168.5	26664	44.6	48.0		
		192.5	53329	50.2	73.33		
		218.6	101325	51.2	83.99	eq. 1	P/Pa

(Continued)

TABLE 6.1.4.4.1 (Continued)

Aqueous solubility		Vapor pressure					
Kuramochi et al.2004		Stull 1947		Walsh & Smith 1961		de Kruif et al. 1981	
shake flask-GC		summary of literature data		manometry		diaphragm gauge	
t/°C	S/(g m ⁻³)	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
ln S = −3151.3/(T/K) + 1.06		mp/°C	87.5	56.4	129.3	A	13.86395
S in mol/L				57.2	136.0	B	3864.8
				57.3	141.3		
				64.3	238.7		
				71.8	420.0		
				80.5	791.9		
				mp/°C	87.24		
				eq. 1	P/mmHg		
				A	11.592		
				B	3826.2		
				ΔH _{subl} /(kJ mol ⁻¹) = 73.26			

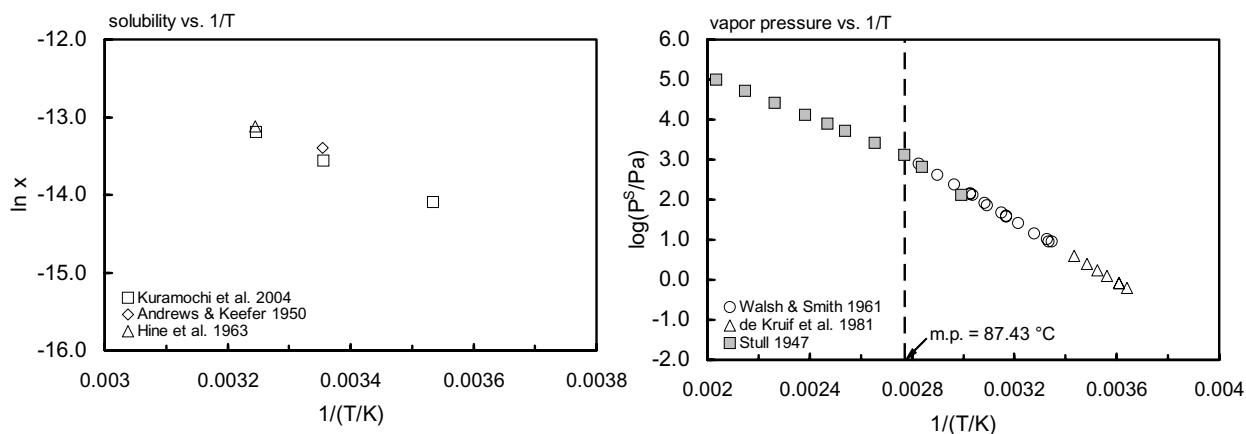
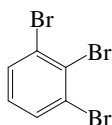


FIGURE 6.1.4.4.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,4-dibromobenzene.

6.1.4.5 1,2,3-Tribromobenzene

Common Name: 1,2,3-Tribromobenzene

Synonym:

Chemical Name: 1,2,3-tribromobenzene

CAS Registry No: 608-21-9

Molecular Formula: $C_6H_3Br_3$

Molecular Weight: 314.800

Melting Point ($^{\circ}C$):

87.8 (Weast 1982–83)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

2.658 (Weast 1982–83, Horvath 1982)

Molar Volume (cm^3/mol):

137.7 (Ruelle & Kesselring 1997)

118 (calculated-density, Wang et al. 1992)

165.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.242 (mp at $87.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.94 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.98; 4.25 (quoted exptl value; calculated-molar volume, Wang et al. 1992)

4.57; 4.42 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

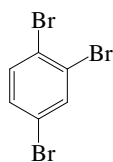
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 3\ d$ in guppy (for tribromobenzenes, Niimi 1986).

6.1.4.6 1,2,4-Tribromobenzene



Common Name: 1,2,4-Tribromobenzene

Synonym:

Chemical Name: 1,2,4-tribromobenzene

CAS Registry No: 615-54-3

Molecular Formula: $C_6H_3Br_3$

Molecular Weight: 314.800

Melting Point ($^{\circ}C$):

44.5 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

275 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

137.7 (Ruelle & Kesselring 1997)

165.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.644 (mp at $44.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

9.96 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

10.1 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)

3.67, 7.21, 11.0 (10, 25, $35^{\circ}C$, generator column-HPLC, Kuramochi et al. 2004)

$\ln [S/(mol/L)] = -3836.9/(T/K) + 2.19$; temp range 10 – $35^{\circ}C$ (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

31.9 (derived from γ_w , infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.51 (shake flask-GC, Watarai et al. 1982)

4.54 (Oliver & Niimi 1984)

4.32 (GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

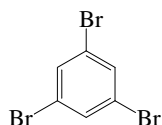
3.63 (rainbow trout, Oliver 1984, Oliver & Niimi 1984, Oliver 1987)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 3$ d in guppy (for tribromobenzenes, Niimi 1987)

6.1.4.7 1,3,5-Tribromobenzene

Common Name: 1,3,5-Tribromobenzene

Synonym:

Chemical Name: 1,3,5-tribromobenzene

CAS Registry No: 626-39-1

Molecular Formula: $C_6H_3Br_3$

Molecular Weight: 314.800

Melting Point ($^{\circ}C$):

122.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

271 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

137.7 (Ruelle & Kesselring 1997)

165.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.11 (mp at $122.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

200 (shake flask-residue volume method, Booth & Everson 1948)

0.04 (Stephen & Stephen 1963)

0.787 (shake flask-UV, Yalkowsky et al. 1979)

0.789 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

5.187 (GC-RT correlation, Watanabe & Tatsukawa 1989)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.51 (shake flask-GC, Watarai et al. 1982)

5.07 (calculated-fragment const., Yalkowsky et al. 1983)

4.60, 4.63 (HPLC-RT correlation, Garst 1984)

5.26 (HPLC-RT correlation, Gobas et al. 1989)

5.18 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

4.51 (recommended, Sangster 1993)

4.51 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.70 (rainbow trout, Oliver & Niimi 1984, Oliver 1987)

3.26–4.08 mean 3.97; 3.53–4.20 mean 4.08 (rainbow trout, wet wt. basis, $15^{\circ}C$, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)

4.42 (guppy, lipid-weight based, Gobas et al. 1989)

3.23; 3.70, 3.97, 4.08 (*Poecilia reticulata*; *Oncorhynchus mykiss*, quoted values, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: pseudo-first order reaction rate constant in dilute aqueous solution $k = 0.005 \text{ min}^{-1}$ with $t_{1/2} = 140.5 \text{ min}$. (Peijeneburg et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$\log k_1 = 2.85 \text{ d}^{-1}$; $\log k_2 = -0.38 \text{ d}^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Air:

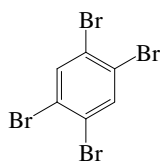
Surface water: pseudo-first order reaction rate constant for direct photolysis in dilute aqueous solution $k = 0.005 \text{ min}^{-1}$ with $t_{1/2} = 140.5 \text{ min}$. (Peijeneburg et al. 1992).

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 3 \text{ d}$ (guppy, for tribromobenzenes, Niimi 1987)

6.1.4.8 1,2,4,5-Tetrabromobenzene

Common Name: 1,2,4,5-Tetrabromobenzene

Synonym:

Chemical Name: 1,2,4,5-tetrabromobenzene

CAS Registry No: 636-28-2

Molecular Formula: $C_6H_2Br_4$

Molecular Weight: 393.696

Melting Point ($^{\circ}C$):

182 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

3.072 (Weast 1982–83)

Molar Volume (cm^3/mol):

128.2 (calculated-density, Wang et al. 1992)

153.8 (Ruelle & Kesselring 1997)

189.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0288 (mp at $182^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0433 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

0.0434 (recommended-tentative, IUPAC Solubility Data Series, Hovrath & Getzen 1985)

0.044 (shake flask-GC, Kim & Saleh 1990)

0.0182, 0.0435, 0.0778 (10, 25, $35^{\circ}C$, generator column-HPLC, Kuramochi et al. 2004)

$\ln [S/(mol/L)] = -4967.5/(T/K) + 0.681$; temp range 10 – $35^{\circ}C$ (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$):

0.157 (GC-RT correlation, Watanabe & Tatsukawa 1989)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

376 (derived from γ_w , infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.13 (shake flask-GC, Watarai et al. 1982)

5.25 (HPLC-RT correlation, Garst 1984)

5.56 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.13 (recommended, Sangster 1993)

5.13 (recommended, Hansch et al. 1995)

5.00 (GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.80 (rainbow trout, Banerjee et al. 1980)

2.94–3.68 mean 3.57; 3.40–3.91 mean 3.81 (rainbow trout, wet wt. basis, $15^{\circ}C$, steady-state BCF on 7- to 96-d laboratory study in two tanks of different water concn, Oliver & Niimi 1985)

3.80 (Nendza 1993; quoted, Lu et al. 1999)

3.57 (*Oncorhynchus mykiss*, flow through conditions, Devillers et al. 1996)

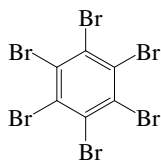
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 4$ d in guppy (for tetrabromobenzenes, Niimi 1987)

6.1.4.9 Hexabromobenzene



Common Name: Hexabromobenzene

Synonym:

Chemical Name: hexabromobenzene

CAS Registry No: 87-82-1

Molecular Formula: C_6Br_6

Molecular Weight: 551.488

Melting Point ($^{\circ}C$):

327 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

186 (Ruelle & Kesselring 1997)

235.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85 (Tittlemier et al. 2002)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.0011 (mp at $327^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and the reported temperature dependence equations):

0.00016 ($22^{\circ}C$, generator column-GC, Opperhuizen 1986)

0.0030 (generator column-GC/ECD, Tittlemier et al. 2002)

0.0000472, 0.00011, 0.000232 (10, 25, $35^{\circ}C$, generator column-HPLC, Kuramochi et al. 2004)

$\ln [S/(mol/L)] = -5484.7/(T/K) - 3.85$; temp range 10 – $35^{\circ}C$ (generator column-HPLC, Kuramochi et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

3.133×10^{-4} (estimated, Lyman et al. 1982)

3.845×10^{-4} (GC-RT correlation, Watanabe & Tatsukawa 1989)

7.50×10^{-4} (supercooled liquid P_L , GC-RT correlation, Tittlemier et al. 2002)

$\log (P_L/Pa) = -4454/(T/K) + 11.82$ (Claiius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.284 (calculated, Meylan & Howard 1991)

0.14 (calculated- P_L/C_L , Tittlemier et al. 2002)

10.8 (derived from γ_w , infinite dilution activity coefficient, Kuramochi et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.15, 6.07 (HPLC-RT correlation, Garst 1984)

7.80 (HPLC-RT correlation, Opperhuizen 1986)

> 6.0 (estimated, Gobas et al. 1987)

7.06 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.07 (recommended, Sangster 1993)

6.07 (Hansch et al. 1995)

6.07 (GC-RT correlation, Kuramochi et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.95–3.08 mean 3.04 (rainbow trout, wet wt., 15°C, steady-state BCF on 21- to 96-d laboratory study, Oliver & Niimi 1985)

1.0 (Kawasaki 1980)

5.0 (Nendza 1993)

4.892, 4.681 (calculated-MCI, calculated- K_{OW} , Lu et al. 1999)

Sorption Partition Coefficient, $\log K_{OC}$:

4.45, 4.68 (estimated-solubility, Lyman et al. 1982; quoted, K_{OW} , Howard 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated volatilization $t_{1/2} = 3.3$ d from a model river is 3.3 d, $t_{1/2} = 114$ months from a model pond with adsorptive processes (Howard 1997)

Photolysis: not expected to occur (Howard 1997)

Oxidation: not expected to occur (Howard 1997)

Hydrolysis: not expected to occur (Howard 1997)

Half-Lives in the Environment:

Air:

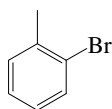
Surface water: estimated volatilization $t_{1/2} = 3.3$ d from a model river, $t_{1/2} = 114$ months from a model pond with adsorptive processes (Howard 1997)

Groundwater:

Sediment:

Soil:

Biota:

6.1.4.10 2-Bromotoluene

Common Name: 2-Bromotoluene

Synonym: *o*-bromotoluene, 1-bromo-2-methylbenzene

Chemical Name: 2-bromotoluene

CAS Registry No: 95-46-5

Molecular Formula: C₇H₇Br

Molecular Weight: 171.035

Melting Point (°C):

– 27.8 (Weast 1982–82; Lide 2003)

Boiling Point (°C):

181.7 (Dreisbach 1959; Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):

1.42322, 1.41774 (20°C, 25°C, Dreisbach 1959)

1.4232 (Weast 1982–83; Lide 2003)

Molar Volume (cm³/mol):

120.2 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

141.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.264, 38.995 (25°C, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

2.423 (Dreisbach 1955)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

51.3 (estimated, Howard 1997)

1007; 105 (quoted, calculated-molar volume and mp, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

186 (interpolated-Antoine eq., Stuckey & Saylor 1940)

$\log P/\text{mmHg} = 7.50879 - 1913.46/(T/K - 38.34)$; temp range 4–75°C (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)

133.3* (24.4, summary of lit. data, Stull 1947)

181 (calculated by formula., Dreisbach 1955)

$\log (P/\text{mmHg}) = 6.90847 - 1549.39/(C + t/^\circ\text{C})$; temp range 80–245°C, (Antoine eq. for liquid state, Dreisbach 1955)

$\log (P/\text{mmHg}) = [-0.2185 \times 11365.0/(T/K)] + 8.396578$; temp range 24.4–181.8°C (Antoine eq., Weast 1972–73)

$\log (P_L/\text{kPa}) = 6.03337 - 1549.39/(T/K - 70.15)$; temp range 353–518 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m³/mol at 25°C):

242 (estimated-group contribution method, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.92 (Hansch & Leo 1979, Hansch et al. 1995)

3.61 (HPLC-*k'* correlation, Hanai et al. 1981)

3.43 (estimated, Howard 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or log K_B :

2.38 (estimated- K_{OW} , Howard 1997)

Sorption Partition Coefficient, log K_{OC} :

2.96 (estimated, Howard 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 1.7$ h from a model river 1-m deep and $t_{1/2} = 14.9$ d from a pond (Howard 1997).

Photolysis:

Oxidation: atmospheric $t_{1/2} \sim 6.2$ d for reaction with hydroxyl radicals in air (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 6.2$ d for reaction with OH radicals in air (Howard 1997).

Surface water: volatilization $t_{1/2} = 1.7$ h from a model river 1-m deep flowing 1 m/s with a wind speed of 5 m/s and $t_{1/2} = 14.9$ d from a model pond with adsorption from water column (Howard 1997).

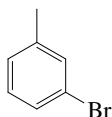
TABLE 6.1.4.10.1
Reported vapor pressures of 2-bromotoluene at various temperatures

Stull 1947

summary of literature data

$t/^{\circ}\text{C}$	P/Pa
24.4	133.3
49.7	666.6
62.3	1333
76.0	2666
91.0	5333
100.0	7999
112.0	13332
133.6	26664
157.3	53329
181.8	101325
mp/ $^{\circ}\text{C}$	-28

6.1.4.11 3-Bromotoluene



Common Name: 3-Bromotoluene

Synonym: *m*-bromotoluene

Chemical Name: 3-bromotoluene

CAS Registry No: 591-17-3

Molecular Formula: C_7H_7Br

Molecular Weight: 171.035

Melting Point ($^{\circ}C$):

−39.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

183.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4099 (Lide 2003)

Molar Volume (cm^3/mol):

121.3 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

141.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

51.3 (estimated, Howard 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($14.8^{\circ}C$, summary of lit. data, Stull 1947)

$\log P/mmHg = 7.75409 - 2049.14/(T/K - 31.44)$; temp range $4-75^{\circ}C$ (Antoine eq. based on exptl. data, Hg manometer, Stuckey & Saylor 1940)

$\log (P/mmHg) = [-0.2185 \times 10537.1/(T/K)] + 7.886560$; temp range $14.8-183.7^{\circ}C$ (Antoine eq., Weast 1972-73)

145 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.86228 - 2085.49/(T/K - 27.333)$; temp range: 287-457 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

445 (estimated-P/C, Howard 1997)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.43 (estimated, Howard 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.38 (estimated- K_{ow} , Howard 1997)

Sorption Partition Coefficient, $\log K_{OC}$:

2.96 (estimated, Howard 1997)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 1.5$ h and 14.9 d from a model river 1-m deep and $t_{1/2} = 14.9$ d from a pond (Howard 1997).

Photolysis:

Oxidation: atmospheric $t_{1/2} \sim 3$ d for reaction with hydroxyl radical in air (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

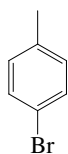
Air: atmospheric $t_{1/2} \sim 3$ d half-life for reaction with hydroxyl radical in air (Howard 1997).

Surface water: volatilization $t_{1/2} = 1.5$ h from a model river 1 m deep flowing 1 m/s with a wind speed of 5 m/s) and $t_{1/2} = 14.9$ d in a model pond with adsorption, from water column (Howard 1997).

TABLE 6.1.4.11.1**Reported vapor pressures of 3-bromotoluene at various temperatures****Stull 1947****summary of literature data**

t/°C	P/Pa
14.8	133.3
50.8	666.6
64.0	1333
78.1	2666
93.9	5333
104.1	7999
117.8	13332
138.0	26664
160.0	53329
183.7	101325
mp/°C	-39.8

6.1.4.12 4-Bromotoluene



Common Name: 4-Bromotoluene

Synonym: *p*-bromotoluene, 4-bromo-1-methylbenzene

Chemical Name: *p*-bromotoluene

CAS Registry No: 106-38-7

Molecular Formula: C₇H₇Br

Molecular Weight: 171.042

Melting Point (°C):

28.5 (Lide 2003)

Boiling Point (°C):

184.3 (Lide 2003)

Density (g/cm³ at 25°C):

1.39953 (Dreisbach 1955)

Molar Volume (cm³/mol):

122.5 (Ruelle & Kesselring 1997)

141.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.74, 39.98 (25°C, bp, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.82 (Dreisbach 1955)

3.5684 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

110 (Hine & Mookerjee 1975)

110; 81.9 (quoted; calculated-molar volume and mp, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* (10.3°C, summary of lit. data, Stull 1947)

153.2 (calculated by formula., Dreisbach 1955)

log (P/mmHg) = 7.00762 – 1612.35/(206.36 + t/°C); temp range 85–250°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/mmHg) = 7.00762 – 1612.35/(t/°C + 206.36); temp range 85–280°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 6.13252 – 1612.35/(T/K – 66.79); temp range 358–523 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 12.8209 – 2.6568 × 10³/(T/K) – 1.4314·log (T/K) – 8.9677 × 10⁻⁴·(T/K) + 3.9733 × 10⁻⁷·(T/K)², temp range 300–699 K (Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

23.82 (calculated-P/C, Howard 1997)

Octanol/Water Partition Coefficient, log K_{ow}:

3.42 (quoted, Howard 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.54 (calculated- K_{OW} , Howard 1997)

Sorption Partition Coefficient, $\log K_{OC}$:

3.10–3.27 (estimated, Howard 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} \sim 9.4$ d for reaction with OH radical in the atmosphere (Howard 1997).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 9.4$ d for reaction with OH radical (Howard 1997).

Surface water: volatilization $t_{1/2} = 4.3$ h from a model river 1 m deep and $t_{1/2} = 14.9$ d from an environmental pond (Howard 1997).

TABLE 6.1.4.12.1

Reported vapor pressures of 4-bromotoluene at various temperatures

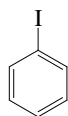
Stull 1947

summary of literature data

$t/^{\circ}\text{C}$	P/Pa
10.3	133.3
47.5	666.6
61.1	1333
75.2	2666
91.8	5333
102.3	7999
116.4	13332
137.4	26664
160.2	53329
184.5	101325
mp/ $^{\circ}\text{C}$	28.5

6.1.5 IODOBENZENES

6.1.5.1 Iodobenzene



Common Name: Iodobenzene

Synonym: phenyl iodide

Chemical Name: iodobenzene

CAS Registry No: 591-50-4

Molecular Formula: C_6H_5I

Molecular Weight: 204.008

Melting Point ($^{\circ}C$):

−31.3 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

188.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.8308 (Weast 1982–83; Lide 2003)

1.8308, 1.8229($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

111.4 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987; Wang et al. 1992)

129.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

40.794 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

340 ($30^{\circ}C$, Gross et al. 1933)

180 (shake flask-UV spectrophotometry, Andrews & Keefer 1950)

228* ($25.1^{\circ}C$, shake flask-spectrophotometry, measured range 10 – $35^{\circ}C$, Vesala 1973)

229 (shake flask-UV spectrophotometry, Vesala 1974)

158 (Deno & Berkheimer 1960)

95* (shake flask-GC, measured range 5 – $45.5^{\circ}C$, Nelson & Smit 1978)

267.6* (summary of literature data, temp range 25 – $50^{\circ}C$, Horvath 1982)

201 (Miller et al. 1985)

226* (recommended, temp range 10 – $45^{\circ}C$, IUPAC Solubility Data Series, Horvath & Getzen 1985)

$S/(g/kg) = 0.59293 - 4.8616 \times 10^{-3} \cdot (T/K) + 1.21754 \times 10^{-5} \cdot (T/K)^2$; temp range 283 – 318 K (regression of literature data, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

213* ($29.3^{\circ}C$, Ramsay-Young method, measured range 29.3 – $100.35^{\circ}C$, Young 1889)

133.3*, 666.6 (24.1 , $50.6^{\circ}C$, summary of lit. data, temp range 24.1 – $188.6^{\circ}C$, Stull 1947)

134.5 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 6.89506 - 1562.87/(201.0 + t/^{\circ}C)$; temp range: 85 – $270^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

132.0 (Antoine eq., Boublik et al. 1973)

$\log(P/mmHg) = 7.01187 - 1640.124/(208.765 + t/^{\circ}C)$; temp range 29.3 – $188.2^{\circ}C$ (Antoine eq. from reported exptl. data of Young 1889, Boublik et al. 1973)

134 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.15935 - 1656.226/(210.496 + t/^{\circ}\text{C})$; temp range 29.3–188.2°C (Antoine eq. from reported exptl. data of Young 1889, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.0119 - 1640.1/(208.8 + t/^{\circ}\text{C})$; temp range 20–188°C (Antoine eq., Dean 1985, 1992)

134.5 (Riddick et al. 1986)

133 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.01996 - 1562.87/(-72.15 + T/\text{K})$; temp range 358–543 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.46493 - 1867.69/(-20.202 + T/\text{K})$; temp range 462–679 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.36129 - 1765.99/(-54.15 + T/\text{K})$; temp range 273–358 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 32.7342 - 3.5824 \times 10^3/(T/\text{K}) - 8.4197 \cdot \log (T/\text{K}) + 2.0073 \times 10^{-10} \cdot (T/\text{K}) + 1.591 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 242–721 K (Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

130 (recommended, Mackay & Shiu 1981)

134 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.25, 3.32 (quoted, calculated-fragment const., Rekker 1977)

3.25 (Hansch & Leo 1979)

3.28 (generator column-HPLC, Wasik et al. 1983)

3.28 (generator column-HPLC, Tewari et al. 1982)

3.23 (HPLC/MS correlation, Burkhard et al. 1985)

3.37 (HPLC-RT correlation, Eadsforth 1986)

3.25 (recommended, Sangster 1989)

3.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}(\text{calc}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs}) = 0.93 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^* = (1.32 \pm 0.19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{\text{OH}} = 1.32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}} = 1.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range 263–393 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 6.1.5.1.1
Reported aqueous solubilities of iodobenzene at various temperatures

$S(\text{wt}\%) = -2.78956 \times 10^{-3} + 1.95862 \times 10^{-3} \cdot (t/^{\circ}\text{C}) - 4.53984 \times 10^{-5} \cdot (t/^{\circ}\text{C})^2 + 5.73315 \times 10^{-7} \cdot (t/^{\circ}\text{C})^3$ (1)

$S(\text{g/kg}) = 0.59293 - 4.816 \times 10^{-3} \cdot (T/\text{K}) + 1.21754 \times 10^{-5} \cdot (T/\text{K})^2$ (2)

Vesala 1973		Nelson & Smit 1978		Horvath 1982		Horvath & Getzen 1985	
shake flask-UV		shake flask-GC		summary of literature data		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	195.29	5	54.9	25	267.6	10	193
15.2	196.56	25	95.0	30	305.9	15	203
19.6	216.42	39	143.8	40	396.1	20	214
25.0	228.45	45.5	207.2	50	533.1	25	226
30.0	236.20					30	238
35.0	251.09			eq. 1	S/wt%	35	251
						40	264
						45	279
						eq. 2	S/(g/kg)

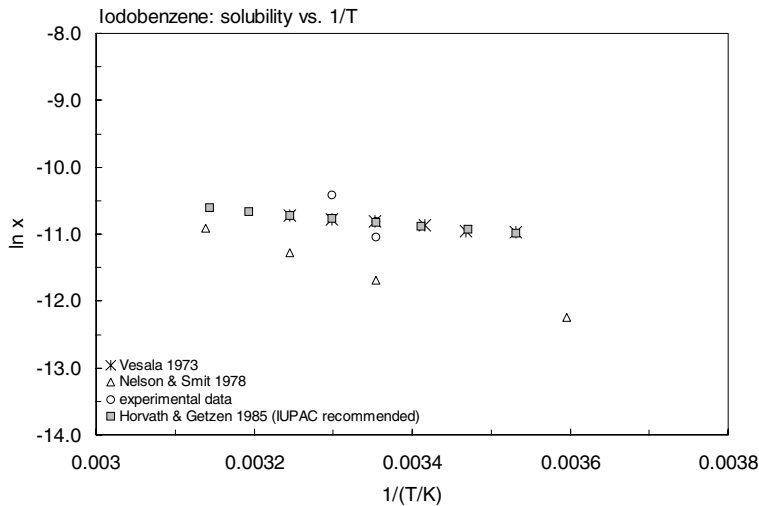


FIGURE 6.1.5.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for iodobenzene.

TABLE 6.1.5.1.2

Reported vapor pressures of iodobenzene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

Young 1889		Stull 1947	
Ramsay-Young method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
29.3	213	24.1	133.3
33	240	50.6	666.6
40.1	367	64	1333
46.3	513	78.3	2666
52.5	753	94.4	5333
57	933	105	7999
61.45	1187	118.3	13332
67.8	1627	139.8	26664
70.9	1927	163.9	53329
78.4	2700	188.6	101325
81.9	3166		
85.5	3673	mp/°C	-28.5
87.45	4026		
88.75	4266		
91.55	4820		
91.6	4820		
94.75	5466		
100.35	6919		

complete set of data see [ref.](#)

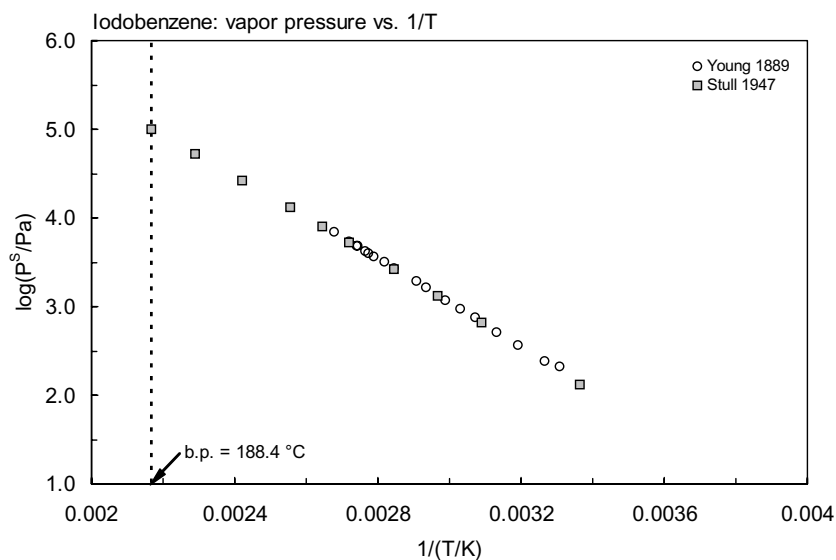
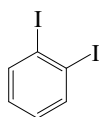


FIGURE 6.1.5.1.2 Logarithm of vapor pressure versus reciprocal temperature for iodobenzene.

6.1.5.2 1,2-Diiodobenzene

Common Name: 1,2-Diiodobenzene

Synonym: *o*-diiodobenzene

Chemical Name: 1,2-Diiodobenzene

CAS Registry No: 615-42-9

Molecular Formula: $C_6H_4I_2$

Molecular Weight: 329.051

Melting Point ($^{\circ}C$):

27 (Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

287 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

2.54 ($20^{\circ}C$, Weast 1982–83, Horvath 1982; Lide 2003)

Molar Volume (cm^3/mol):

162.6 (calculated-Le Bas method at normal boiling point)

134.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.956 (mp at $27^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

14.9 (shake flask-UV, Andrews & Keefer 1950)

19.0 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, log K_{ow} :

4.65 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980)

4.64 (calculated-fragment const., Yalkowsky et al. 1983)

4.65; 4.35 (quoted; calculated-molar volume correlation, Wang et al. 1992)

4.39 (calculated, Müller & Klein 1992)

4.64, 5.24; 4.56 (quoted exptl., predicted; calculated-atom typing scheme, Inel & Iseri 1997)

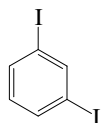
Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.5.3 1,3-Diiodobenzene

Common Name: 1,3-Diiodobenzene

Synonym: *m*-diiodobenzene

Chemical Name: 1,3-Diiodobenzene

CAS Registry No: 626-00-6

Molecular Formula: $C_6H_4I_2$

Molecular Weight: 329.905

Melting Point ($^{\circ}C$):

40.4 (Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Weast 1982–83, Horvath 1982; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

2.47 (Weast 1982–83, Horvath 1982)

Molar Volume (cm^3/mol):

162.6 (calculated-Le Bas method at normal boiling point)

134.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

3.8064 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.706 (mp at $40.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9.67 (shake flask-UV, Andrews & Keefer 1950)

8.88 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.64 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)

4.39 (calculated, Müller & Klein 1992)

4.70 (calculated-molar volume correlation, Wang et al. 1992)

5.25; 4.56 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

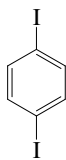
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.5.4 1,4-Diiodobenzene

Common Name: 1,4-Diiodobenzene

Synonym: *p*-diiodobenzene

Chemical Name: 1,4-Diiodobenzene

CAS Registry No: 624-38-4

Molecular Formula: $C_6H_4I_2$

Molecular Weight: 329.905

Melting Point ($^{\circ}C$):

131.5 (Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

285 (sublimation, Weast 1982–83, Horvath 1982; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

162.6 (calculated-Le Bas method at normal boiling point)

134.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.3342 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0902 (mp at $131.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.62 (shake flask-UV, Andrews & Keefer 1950)

1.855 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.545 (extrapolated Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.29504 - 33311.326/(T/K)$; temp range 372–401 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.8859 - 2747.88/(T/K)$; temp range 402–560 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.64 (calculated-fragment const., Yalkowsky et al. 1979; Valvani & Yalkowsky 1980; Yalkowsky et al. 1983; quoted, Wang et al. 1992)

4.39 (calculated, Müller & Klein 1992)

4.11 (shake flask, recommended, Hansch et al. 1995)

4.64, 5.24; 4.56 (quoted exptl., predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

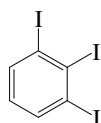
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.5.5 1,2,3-Triiodobenzene



Common Name: 1,2,3-Triiodobenzene

Synonym:

Chemical Name: 1,2,3-Triiodobenzene

CAS Registry No: 608-29-7

Molecular Formula: $C_6H_3I_3$

Molecular Weight: 455.801

Melting Point ($^{\circ}C$):

166 (Weast 1982–83, Horvath 1982)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83, Horvath 1982)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

141 (Wang et al. 1992)

195.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.041 (mp at $166^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.301 (shake flask-UV, Yalkowsky & Valvani 1980)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.86 (quoted, Wang et al. 1992)

6.17; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

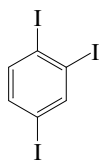
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.5.6 1,2,4-Triiodobenzene

Common Name: 1,2,4-Triiodobenzene

Synonym:

Chemical Name: 1,2,4-Triiodobenzene

CAS Registry No: 615-68-9

Molecular Formula: $C_6H_3I_3$

Molecular Weight: 455.801

Melting Point ($^{\circ}C$):

91.5 (Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83, Horvath 1982; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

195.9 (calculated-Le Bas method at normal boiling point)

145 (Wang et al. 1992)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.223 (mp at $91.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.538 (shake flask-UV, Yalowsky & Valvani 1980)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.85 (quoted, Wang et al. 1992)

6.58; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

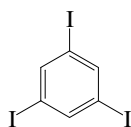
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.5.7 1,3,5-Triiodobenzene



Common Name: 1,3,5-Triiodobenzene

Synonym:

Chemical Name: 1,3,5-Triiodobenzene

CAS Registry No: 626-44-8

Molecular Formula: $C_6H_3I_3$

Molecular Weight: 455.801

Melting Point ($^{\circ}C$):

184.2 (Weast 1982–83, Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83, Horvath 1982; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

131 (Wang et al. 1992)

195.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.0274 (mp at $184.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0706 (shake flask-UV, Yalowsky & Valvani 1980)

0.0644 (quoted, Wang et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.85 (quoted, Wang et al. 1992)

6.90; 5.82 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

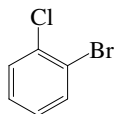
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.6 MIXED HALOGENATED BENZENES**6.1.6.1 2-Bromochlorobenzene**

Common Name: 2-Bromochlorobenzene

Synonym: 2-bromo-1-chlorobenzene

Chemical Name:

CAS Registry No: 108-37-2

Molecular Formula: C_6H_4BrCl

Molecular Weight: 191.453

Melting Point ($^{\circ}C$):

-12.3 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

204 (Weast 1982–83; Horvath 1982; Lide 2003)

Density (g/cm^3):

1.6387 (25 $^{\circ}C$, Weast 1982–83; Horvath 1982)

Molar Volume (cm^3/mol):

117 (calculated-density, Lande & Banerjee 1981; Wang et al. 1992)

116.8 (Ruelle & Kesselring 1997)

140.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

124 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)

124 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25 $^{\circ}C$):

Henry's Law Constant (Pa-m 3 /mol at 25 $^{\circ}C$):

Octanol/Water Partition Coefficient, log K_{ow} :

3.83 (calculated-fragment const., Yalkowsky et al. 1979)

3.86 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky 1983)

3.44 (calculated, Müller & Klein 1992)

3.83; 3.63 (quoted; calculated-molar volume correlation, Wang et al. 1992)

3.83, 3.54; 3.36 (quoted, predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA} :

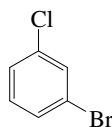
Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.6.2 3-Bromochlorobenzene



Common Name: 3-Bromochlorobenzene

Synonym: *m*-bromochlorobenzene, 3-bromo-1-chlorobenzene, 1-bromo-3-chlorobenzene

Chemical Name: 3-bromochlorobenzene

CAS Registry No: 108-37-2

Molecular Formula: C₆H₄BrCl

Molecular Weight: 191.453

Melting Point (°C):

−21.5 (Dreisbach & Martin 1949, Weast 1982–83; Horvath 1982; Lide 2003)

21 (Stephenson & Malanowski 1987)

Boiling Point (°C):

196 (Weast 1982–83; Horvath 1982, Stephenson & Manlanowski 1987; Lide 2003)

Density (g/cm³):

1.62745, 1.62065 (20°C, 25°C, Dreisbach & Martin 1949)

1.602 (20°C, Weast 1982–83; Horvath 1982)

1.5771 (20°C, Lide 2003)

Molar Volume (cm³/mol):

117.4 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)

140.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

118 (shake flask-UV, Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983)

118 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

log (P/mmHg) = 7.37230 − 1912.7/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

99.2 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.4972 − 1912.7/(T/K − 43.15); temp range 252–469 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

3.83 (calculated-fragment const., Yalkowsky et al. 1979)

3.83 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky et al. 1983)

3.74 (HPLC-k' correlation, Hanai et al. 1981)

3.72 (calculated, Müller & Klein 1992)

3.61 (calculated-molar volume correlation, Wang et al. 1992)

3.54; 3.36 (predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, log K_{OA}:

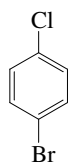
Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.6.3 4-Bromochlorobenzene



Common Name: 4-Bromochlorobenzene

Synonym: 4-bromo-1-chlorobenzene, 1-bromo-4-chlorobenzene

Chemical Name: 4-bromochlorobenzene

CAS Registry No: 106-39-8

Molecular Formula: C_6H_4BrCl

Molecular Weight: 191.453

Melting Point ($^{\circ}C$):

68 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

196 (Weast 1982–83; Horvath 1982, Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

1.576 (71 $^{\circ}C$, Weast 1982–83; Horvath 1982)

Molar Volume (cm^3/mol):

121.5 (calculated-density, Stephenson & Malanowski 1987)

140.2 (calculated-Le Bas method at normal boiling point)

126.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.376 (mp at 68 $^{\circ}C$)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

44.9; 37.3 (shake flask-UV; calculated- K_{ow} , Yalkowsky et al. 1979, Yalkowsky & Valvani 1980, Yalkowsky et al. 1983; quoted, Lande & Banerjee 1981; Horvath 1982; Müller & Klein 1992)

44.9; 37.3 (quoted; calculated- K_{ow} , Valvani & Yalkowsky 1980)

44.2 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

45; 11.31 (quoted; calculated-molar volume correlation, Wang et al. 1992)

44.9; 50.4 (quoted; calculated-group contribution method; Kühne et al. 1995)

44.9; 51.5 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

133.3* (32.0 $^{\circ}C$, summary of literature data, temp range 32.0–196.9 $^{\circ}C$, Stull 1947)

33.3* (24.2 $^{\circ}C$, manometry, measured range 21.4–64.4 $^{\circ}C$, Walsh & Smith 1961)

34.45 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 16671.8/(T/K)] + 11.629$; temp range 23–63 $^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 11451.1/(T/K)] + 8.222763$; temp range 32–196 $^{\circ}C$ (Antoine eq., Weast 1972–73)

32.12 (calculated-bp, Mackay et al. 1982)

37.72 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.478 - 3548.4/(T/K)$; temp range 294–337 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.71377 - 2074.22/(T/K - 35.248)$; temp range 333–470 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at 25 $^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.86 (calculated-fragment const., Yalkowsky et al. 1979)
- 3.83 (calculated-fragment const., Valvani & Yalkowsky 1980; Yalkowsky 1983; quoted, Malihot & Peters 1988)
- 3.72 (calculated, Müller & Klein 1992)
- 3.83; 4.29 (quoted; calculated-molar volume correlation, Wang et al. 1992)
- 3.83, 3.73; 3.36 (quoted, predicted; calculated-atom typing scheme, Inel & Iseri 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 6.1.6.3.1
Reported vapor pressures of 4-bromochlorobenzene at various temperatures

Stull 1947		Walsh & Smith 1961	
summary of literature data		manometry	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
32.0	133.3	21.4	22.7
59.5	666.6	24.2	33.3
72.7	1333	26.1	37.3
87.8	2666	29.0	53.3
103.8	5333	30.7	58.7
114.8	7999	35.4	96.0
128.0	13332	35.6	93.3
149.5	26664	40.5	144.0
172.6	53329	40.6	144.0
196.9	101325	44.5	200.0
		45.6	221.3
		48.9	284
		49.9	313.3
		53.0	401.3
		54.7	457.3
		57.1	545.3
		59.9	673.3
		60.7	710.6
		64.0	902.6
		64.4	911.9

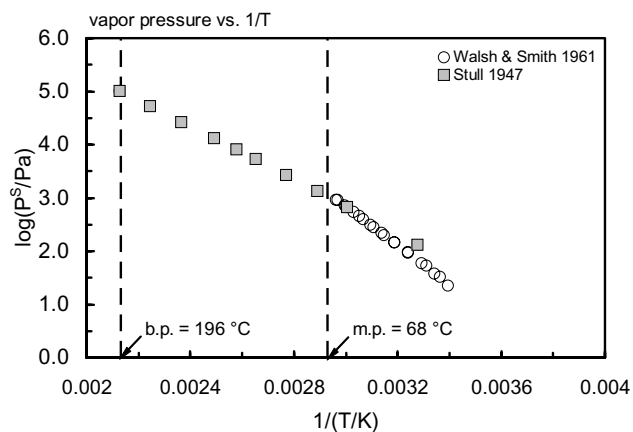
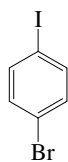


FIGURE 6.1.6.3.1 Logarithm of vapor pressure versus reciprocal temperature for 4-bromochlorobenzene.

6.1.6.4 4-Bromoiodobenzene

Common Name: 4-Bromoiodobenzene

Synonym: 4-bromo-1-iodobenzene

Chemical Name:

CAS Registry No: 589-87-7

Molecular Formula: C_6H_4BrI

Molecular Weight: 282.904

Melting Point ($^{\circ}C$):

92 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

252 (Weast 1982–83; Horvath 1982; Lide 2003)

Density (g/cm^3):

2.235 (Weast 1982–83; Horvath 1982; Lide 2003)

Molar Volume (cm^3/mol):

152.6 (calculated-Le Bas method at normal boiling point)

128.1 (Rulle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.13 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.22 (mp at $92^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

7.8 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980, Valvani & Yalkowsky 1980)

7.94 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.36 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)

4.62; 4.10 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

4.13 (calculated, Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

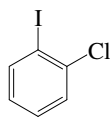
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.6.5 2-Chloriodobenzene



Common Name: 2-Chloriodobenzene

Synonym: 2-chloro-1-iodobenzene

Chemical Name:

CAS Registry No: 615-41-8

Molecular Formula: $\text{ClC}_6\text{H}_4\text{I}$

Molecular Weight: 238.453

Melting Point ($^{\circ}\text{C}$):

0.7 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

234.5 (Weast 1982–83; Horvath 1982; Lide 2003)

Density (g/cm^3):

1.9515 (Weast 1982–83; Horvath 1982)

1.9255 (20°C , Lide 2003)

Molar Volume (cm^3/mol):

150.2 (calculated-Le Bas method at normal boiling point)

134.6 (Rulle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

68.8 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

68.68 (quoted, Horvath 1982; IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.12 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)

3.98 (calculated, Müller & Klein 1992)

2.54; 3.89 (quoted; calculated-molar volume correlation, Wang et al. 1992)

4.05, 3.82 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

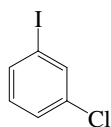
Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.6.6 3-Chloriodobenzene

Common Name: 3-Chloriodobenzene

Synonym: 3-chloro-1-iodobenzene

Chemical Name:

CAS Registry No: 625-99-0

Molecular Formula: $\text{ClC}_6\text{H}_4\text{I}$

Molecular Weight: 238.453

Melting Point ($^{\circ}\text{C}$):

Boiling Point ($^{\circ}\text{C}$):

230 (Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.9515 (25°C , Weast 1982–83)

1.9255 (20°C , Horvath 1982)

Molar Volume (cm^3/mol):

150.2 (calculated-Le Bas method at normal boiling point)

124.9 (Rulle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C , F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

68.8 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

67.4 (quoted, Horvath 1982; IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

4.12 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky 1980)

4.05, 3.82 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

3.98 (calculated, Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

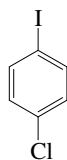
Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.1.6.7 4-Chloriodobenzene



Common Name: 4-Chloriodobenzene

Synonym: 4-chloro-1-iodobenzene

Chemical Name:

CAS Registry No: 637-87-6

Molecular Formula: $\text{ClC}_6\text{H}_4\text{I}$

Molecular Weight: 238.453

Melting Point ($^{\circ}\text{C}$):

57 (Weast 1982–83; Horvath 1982; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

227 (Weast 1982–83; Horvath 1982; Lide 2003)

Density (g/cm^3):

1.886 (57°C , Weast 1982–83; Horvath 1982)

Molar Volume (cm^3/mol):

122 (calculated-density, Lande & Banerjee 1981)

126.4 (Stephenson & Malanowski 19987; Rulle & Kesselring 1997)

127 (Wang et al. 1992)

150.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F: 0.4825)

Water Solubility (g/m^3 or mg/L at 25°C):

22.5 (shake flask-UV, Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

31.11 (quoted, IUPAC Solubility Data Series, Horvath & Getzen 1985)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

16.26 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 8.944 - 3200/(T/\text{K})$; temp range 303–323 K (Antoine eq.-I, solid state, Stephenson & Malanowski 1987)

$\log (P_l/\text{kPa}) = 5.63678 - 1465.651/(T/\text{K} - 102.487)$; temp range 333–500 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C): k'

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.12 (calculated-fragment const., Yalkowsky et al. 1979, Valvani & Yalkowsky)

4.06 (HPLC- k' correlation, Hanai et al. 1981)

3.98 (calculated, Müller & Klein 1992)

4.47 (calculated-molar volume correlation, Wang et al. 1992)

4.34; 3.82 (predicted; calculated-atom typing scheme, Onel & Iseri 1997)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

6.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 6.2.1

Summary of physical properties of chlorobenzenes and other halogenated mononuclear aromatics

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/cm³ at 20°C	Molar volume, V _M cm³/mol	
								from ρ ^(a)	Le Bas
Chlorobenzenes:									
Chlorobenzene	108-90-7	C ₆ H ₅ Cl	112.557	−45.31	131.72	1	1.1058	101.79	116.9
1,2-Dichloro-	95-50-1	C ₆ H ₄ Cl ₂	147.002	−17.0	180	1	1.3059	112.57	137.9
1,3-Dichloro-	541-73-1	C ₆ H ₄ Cl ₂	147.002	−24.8	173	1	1.2884	114.10	137.8
1,4-Dichloro-	106-46-7	C ₆ H ₄ Cl ₂	147.002	53.09	174	0.530	1.2457	118.01	137.8
1,2,3-Trichloro-	87-61-6	C ₆ H ₃ Cl ₃	181.447	51.3	218.5	0.552		125‡	158.7
1,2,4-Trichloro-	120-82-1	C ₃ H ₃ Cl ₃	181.447	16.92	213.5	1	1.4542	124.77	158.7
1,3,5-Trichloro-	108-70-3	C ₆ H ₃ Cl ₃	181.447	62.8	208	0.426		125‡	158.7
1,2,3,4-Tetrachloro-	634-66-2	C ₆ H ₂ Cl ₄	215.892	47.5	254	0.602		142‡	179.6
1,2,3,5-Tetrachloro-	634-90-2	C ₆ H ₂ Cl ₄	215.892	54.5	246	0.514		142‡	179.6
1,2,4,5-Tetrachloro-	95-94-3	C ₆ H ₂ Cl ₄	215.892	139.5	244.5	0.0753		142‡	179.6
Pentachlorobenzene	608-93-5	C ₆ HCl ₅	250.337	86	277	0.252		166‡	200.5
Hexachlorobenzene	118-74-1	C ₆ Cl ₆	284.782	228.83	325	0.0100		186‡	221.4
Chlorotoluenes:									
2-Chlorotoluene	95-49-8	C ₇ H ₇ Cl	126.584	−35.8	159.0	1	1.0825	116.94	139.1
3-Chlorotoluene	108-41-8	C ₇ H ₇ Cl	126.584	−47.8	161.8	1	1.0722	118.06	139.1
4-Chlorotoluene	106-43-4	C ₇ H ₇ Cl	126.584	7.5	162.4	1	1.0697	118.34	139.1
2,4-Dichlorotoluene	95-73-8	C ₇ H ₆ Cl ₂	161.029	−13.5	201	1	1.2476	129.07	160.0
2,6-Dichlorotoluene	118-69-4	C ₇ H ₆ Cl ₂	161.029	25.8	198	1	1.2686	126.93	160.0
3,4-Dichlorotoluene	95-75-0	C ₇ H ₆ Cl ₂	161.029	−15.2	208.9	1	1.2564	128.17	160.0
2,3,6-Trichlorotoluene	2077-46-5	C ₇ H ₅ Cl ₃	195.474	45.5	229.5	0.629			180.9
2,4,5-Trichlorotoluene	6639-30-1	C ₇ H ₅ Cl ₃	195.474	82.4	231	0.273			180.9
α-Chlorotoluene	100-44-7	C ₇ H ₇ Cl	126.584	−45	179	1	1.1004	115.03	139.1
α, α, α-Trichlorotoluene	98-07-7	C ₇ H ₅ Cl ₃	195.474	−4.42	221	1	1.3723	142.44	180.9
Pentachlorotoluene	877-11-2	C ₇ H ₃ Cl ₅	264.364	224.8	301	0.0110			222.7
o-Chlorostyrene	2039-87-4	C ₈ H ₇ Cl	138.595	−63.1	188.7	1	1.1000	126.00	153.9
m-Chlorostyrene	2039-85-2	C ₈ H ₇ Cl	138.595				1.1033	125.62	153.9
p-Chlorostyrene	1073-67-2	C ₈ H ₇ Cl	138.595	15.9	192	1	1.0868	127.53	153.9
Octachlorostyrene	29082-74-4	C ₈ Cl ₈	379.710	99		0.188			300.2

(Continued)

TABLE 6.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/cm³ at 20°C	Molar volume, V _M cm³/mol	
								from ρ ^(a)	Le Bas
Fluorobenzenes:									
Fluorobenzene	462-06-6	C ₆ H ₅ F	96.102	-42.18	84.73	1	1.0225	93.99	101.0
1,2-Difluorobenzene	367-11-3	C ₆ H ₄ F ₂	114.093	-47.1	94	1	1.158	98.53	106.0
1,3-Difluorobenzene	372-18-9	C ₆ H ₄ F ₂	114.093	-69.12	82.6	1	1.1572	98.59	106.0
1,4-Difluorobenzene	540-36-3	C ₆ H ₄ F ₂	114.093	-23.55	89	1	1.1701	97.51	106.0
1,2,4-Trifluorobenzene	367-23-7	C ₆ H ₃ F ₃	132.083		90	1			111.0
1,3,5-Trifluorobenzene	372-38-3	C ₆ H ₃ F ₃	132.083	-5.5	75.5	1		103.4†	111.0
1,2,3,4-Tetrafluorobenzene	551-62-2	C ₆ H ₂ F ₄	150.074		94.3	1		105.5†	116.0
1,2,3,5-Tetrafluorobenzene	2367-82-0	C ₆ H ₂ F ₄	150.074	-46.25	84.4	1		107.7†	116.0
1,2,4,5-Tetrafluorobenzene	327-54-8	C ₆ H ₂ F ₄	150.074	3.88	90.2	1	1.4255	105.28	116.0
Pentafluorobenzene	363-72-4	C ₆ HF ₅	168.064	-47.4	85.74	1		111.0†	121.0
Hexafluorobenzene	392-56-3	C ₆ F ₆	180.054	5.03	80.26	1	1.6184	111.25	126.0
Pentafluorotoluene	771-56-2	C ₇ H ₃ F ₅	182.091	-29.78	117.5	1	1.440	126.45	143.2
Chloropentafluorobenzene	344-07-0	C ₆ ClF ₅	202.509		117.96				141.9
Pentafluorophenol	771-61-9	C ₆ HF ₅ O	184.063	37.5	145.6	0.754			128.4
Bromobenzenes and bromotoluenes:									
Bromobenzene	108-86-1	C ₆ H ₅ Br	157.008	-30.72	156.06	1	1.4950	105.02	119.3
1,2-Dibromobenzene	583-53-9	C ₆ H ₄ Br ₂	235.904	7.1	225	1	1.9843	118.89	142.6
1,3-Dibromobenzene	108-36-1	C ₆ H ₄ Br ₂	235.904	-7.0	218	1	1.9523	120.83	142.6
1,4-Dibromobenzene	106-37-6	C ₆ H ₄ Br ₂	235.904	87.43	218.5	0.244	1.5742	149.86	142.6
1,2,3-Tribromobenzene	608-21-9	C ₆ H ₃ Br ₃	314.800	87.8		0.242	2.6580	118.43	165.9
1,2,4-Tribromobenzene	615-54-3	C ₆ H ₃ Br ₃	314.800	44.5	275	0.644			165.9
1,3,5-Tribromobenzene	626-39-1	C ₆ H ₃ Br ₃	314.800	122.8	271	0.110			165.9
1,2,4,5-Tetrabromobenzene	636-28-2	C ₆ H ₂ Br ₄	393.696	182		0.0288	3.0720	128.16	189.2
Hexabromobenzene	87-82-1	C ₆ Br ₆	551.488	327		0.0011			235.8
2-Bromotoluene	95-46-5	C ₇ H ₇ Br	171.035	-27.8	181.7	1	1.4232	120.18	141.5
3-Bromotoluene	591-17-3	C ₇ H ₇ Br	171.035	-39.8	183.7	1	1.4099	121.31	141.5
4-Bromotoluene	106-38-7	C ₇ H ₇ Br	171.035	28.5	184.3	1			141.5
Iodobenzenes:									
Iodobenzene	591-50-4	C ₆ H ₅ I	204.008	-31.3	188.4	1	1.8308	111.43	129.3
1,2-Diiodobenzene	615-42-9	C ₆ H ₄ I ₂	329.905	27	287	0.956	2.5400	129.88	162.6
1,3-Diiodobenzene	626-00-6	C ₆ H ₄ I ₂	329.905	40.4	285	0.706			162.6
1,4-Diiodobenzene	624-38-4	C ₆ H ₄ I ₂	329.905	131.5	285	0.0902			162.6

1,2,3-Triiodobenzene	608-29-7	C ₆ H ₃ I ₃	455.801	166	sublim	0.0410		141§	195.9
1,2,4-Triiodobenzene	615-68-9	C ₆ H ₃ I ₃	455.801	91.5	sublim	0.223		145§	195.9
1,3,5-Triiodobenzene	626-44-8	C ₆ H ₃ I ₃	455.801	184.2	sublim	0.0274		131§	195.9
Mixed halogenated benzenes:									
2-Bromochlorobenzene	694-80-4	C ₆ H ₄ BrCl	191.453	-12.3	204	1		117§	140.2
3-Bromochlorobenzene	108-37-2	C ₆ H ₄ BrCl	191.453	-21.5	196	1	1.5771	121.40	140.2
4-Bromochlorobenzene	106-39-8	C ₆ H ₄ BrCl	191.453	68	196	0.379		121.5†	140.2
4-Bromoiodobenzene	589-87-7	C ₆ H ₄ BrI	282.904	92	252	0.220	2.2350	126.58	152.6
2-Chloroiodobenzene	615-41-8	ClC ₆ H ₄ I	238.453	0.7	234.5	1	1.9255	123.84	150.2
3-Chloroiodobenzene	625-99-0	ClC ₆ H ₄ I	238.453		230	1	1.9255	123.84	150.2
4-Chloroiodobenzene	637-87-6	ClC ₆ H ₄ I	238.453	57	227	0.485		127§	150.2

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$

(a) † Chiou 1985 (liquid molar volume), ‡ Stephenson & Malanowski 1987, §Wang et al. 1992, and calculated as MW/p at 20°C for this work

TABLE 6.2.2

Summary of selected physical-chemical properties of chlorobenzenes and other halogenated mononuclear aromatics at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m ³ /mol) calculated P/C
	Vapor pressure		Solubility			log K _{OW}	
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		
Chlorobenzenes:							
Chlorobenzene	1580	1580	484	4.3000	4.2300	2.80	367
1,2-Dichloro-	170	170	140	0.9523	0.9523	3.40	178
1,3-Dichloro-	260	260	120	0.8163	0.8163	3.40	318
1,4-Dichloro-	130	245	80	0.544	1.0268	3.40	242
1,2,3-Trichloro-	28	50.72	21	0.1157	0.2100	4.10	242
1,2,4-Trichloro-	40	40	40	0.2204	0.2204	4.10	277
1,3,5-Trichloro-	25	78.05	5.3	0.0292	0.0686	4.10	856
1,2,3,4-Tetrachloro-	4.0	6.64	7.8	0.0361	0.0600	4.50	111
1,2,3,5-Tetrachloro-	9.8	19.01	3.6	0.0167	0.0324	4.50	588
1,2,4,5-Tetrachloro-	0.72	9.56	1.27	0.00588	0.0781	4.50	122
Pentachlorobenzene	0.22	0.8730	0.65	0.00260	0.0103	5.00	85
Hexachlorobenzene	0.0023	0.23	0.005	0.0000176	0.00176	5.50	131

TABLE 6.2.3

Suggested half-life classes of chlorobenzenes and other halogenated mononuclear aromatics in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Chlorobenzene	4	6	7	8
1,2-Dichloro-	5	6	7	8
1,3-Dichloro-	5	6	7	8
1,4-Dichloro-	5	6	7	8
1,2,3-Trichloro-	5	6	7	8
1,2,4-Trichloro-	5	6	7	8
1,3,5-Trichloro-	5	6	7	8
1,2,3,4-Tetrachloro-	6	7	7	8
1,2,3,5-Tetrachloro-	6	7	7	8
1,2,4,5-Tetrachloro-	6	7	7	8
Pentachlorobenzene	7	8	8	8
Hexachlorobenzene	8	9	9	9
Fluorobenzene	4	5	6	7
Bromobenzene	4	6	7	8
Iodobenzene	4	6	7	8

where,

Class	Mean half-life (hours)	Range (hours)
1	5	<10
2	17 (~1 day)	10–30
3	55 (~2 days)	30–100
4	170 (~1 week)	100–300
5	550 (~3 weeks)	300–1,000
6	1,700 (~2 months)	1,000–3,000
7	5,500 (~8 months)	3,000–10,000
8	17,000 (~2 years)	10,000–30,000
9	55,000 (~6 years)	>30,000

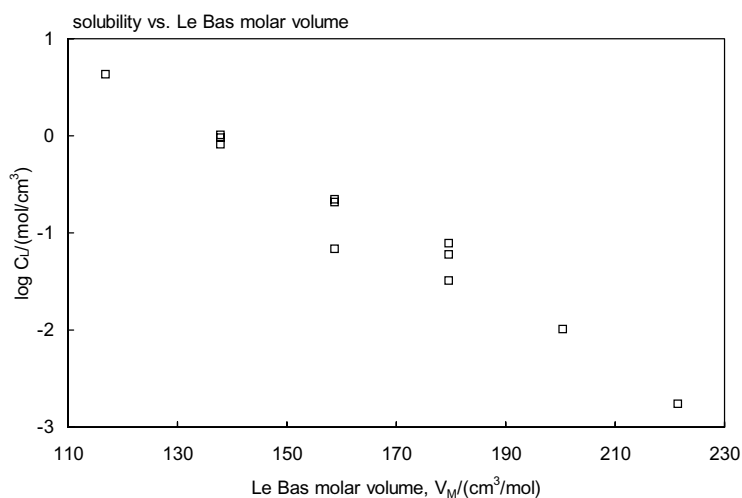


FIGURE 6.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for chlorobenzenes.

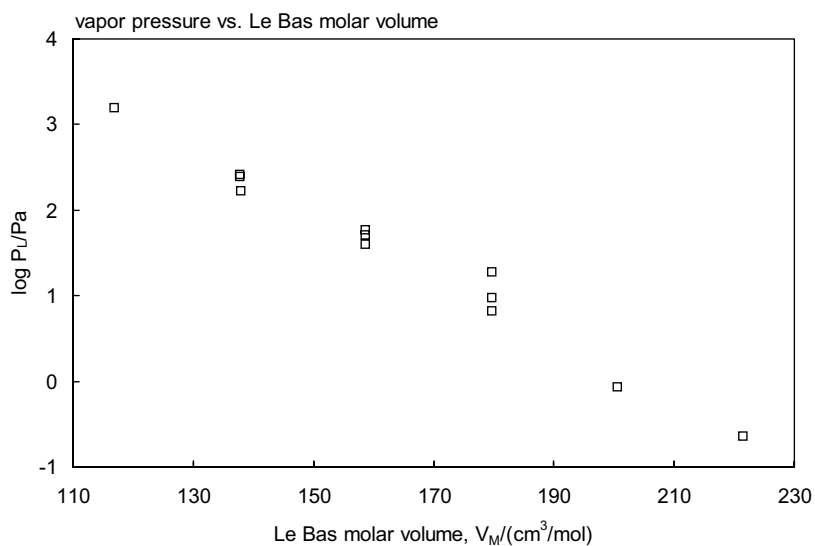


FIGURE 6.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for chlorobenzenes.

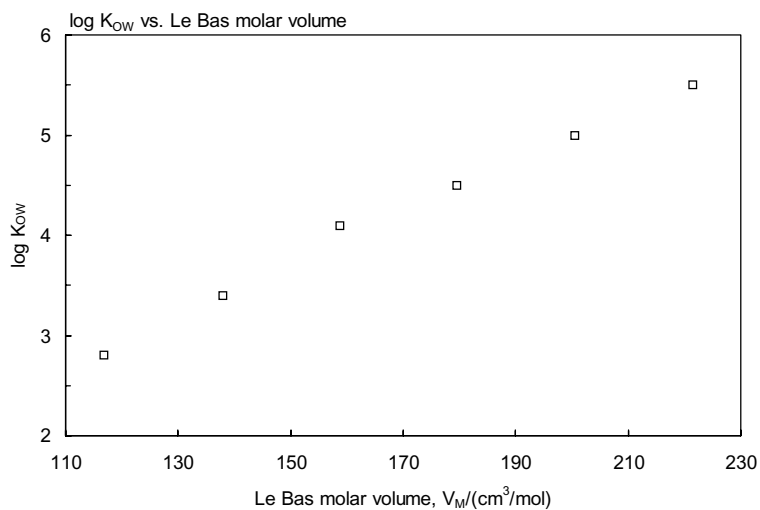


FIGURE 6.2.3 Octanol-water partition coefficient versus Le Bas molar volume for chlorobenzenes.

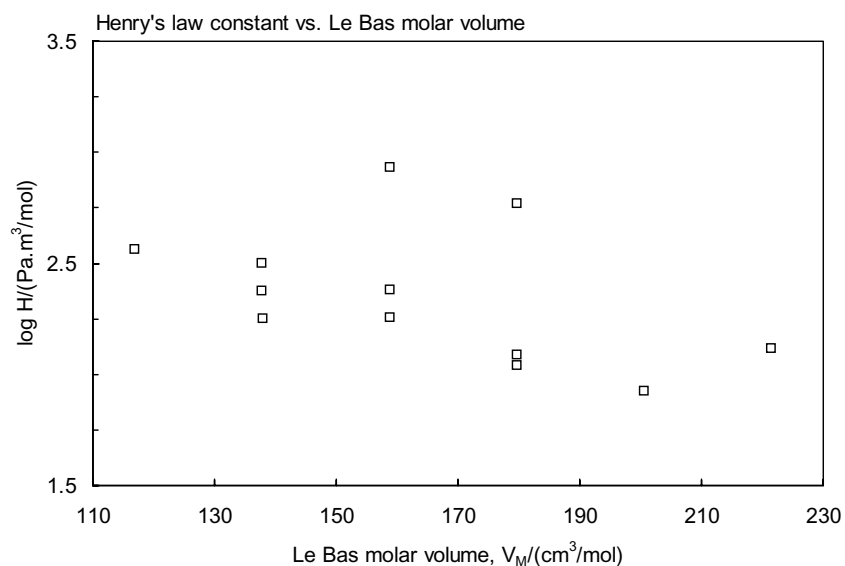


FIGURE 6.2.4 Henry's law constant versus Le Bas molar volume for chlorobenzenes.

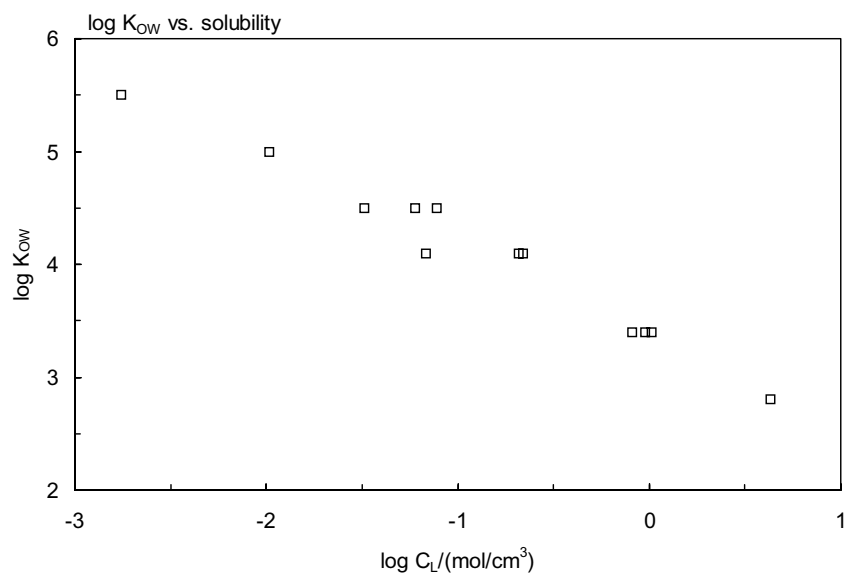


FIGURE 6.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) chlorobenzenes.

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7 Polychlorinated Biphenyls (PCBs)

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7.1.1.187	2,2',3,4',5,5',6-Heptachlorobiphenyl (PCB-187)	1947
7.1.1.188	2,2',3,4',5,6,6'-Heptachlorobiphenyl (PCB-188)	1950
7.1.1.189	2,3,3',4,4',5,5'-Heptachlorobiphenyl (PCB-189)	1952
7.1.1.190	2,3,3',4,4',5,6-Heptachlorobiphenyl (PCB-190)	1954
7.1.1.191	2,3,3',4,4',5',6-Heptachlorobiphenyl (PCB-191)	1956
7.1.1.192	2,3,3',4,5,5',6-Heptachlorobiphenyl (PCB-192)	1958
7.1.1.193	2,3,3',4',5,5',6-Heptachlorobiphenyl (PCB-193)	1960
7.1.1.194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl (PCB-194)	1962
7.1.1.195	2,2',3,3',4,4',5,6-Octachlorobiphenyl (PCB-195)	1965
7.1.1.196	2,2',3,3',4,4',5,6'-Octachlorobiphenyl (PCB-196)	1967
7.1.1.197	2,2',3,3',4,4',6,6'-Octachlorobiphenyl (PCB-197)	1969
7.1.1.198	2,2',3,3',4,5,5',6-Octachlorobiphenyl (PCB-198)	1971
7.1.1.199	2,2',3,3',4,5,5',6'-Octachlorobiphenyl (PCB-199)	1973
7.1.1.200	2,2',3,3',4,5,6,6'-Octachlorobiphenyl (PCB-200)	1975
7.1.1.201	2,2',3,3',4,5',6,6'-Octachlorobiphenyl (PCB-201)	1977
7.1.1.202	2,2',3,3',5,5',6,6'-Octachlorobiphenyl (PCB-202)	1979
7.1.1.203	2,2',3,4,4',5,5',6-Octachlorobiphenyl (PCB-203)	1983

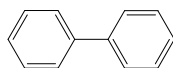
7.1.1.204	2,2',3,4,4',5,6,6'-Octachlorobiphenyl (PCB-204)	1985
7.1.1.205	2,3,3',4,4',5,5',6-Octachlorobiphenyl (PCB-205)	1987
7.1.1.206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl (PCB-206)	1989
7.1.1.207	2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl (PCB-207)	1991
7.1.1.208	2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl (PCB-208)	1993
7.1.1.209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl (PCB-209)	1995
7.1.2	Isomer groups	1999
7.1.2.1	Monochlorobiphenyl	1999
7.1.2.2	Dichlorobiphenyl	2001
7.1.2.3	Trichlorobiphenyl	2003
7.1.2.4	Tetrachlorobiphenyl	2005
7.1.2.5	Pentachlorobiphenyl	2007
7.1.2.6	Hexachlorobiphenyl	2009
7.1.2.7	Heptachlorobiphenyl	2011
7.1.2.8	Octachlorobiphenyl	2013
7.1.2.9	Nonachlorobiphenyl	2014
7.1.3	Aroclor mixtures	2015
7.1.3.1	Aroclor 1016	2015
7.1.3.2	Aroclor 1221	2017
7.1.3.3	Aroclor 1232	2019
7.1.3.4	Aroclor 1242	2021
7.1.3.5	Aroclor 1248	2024
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7.1 LIST OF CHEMICALS AND DATA COMPILATIONS

7.1.1 PCB CONGENERS

7.1.1.0 Biphenyl

(See also [Chapter 4](#), Polynuclear Aromatic Hydrocarbons [PAHs] and Related Aromatic Hydrocarbons)



Common Name: Biphenyl

Synonym: diphenyl, phenylbenzene

Chemical Name: biphenyl

CAS Registry No: 92-52-4

Molecular Formula: $C_{12}H_{10}$

Molecular Weight: 154.207

Melting Point ($^{\circ}C$):

68.93 (Lide 2003)

Boiling Point ($^{\circ}C$):

256.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.866 ($20^{\circ}C$, Weast 1982–1983)

1.04 (Lide 2003)

Molar Volume (cm^3/mol):

148.3 ($20^{\circ}C$, calculated-density)

184.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.58 (Parks & Huffman 1931)

18.66 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

51.05 (Miller et al. 1984)

54.81, 59.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.371 (mp at $68.93^{\circ}C$)

0.35 (Mackay et al. 1980,1983; Shiu & Mackay 1986; Shiu et al. 1987)

0.381 (calculated, $\Delta S_{fus} = 54 J/mol K$, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5.94 (shake flask-UV, Andrews & Keefer 1949)

7.48* (shake flask-UV, measured range 0.4 – $42.8^{\circ}C$, Bohon & Claussen 1951)

3.87 (shake flask-UV, Sahyun 1966)

7.08* (shake flask-UV, measured range 0 – $64.5^{\circ}C$, Wauchope & Getzen 1972)

$R \cdot \ln x = -4520/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 298.15]^2 - 20.8 + 0.0273 \cdot (T/K)$, temp range 24.6 – $73.4^{\circ}C$ (shake flask-UV measurements, Wauchope & Getzen 1972)

7.45 (shake flask-GC, Eganhouse & Calder 1976)

7.0 (shake flask-fluorescence, Mackay & Shiu 1977)

8.50 (shake flask-nephelometry, Hollifield 1979)

7.51 (shake flask-LSC, Banerjee et al. 1980)

8.09 (TLC-RT correlation, Bruggeman et al. 1982)

6.71 (generator column-GC/ECD, Miller et al. 1984, 1985; quoted, Hawker 1989b)

7.09 (recommended, Pearlman et al. 1984)

7.05 (vapor saturation-UV, Akiyoshi et al. 1987)

6.5 ($29^{\circ}C$, shake flask-GC/FID; Stucki & Alexander 1987)

7.20, 7.55 (generator column-HPLC/UV, Billington et al. 1988)

9.96, 9.96, 9.96, 10.67 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.2* (recommended, IUPAC Solubility Data Series, Shaw 1989)

$\log [S_L/(\text{mol/L})] = 1.872 - 973.4/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -1.5792 - 3669.26/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

5.37, 5.32 (generator column-GC/ECD, different flow rates, Oleszek-Kudlak et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7933* (162.5°C, isoteniscope-manometer, measured range 162.5–255.2°C, Chipman & Peltier 1929)

104* (69.20°C, temp range 69.20–271.2°C, Cunningham 1930; quoted, Boublik et al. 1984)

133.3* (70.6°C, summary of literature data, temp range 70.6–254.0°C, Stull 1947)

1.30 (effusion method, measured range 4.0–34.5°C, Bright 1951)

$\log (P/\text{mmHg}) = 10.38 - 3799/(T/K)$; temp range: 4.0–34.5°C (Antoine eq., effusion, Bright 1951)

0.031 (manometry, Augood et al. 1953; selected, Bidleman 1984)

1.273* (effusion method, measured range 15.05–40.55°C, Bradley & Cleasby 1953)

$\log (P/\text{cmHg}) = 11.282 - 4263/(T/K)$; temp range 15.05–40.55°C (Antoine eq., Bradley & Cleasby 1953)

$\log (P/\text{mmHg}) = [-0.2185 \times 12910.0/(T/K)] + 8.218583$; temp range 70.6–254.9°C (Antoine eq., Weast 1972–73)

1.41* (effusion method, interpolated-Antoine eq., measured range 24.9–50.33°C, Radchenko & Kitiagorodskii 1974)

$\log (P/\text{mmHg}) = 12.6789 - 4367.436/(T/K)$; temp range; 24.9–50.33°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)

2040* (123.0°C, pressure transducer, measured range 123.0–327.55°C, Nasir et al. 1980)

1.40 (HPLC-RT correlation, Swann et al. 1983)

$\log (P/\text{atm}) = [1 - 528.437/(T/K)] \times 10^4 \{0.821410 - 2.73337 \times 10^{-4} \cdot (T/K) + 1.02285 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 342.35–673.15 K (Cox eq., Chao et al. 1983)

3.35, 3.41 (P_{GC} by GC-RT correlation, different GC columns, Bidleman 1984)

5.608 (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)

$\log (P/\text{kPa}) = 6.36895 - 1997.558/(202.608 + t/^\circ\text{C})$, temp range: 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.15* (24.7°C, gas saturation-GC/FID, measured range 5.2–24.7°C, Burkhard et al. 1984)

$\log (P/\text{Pa}) = 14.840 - 4402.1/(T/K)$, temp range: 5.2–24.7°C (gas saturation data, Clapeyron eq., Burkhard et al. 1984)

2.03 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

$\log (P/\text{mmHg}) = 7.24541 - 1998.725/(202.733 + t/^\circ\text{C})$, temp range: 69–271°C (Antoine eq., Dean 1985, 1992)

5.61; 6.62 (supercooled liquid P_L , quoted lit.; GC-RT correlation, Foreman & Bidleman 1985)

2.43; 6.90 (selected P_S ; supercooled liq. P_L , Shiu & Mackay 1986; Shiu et al. 1987; Sklarew & Girvin 1987)

1.443; 1.23 (P_S , interpolated-Antoine equations; Stephenson & Malanowski 1987)

$\log (P_S/\text{kPa}) = 11.71929 - 4143.054/(T/K)$; temp range 297–324 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_S/\text{kPa}) = 28.5175 - 21141.5/(374.85 + T/K)$; temp range: 283–342 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.37526 - 1794.8/(-74.85 + T/K)$, temp range: 390–563 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

5.10, 5.00 (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)

3.35 (P_{GC} by GC-RT correlation, Hinckley et al. 1990)

0.422–2.54; 2.03–7.04 (quoted range of lit. P_S values; lit. P_L values, Delle Site 1997)

5.31; 2.02 (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/\text{Pa}) = 11.05 - 3201/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 8.20 - 2228/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P/\text{kPa}) = 14.840 - 4402.1/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

3.63; 0.822 (supercooled liquid P_L , calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

$\log (P_L/\text{Pa}) = -3265/(T/K) + 11.51$; $\Delta H_{vap} = -62.5 \text{ kJ}\cdot\text{mol}^{-1}$ (GC-RT correlation, Lei et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 41.34 (batch stripping-GC, Mackay et al. 1979)
- 30.4 (batch stripping-GC, Mackay et al. 1980;)
- 11.55 (gas stripping-GC, Warner et al. 1987)
- 19.57 (wetted-wall column-GC, Fendinger & Glotfelty 1990)
- 31.20 (gas stripping-GC, Shiu & Mackay 1997)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 6.33 - 1255/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.16 (shake flask-UV, Rogers & Cammarata 1969)
- 4.09 (shake flask, Leo et al. 1971; Hansch & Leo 1979)
- 4.04 (shake flask, Hansch et al. 1973)
- 4.17, 4.09, 3.16, 4.04 (Neely et al. 1974; Hansch & Leo 1979)
- 3.95 (HPLC- k' correlation, Rekker & De Kort 1979)
- 3.75 (HPLC-RT correlation, Veith et al. 1979a)
- 4.04 (shake flask-HPLC, Banerjee et al. 1980)
- 3.88 (lit. average, Kenaga & Goring 1980)
- 4.10 (RP-TLC- k' correlation, Bruggeman et al. 1982)
- 4.08 (HPLC- k' correlation, Hammers et al. 1982)
- 3.70 (HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)
- 3.16–4.09, 3.91 (shake flask, range, average, Eadsforth & Moser, 1983)
- 3.91–4.15, 4.05 (HPLC, range, average, Eadsforth & Moser 1983)
- 4.03 (HPLC- k' correlation, Hafkenscheid & Tomlinson 1983)
- 3.93 (HPLC correlation; Harnisch et al. 1983)
- 3.76 (generator column-GC/ECD, Miller et al. 1984,1985)
- 3.89 (generator column-HPLC, Woodburn et al. 1984)
- 3.79 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 4.11–4.13 (HPLC-RV correlation, quoted exptl., Garst 1984)
- 4.10 (HPLC-RV correlation, Garst & Wilson 1984)
- 4.05 (HPLC-RT correlation, Eadsforth 1986)
- 3.81 (shake flask-GC, Menges & Armstrong 1986)
- 4.13 (HPLC-RT correlation, Wang et al. 1991)
- 3.63 (HPLC- k' correlation; De Kock & Lord 1987)
- 3.89 (generator column-GC, Doucette & Andren 1987,1988)
- 4.14, 4.06, 4.00, 3.94 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 3.69 (HPLC-RT correlation, Doucette & Andren 1988)
- 3.75 (HPLC-RT correlation, Sherblom & Eganhouse 1988)
- 4.008; 4.10 (slow stirring-GC; calculated- π const., De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 3.98 (recommended, Sangster 1989, 1993)
- 4.29 (dual-mode centrifugal partition chromatography, Gluck & Martin 1990)
- 4.26 (HPLC- k' correlation, Noegrohati & Hammers 1992)
- 4.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 6.92, 6.09; 6.09 (0, 20°C , multi-column GC- k' correlation; calculated at 20°C , Zhang et al. 1999)
- 6.15 (calculated- S_{oct} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 2.64 (trout, calculated- k_1/k_2 , Neely et al. 1974)
- 3.12 (rainbow trout, Veith et al. 1979; Veith & Kosian 1983)
- 2.53 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 2.73, 2.45, 3.41 (algae, fish, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC} :

- 3.15 (soil, Kenaga 1980)
 3.0, 3.27 (Aldrich humic acid, reversed phase separation, Landrum et al. 1984)
 3.57, 3.77 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with 9.6 mg/L DOC, Landrum et al. 1984)
 5.58, 4.04 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 mg/L DOC, Landrum et al. 1984)
 5.68, 5.34, 5.23, 3.57 (humic materials in natural water: Huron River 6.7% DOC spring, Grand River 10.7% DOC spring, Lake Michigan 4.7% DOC spring, Lake Erie 9.6% DOC spring, RP-HPLC separation method, Landrum et al. 1984)
 3.52, 2.94 (Apison soil 0.11% OC, Dormont soil 1.2% OC, batch equilibrium, Southworth & Keller 1986)
 3.40 (calculated, soil, Chou & Griffin 1986)
 3.04, 3.32, 3.26, 3.04, 3.08 (5 soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
 4.20; 3.30 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
 3.03, 3.12 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average values, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization/Evaporation: $t_{1/2} = 7.52$ d evaporation from water depth of 1 m (Mackay & Leinonen 1975)
 rate of volatilization $k = 0.92 \text{ g m}^{-2} \text{ h}^{-1}$ (Mackay 1986; Metcalfe et al. 1988).
 Photolysis: $k = 5.1 \times 10^{-4} \text{ h}^{-1}$ to $7.4 \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO^- in the gas (Dilling et al. 1988);
 photodegradation $k = 5.1 \times 10^{-4} \text{ min}^{-1}$ and $t_{1/2} = 22.61$ h in methanol-water (3:7, v/v) with initial concentration of 16.2 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991).
 Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH} = (8.06 \pm 0.77) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated lifetime of ~ 3 d, and $k_{O_3} < 2.0 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 ± 1 K (relative rate method, Atkinson et al. 1984)
 $k_{OH} = (8.5 \pm 0.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1985)
 $k_{OH} = (7 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)
 $k_{OH}(\text{calc}) = 7.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = (5.8 - 8.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 3 d (Atkinson 1987a)
 $k_{OH}(\text{calc}) = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (SAR structure-activity relationship, Atkinson 1987b)
 $k_{O_3} < 2 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH} = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{N_2O_5} < 2.0 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with N_2O_5 at room temp (Atkinson & Aschmann 1988)
 $k_{OH}^* = 7.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)
 $k_{OH}(\text{calc}) = 6.44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)
 $k_{OH}(\text{exptl}) = 7.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 6.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 2.0 d (Kwok et al. 1995)

Hydrolysis:

- Biodegradation: 100% degraded by activated sludge in 47 h cycle (Monsanto Co. 1972)
 $k = 109 \text{ yr}^{-1}$ in the water column and $k = 1090 \text{ yr}^{-1}$ in the sediment, microbial degradation pseudo first-order rate constant (Wong & Kaiser 1975; selected, Neely 1981)
 $k = 9.3\text{--}9.8 \text{ nmol L}^{-1} \text{ d}^{-1}$ with an initial biphenyl concentration of $4.4\text{--}4.7 \text{ } \mu\text{mol/L}$, and $k = 3.2 \text{ nmol L}^{-1} \text{ d}^{-1}$ with initial concentration of $2.9 \text{ } \mu\text{mol/L}$, rate of biodegradation in water from Port Valdez (estimated, Reichardt et al. 1981)
 $t_{1/2} = 1.5$ d, estimated by using water die-away test (Bailey et al. 1983)
 $t_{1/2}(\text{aq. aerobic}) = 36\text{--}168$ h, based on river die-away test data and activated sludge screening test data (Howard et al. 1991)
 $t_{1/2}(\text{aq. anaerobic}) = 144\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

removal rate of 5.3 and 0.52 mg (g of volatile suspended solid d)⁻¹, degradation by bacteria from creosote-contaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne & Strand 1998)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 6.79 \text{ h}^{-1}$; $k_2 = 0.0155 \text{ h}^{-1}$ (trout muscle, Neely et al. 1974; Neely 1979)

$k_1 = 6.8 \text{ h}^{-1}$; $1/k_2 = 65 \text{ h}$ (trout, quoted, Hawker & Connell 1985)

$\log k_1 = 2.21 \text{ d}^{-1}$; $\log 1/k_2 = 0.43 \text{ d}$ (fish, Connell & Hawker 1988)

$\log k_2 = -0.43 \text{ d}^{-1}$ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air: calculated lifetime of ~3 d due to reaction with OH radical, assuming an average daytime atmospheric OH radical concn of $\sim 1 \times 10^6 \text{ molecule/cm}^3$ (Atkinson et al. 1984);

estimated atmospheric lifetime of ~2.7 d due to reaction with the OH radical for a 24-h average OH radical concn of $5 \times 10^5 \text{ cm}^{-3}$ (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 9 d due to the rate constants of gas-phase reaction with OH radical (Atkinson 1987);

$t_{1/2} = 7.8\text{--}110 \text{ h}$, based on photooxidation half-life in air (Howard et al. 1991);

tropospheric lifetime of 2.0 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for biphenyl (Kwok et al. 1995).

Surface water: $t_{1/2} \sim 1.5 \text{ d}$ in river water (Bailey et al. 1983);

$t_{1/2} = 36\text{--}168 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
photolysis $t_{1/2} = 19.18 \text{ min}$ in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2} = 72\text{--}336 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 36\text{--}168 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota: estimated $t_{1/2} = 29 \text{ h}$ from fish in simulated ecosystem (Neely 1980).

TABLE 7.1.1.0.1

Reported aqueous solubilities of biphenyl at various temperatures:

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
			experimental		smoothed		
0.40	2.83	24.6	7.13	0	2.64	0	2.72
2.4	2.97	24.6	7.29	24.6	6.96	10	4.1
5.2	3.38	24.6	7.35	25	7.08	20	6.3
7.6	3.64	29.9	8.77	29.9	8.73	25	7.2
10	4.06	29.9	8.64	30.3	8.88	30	9.1
12.6	4.58	29.9	8.95	38.4	12.7	40	14.4
14.9	5.11	30.3	8.55	40.1	13.8	50	22
15.9	5.27	30.3	8.54	47.5	19.5	69	37
25	7.48	30.3	8.48	50	22.0		
25.6	7.78	38.4	13.2	50.1	22.1		
30.1	9.64	38.4	13.3	50.2	22.2		
30.4	9.58	38.4	13.5	54.7	27.7		
33.3	11.0	40.1	13.1	59.2	34.8		
34.9	11.9	40.1	13.4	60.5	37.2		
36	12.5	40.1	13.4	64.5	45.9		
42.8	17.2	47.5	18.8				
		47.5	19.0	temp dependence eq. 1			

TABLE 7.1.1.0.1 (Continued)

Bohon & Claussen 1951		Wauchope & Getzen 1972				Shaw 1989	
shake flask-UV		shake flask-UV				IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
for supercooled liquid:		47.5	18.7	ln x	mole fraction		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) =$		50.1	20.6	ΔH_{fus}	18.9 ± 0.50		
at 275 K	7.03	50.1	21.6	10 ² ·b	2.73 ± 0.12		
280 K	10.13	50.1	21.8	c	20.8 ± 0.4		
285 K	11.25	50.2	20.7				
290 K	12.55	50.2	21.8				
295 K	13.43	54.7	28.3				
300 K	15.02	54.7	28.8				
305 K	18.58	59.2	36.4				
310 K	21.42	59.2	36.3				
315 K	21.09	59.2	36.0				
		60.5	40.4				
		64.5	43.7, 44.7				
		64.5	46.5				
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.91$							

Empirical temperature dependence equations:
Wauchope & Getzen (1972): $R \cdot \ln x = -[H_{\text{fus}}/(T/K)] + (0.000408)[(T/K) - 291.15]^2 - c + b \cdot (T/K)$ (1)

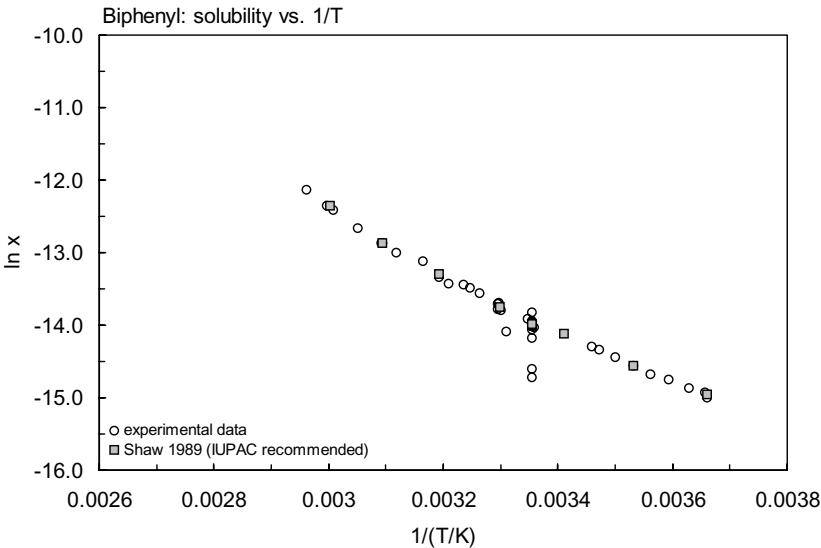


FIGURE 7.1.1.0.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for biphenyl.

TABLE 7.1.1.0.2

Reported vapor pressures of biphenyl at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C/(T/K)^2$	(5)		

1.

Chipman & Peltier 1929		Stull 1947		Bright 1951		Bradley & Cleasby 1953	
isoteniscope-manometer		summary of literature data		effusion		effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
162.5	7933	70.6	133.3	Data presented in graph		15.05	0.416
172.3	10959	101.8	666.6	25	0.579	20.7	0.7786
177.7	12799	117.0	1333		(interpolated)	24.7	1.2252
183.5	15705	134.2	2666	eq. 1	P/mmHg	24.0	1.1825
191.6	19972	152.5	5333	A	10.38	24.1	1.184
198.75	24691	165.2	7999	B	3799	27.05	1.600
293.8	28504	180.7	13332	temp range 4.9–34.5°C		29.15	2.053
211.25	34677	204.2	26664			32.45	2.973
220.05	43756	229.4	53329	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 72.80$		35.05	3.866
229.8	56329	254.0	101325			37.9	5.160
238.2	68901					40.55	6.693
247.7	85580	mp/°C	69.5			23.05	1.027
253.7	98019					36.5	1.533
255.2	101178					31.25	2.546
						35.9	4.133
bp/°C	266.25						
$\Delta H_v/(\text{kJ mol}^{-1}) = 44.99$						eq. 1	P/mmHg
at bp						A	11.282
						B	4262
eq. 5	P/mmHg					temp range 15–41°C	
A	7.0220						
B	1723						
C	245700						
temp range 162–322°C							

TABLE 7.1.1.0.2 (Continued)

2.

Radchenko& K. 1974		Nasir et al. 1980		Burkhard et al. 1984		Cunningham 1930	
Knudsen effusion		pressure transducer		gas saturation-GC		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.9	1.433	123.0	2040	5.2	0.106	69.20	104
31.75	2.976	143.81	4773	14.9	0.361	93.3	413
33.7	3.734	164.69	9962	24.7	1.15	148.7	4833
35.5	4.538	181.28	16447			160.0	7239
37.6	5.726	200.87	28599	eq. 1	P/Pa	171.1	10548
39.57	6.913	223.66	51518	A	14.840	182.2	15031
41.52	8.26	245.65	86254	B	4402.1	193.3	21098
43.48	10.26	257.91	111343			204.4	28958
45.45	12.35	274.09	154493			215.6	39093
47.4	15.49	296.14	235345			226.7	51986
50.0	19.46	315.19	329300			237.8	68051
		327.55	400175			248.9	88252
eq. 1	P/mmHg					255.3	101353
A	12.6789	data fitted to				260.0	112384
B	4367.436	Chebyshev polynomial				271.2	142032
for temp range 24.9–50°C							
						eq. 2	P/kPa
						A	6.36895
						B	1997.558
						C	202.608
						bp/°C	255.208
Sharma & Palmer 1974							
gas saturation-GC							
t/°C	P/Pa						
53.05	16.0						
61.05	34.66						
71.95	92.0						
81.05	220.0						

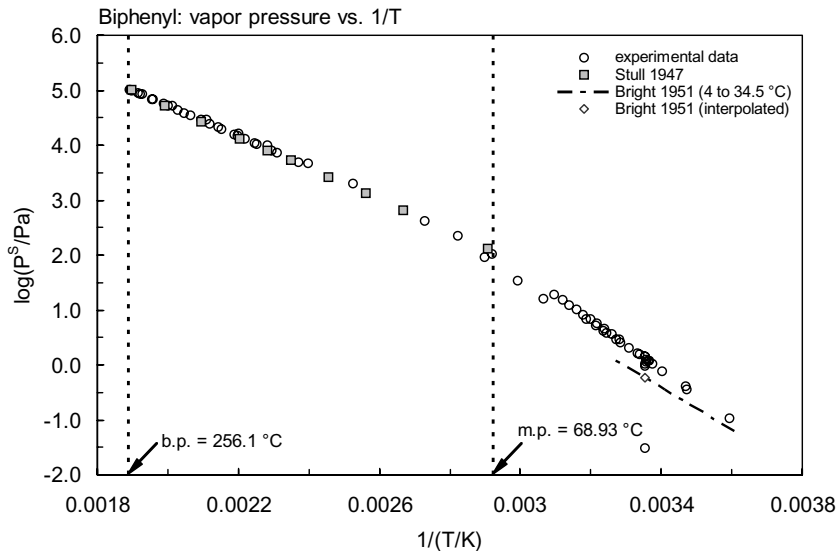
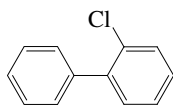


FIGURE 7.1.1.0.2 Logarithm of vapor pressure versus reciprocal temperature for biphenyl.

7.1.1.1 2-Chlorobiphenyl (PCB-1)



Common Name: 2-Chlorobiphenyl

Synonym: PCB-1, *o*-chlorobiphenyl, 2-chloro-1,1'-biphenyl

Chemical Name: 2-chlorobiphenyl

CAS Registry No: 2051-60-7

Molecular Formula: C₁₂H₉Cl

Molecular Weight: 188.652

Melting Point (°C):

34 (Beaven et al. 1961; Weast 1972–73, 1982–83; Lide 2003)

Boiling Point (°C):

274 (Weast 1972–73, 1982–83; Lide 2003)

Density (g/cm³ at 20°C): 0.9837

Molar Volume (cm³/mol):

205.5 (calculated-Le Bas method at normal boiling point)

172.9 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

57.8 (Geidarov et al. 1975)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

72.3 (Geidarov et al. 1975)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.52 (Geidarov et al. 1975)

15.3 (differential scanning calorimetry, Miller et al. 1984)

14.54 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

47.66 (Geidarov et al. 1975)

50.21 (Miller et al. 1984)

Fugacity Ratio at 25°C, F (assuming ΔS_{fus} = 56 J/mol K), F: 0.816 (mp at 34°C)

Water Solubility (g/m³ or mg/L at 25°C):

1.60 (Webb 1970)

0.90 (Hoover 1971)

5.90 (shake flask-GC/ECD, Wallnöfer et al. 1973)

4.13 (generator column-GC/ECD, Weil et al. 1974)

5.08 (supercooled liquid S_L, shake flask-GC/ECD, Chiou et al. 1983)

5.06 (generator column-GC/ECD, Miller et al. 1984,1985)

4.13, 4.74, 14.0, 4.13 (RP-HPLC-*k'* correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (89.3°C, summary of literature data, temp range 89.3–267.5°C, Stull 1947)

log (P/mmHg) = (8.306 ± 0.087) – (3018 ± 45)/(T/K), temp range: 410–510 K (static method-quartz manometer measurements, Geidarov et al. 1975)

1.84 (supercooled liquid P_L, extrapolated Antoine eq., Weast 1976–77)

1.12 (Neely 1981,1983)

0.605; 0.159; 0.367* (Knudsen effusion; torsion effusion; torsion-Knudsen effusion, extrapolated from exptl. derived Antoine eq., measured range 33–110°C, Ferro et al. 1983)

$\log (P_L/\text{kPa}) = -3893/(T/\text{K}) + 9.99$; temp range: 33–77°C (Knudsen effusion data, Ferro et al. 1983)
 $\log (P_L/\text{kPa}) = -4406/(T/\text{K}) + 10.98$; temp range: 64–110°C (torsion effusion data, liquid, Ferro et al. 1983)
 $\log (P_L/\text{kPa}) = -(4149 \pm 230)/(T/\text{K}) + (10.48 \pm 0.50)$; temp range: 33–110°C (torsion-Knudsen effusion data, Ferro et al. 1983)
 1.096, 1.456 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
 1.892, 2.56 (supercooled liquid P_L from P_{GC} , GC-RT correlation, different stationary phases, Bidleman 1984)
 0.755 (GC-RI correlation, Burkhard et al. 1985a)
 0.926 (GC-RI correlation, supercooled liquid P_L , Burkhard et al. 1985b)
 2.20 (supercooled liquid P_L , GC-RT correlation, Foreman & Bidleman 1985)
 1.096 (P_{GC} by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
 $\log (P_L/\text{Pa}) = -3366/(T/\text{K}) + 11.57$ (GC-RT correlation, Falconer & Bidleman 1994)
 0.27–2.70; 0.367–2.56 (literature P_s range; literature supercooled liquid P_L range, Delle Site 1997)
 $\log (P/\text{kPa}) = 9.99 - 3893/(T/\text{K})$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

28.9 (calculated-P/C, Burkhard et al. 1985b)
 70.1 (calculated-P/C, Shiu & Mackay 1986)
 74.6 (Dow Chemical, Neely 1982)
 30.18 (calculated-QSPR, Dunnivant et al. 1992)
 5.13, 8.32, 13.17, 20.43 ± 0.52 , 29.3 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(42.7/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.104/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
 22.0 (gas stripping-GC, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 43 \pm 6 \text{ kJ/mol}$, $\Delta S_H = 0.10 \pm 0.02 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.54 (shake flask-GC, Tulp & Hutzinger 1978)
 4.80 (Hansch & Leo 1979)
 4.35 (HPLC-RT correlation, Veith et al. 1979)
 4.10 (HPLC-RT correlation, McDuffie 1981)
 4.59 ± 0.1 ; 4.56 (shake flask-GC; RP-TLC- k' correlation, Bruggeman et al. 1982)
 3.75 (HPLC-RT correlation, Woodburn 1982)
 4.51 (shake flask-GC, Chiou et al. 1983)
 4.50 (generator column-GC, Miller et al. 1984, 1985)
 4.38 (generator column-HPLC, Woodburn et al. 1984)
 3.90, 4.60 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
 4.44 (HPLC-RP/MS correlation, Burkhard & Kuehl 1986)
 4.38 (generator column-GC/ECD, Doucette & Andren 1987)
 4.33, 4.39, 4.53, 4.43 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 3.92 (HPLC-RT correlation, Doucette & Andren 1988)
 4.531 ± 0.029 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 4.52 (recommended, Sangster 1989, 1993)
 4.68 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 4.53 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated:

7.54, 6.65 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 6.04 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, log K_{OC} :

- 3.50 (Woodburn silt loam soil, batch equilibrium isotherm-GC/ECD, Chiou et al. 1983)
 4.35 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 3.47 (calculated, soil, Chou & Griffin 1986)
 2.59 (Borden soil 0.29% OC, Hu et al. 1995)

Sorption Partition Coefficient, log K_{OM} :

- 3.23 (soil organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

$k(\text{calc}) = 3.7 \times 10^{-4} \text{ d}^{-1}$ and with $t_{1/2} = 18 \text{ yr}$, calculated sunlight photolysis rate constant in surface water at 40°N in summer (Dulin et al. 1986)

$k(\text{calc}) = 3.0 \text{ h}^{-1}$ maximum summer photolysis rate, at midday under clear skies (Bunce et al. 1989)
 $t_{1/2} = 31 \text{ d}$ under sunlight in water (Mansour & Feicht 1994)

$k = 0.081 \text{ min}^{-1}$ at pH 3, $k = 0.045 \text{ min}^{-1}$ at pH 7 and $k = 0.035 \text{ min}^{-1}$ at pH 10 with half-lives of 9, 15 and 20 min, respectively, in aqueous solutions when irradiated by UVA-340 light tubes in the presence of 25 $\mu\text{g/mL}$ of TiO_2 ;

$k = (0.043\text{--}0.045) \text{ min}^{-1}$ with $t_{1/2} = 15\text{--}16 \text{ min}$, $k = (0.082\text{--}0.091) \text{ min}^{-1}$ with $t_{1/2} = 8 \text{ min}$, and $k = (0.21\text{--}0.29) \text{ min}^{-1}$ with $t_{1/2} = 2\text{--}3 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively;
 $k = (0.043\text{--}0.044) \text{ min}^{-1}$ with $t_{1/2} = 15\text{--}16 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ;

$k = (0.030\text{--}0.055) \text{ min}^{-1}$ with $t_{1/2} = 13\text{--}22 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.9 \pm 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K with estimated atmospheric lifetime of ~8 d (relative rate method, Atkinson & Aschmann 1985)

$k_{OH} = 1.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to the $\text{C}_6\text{H}_4\text{Cl}$ ring (ring B), $k_{OH} = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to ring A, and $k_{OH} = 2.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)

$k_{OH}(\text{calc}) = (2.8\text{--}5.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = (3.1\text{--}4.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)

$k_{OH} = 2.82 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1989)

$k_{OH}(\text{exptl}) = (2.8\text{--}5.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = (3.2\text{--}4.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{1/2} = 100 \text{ h}$ biodegradation by bacteria (Wong & Kaiser 1975);

within 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

$k = 63 \text{ yr}^{-1}$ microbial degradation pseudo first-order rate constant of in the water column and $k = 630 \text{ yr}^{-1}$ in the sediment (Wong & Kaiser 1975; quoted, Neely 1981);

$k = 4.1 \text{ nmol L}^{-1} \text{ d}^{-1}$ biodegradation rate in water from Port Valdez with an initial concn of 1.5 $\mu\text{mol/L}$ (data of Aug. 1977, Reichardt et al. 1981) and $k = 1.2 \text{ nmol L}^{-1} \text{ d}^{-1}$ with initial concn of 4.5 $\mu\text{mol/L}$ (data of Aug. 1978, Reichardt et al. 1981); and $t_{1/2} = 2\text{--}3.5 \text{ d}$, an initial concn of 1–100 $\mu\text{g/L}$ by river dieaway test (Bailey et al. 1983)

$k = 1.10 \mu\text{g mL}^{-1} \text{ d}^{-1}$, the degradation rate at 30 $\mu\text{g mL}^{-1}$, under culture conditions include river water as supportive medium and mixed bacterial cultures obtained from river sediments (Kong & Sayler 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of ~8 d due to reaction with the OH radical for a 24-h average OH radical concn of $5 \times 10^5 \text{ cm}^{-3}$ (Atkinson & Aschmann 1985);
 calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radical for mono-chlorobiphenyls (Atkinson 1987);
 photolysis $t_{1/2}$ ~10–25 h for noontime summer sunshine, or more realistically, several days (Bunce et. 1989);
 tropospheric lifetime of 3 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);
 tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2}$ = 1.4 d in Lake Michigan (Neely 1983);
 photolysis $t_{1/2}$ = 18 yr in surface water at 40° L in summer (Dulin et al. 1986);
 photolysis $t_{1/2}$ = 31 d under sunlight (Mansour & Feicht 1994);
 half-lives in aqueous solutions with initial concn of 265 ng/mL, $t_{1/2}$ = 9 min at pH 3, $t_{1/2}$ = 15 min at pH 7 and $t_{1/2}$ = 20 min at pH 10 when irradiated by UVA-340 light tubes (simulated sun light) in the presence of 25 µg/mL TiO_2 , half-lives of 15–16 min, 8 min and 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO_2 , respectively; half-lives of 15–16 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 ; $t_{1/2}$ = 13–22 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 7.1.1.1.1

Reported vapor pressures of 2-chlorobiphenyl (PCB-1) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$	(3)		
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		Geidarov et al. 1975		Ferro et al. 1983			
compiled literature data		static-quartz manometer		torsion effusion		Knudsen	average
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	P/Pa	P/Pa
89.3	133.3	exptl data presented as eq. 1		50	10.3	17.3	13.8
109.8	666.7			54	10.9	19.2	10.0
134.7	1333			59	16.2	24.8	20.5
151.2	2666			63	25.6	36.9	32.2
169.9	5333	range: 137–267°C		cell C			
182.1	7999			50	8.1	12.8	10.4
197.0	13333	mp/°C	31.61	59	15.8	22.9	20.6
219.6	26664	bp/°C	24	69	34.1	51.1	46.1
243.8	53329			73	44.3	65.5	59.0
267.5	101325	$\Delta H_v/(\text{kJ mol}^{-1}) = 57.78$		77	63.3	85.8	78.0
		$\Delta H_{fus}/(\text{kJ mol}^{-1}) = 14.52$		81	83.5	115	99.2

(Continued)

TABLE 7.1.1.1.1 (Continued)

Stull 1947		Geidarov et al. 1975		Ferro et al. 1983			
compiled literature data		static-quartz manometer		torsion effusion		Knudsen	average
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	P/Pa	P/Pa
mp/°C	34.0	$\Delta S_{\text{fus}}/(\text{J mol}^{-1}\text{K}^{-1}) = 47.66$ $\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 72.30$		86	120	163	142
				cell B			
				28	0.762	1.50	1.13
				33	1.52	2.36	1.93
				37	2.30	3.42	2.85
				40	3.05	4.13	3.59
				46	3.81	5.17	4.50
				50	4.57	6.10	5.34
				54	6.10	9.69	7.90
				eq. 1	P/mmHg	P/mmHg	P/mmHg
				A	10.98	9.99	10.48
				B	4406	3898	4149
				temp range: 64–110°C		33–86°C	
				$\Delta H_{\text{V}}/(\text{kJ mol}^{-1}) = 79.4$			

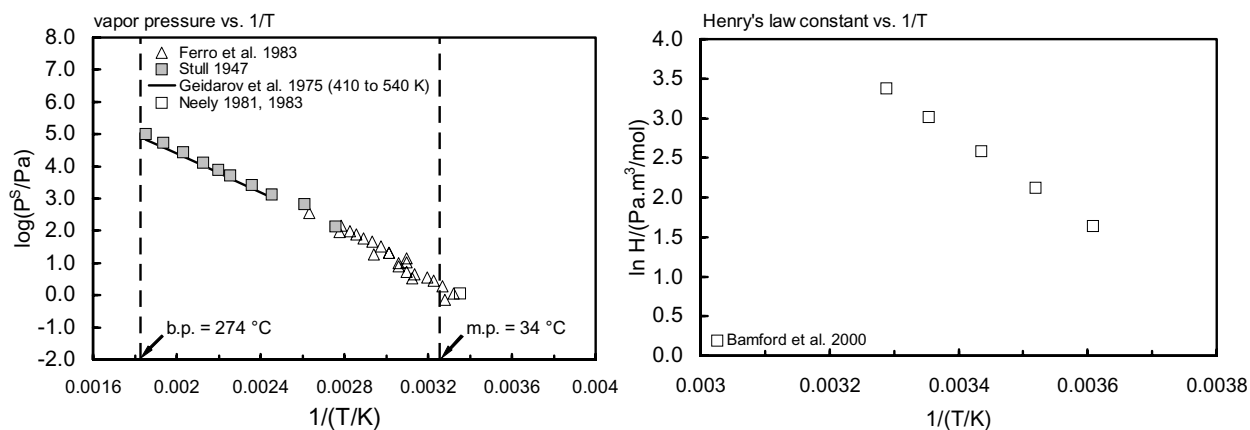
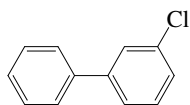


FIGURE 7.1.1.1.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for 2-chlorobiphenyl (PCB-1).

7.1.1.2 3-Chlorobiphenyl (PCB-2)



Common Name: 3-Chlorobiphenyl

Synonym: PCB-2, *m*-chlorobiphenyl, 3-chloro-1,1'-biphenyl

Chemical Name: 3-chlorobiphenyl

CAS Registry No: 2051-61-8

Molecular Formula: $C_{12}H_9Cl$

Molecular Weight: 188.652

Melting Point ($^{\circ}C$):

16 (Weast 1972–73, 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

284.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$): 0.9837

Molar Volume (cm^3/mol):

205.5 (calculated-Le Bas method at normal boiling point)

172.9 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.31 (Miller et al. 1984)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 1.0 (mp at $16^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.50 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

1.30 (generator column-GC/ECD, Weil et al. 1974)

0.56, 0.82, 0.88, 0.86 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

3.63 (generator column-HPLC/UV, Billington et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.723 (extrapolated P_L , Antoine eq., Weast 1972–73)

0.711; 4.01; 0.362* (Knudsen effusion; torsion effusion; torsion-Knudsen effusion, extrapolated from exptl. derived Antoine eq., measured range 37 – $129^{\circ}C$, Ferro et al. 1983)

$\log(P_L/kPa) = -3458/(T/K) + 8.45$; temp range: 37 – $86^{\circ}C$ (Knudsen effusion data, liquid, Ferro et al. 1983)

$\log(P_L/kPa) = -3371/(T/K) + 8.91$; temp range: 68 – $129^{\circ}C$ (torsion effusion data, liquid, Ferro et al. 1983)

$\log(P_L/kPa) = -(3614 \pm 188)/(T/K) + (8.68 \pm 0.47)$; temp range: 37 – $129^{\circ}C$ (torsion-Knudsen effusion data, Ferro et al. 1983)

0.98, 1.01 (supercooled P_L , GC-RT correlation with different stationary phases, Bidleman 1984)

0.366 (GC-RI correlation, Burkhard et al. 1985a)

0.362 (liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.997 (liquid P_L , GC-RT correlation, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -3476/(T/K) + 11.65$ liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.220–1.01 (quoted lit. range, Delle Site 1997)

$\log(P/Pa) = 11.64178 - 3514.98/(T/K)$ temp range 5 – $50^{\circ}C$ (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

14.49 (calculated- P/C , Burkhard et al. 1985b)

75.55 (calculated- P/C , Shiu & Mackay 1986)

62.11 (Dow Chemical, Neely 1982)

27.78 (calculated-QSAR, Dunnivant et al. 1992)

- 20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.54 (shake flask-GC/ECD, Tulp & Hutzinger 1978)
 4.35 (HPLC-RT correlation, Veith et al. 1979)
 4.80 (Hansch & Leo 1979)
 4.71 \pm 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)
 4.72 (RP-TLC-retention time correlation, Bruggeman et al. 1982)
 4.35 (HPLC-RT correlation, Woodburn 1982)
 4.58 (generator column-HPLC, Woodburn et al. 1984)
 3.75 (HPLC-RT correlation, Woodburn et al. 1984)
 4.60 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
 4.60 (selected, Shiu & Mackay 1986)
 4.58 (generator column-GC/ECD, Doucette & Andren 1987)
 4.65 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
 4.58 (recommended, Sangster 1989, 1993)
 4.72 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 4.58 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 7.86, 6.99 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 6.88 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.42 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 3.62 (calculated-S, soil, Chou & Griffin 1986)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

$t_{1/2} = 45$ d under sunlight in water (Mansour & Feicht 1994)
 $k(\text{calc}) = 0.5 \text{ h}^{-1}$, maximum summer photolysis rate, at midday under clear skies (Bunce et al. 1989)
 $k = (0.036\text{--}0.045) \text{ min}^{-1}$ with $t_{1/2} = 15\text{--}19$ min, $k = (0.069\text{--}0.085) \text{ min}^{-1}$ with $t_{1/2} = 8\text{--}10$ min, and
 $k = (0.18\text{--}0.23) \text{ min}^{-1}$ with $t_{1/2} = 3\text{--}4$ min in aqueous Aroclor 1248 solution containing 45 ng/mL
 of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively;
 rate constant of $k = (0.027\text{--}0.042) \text{ min}^{-1}$ with $t_{1/2} = 16\text{--}26$ min in aqueous Aroclor mixtures (Aroclor
 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in
 the presence of 100 $\mu\text{g/mL}$ TiO_2 ;
 $k = (0.033\text{--}0.036) \text{ min}^{-1}$ with $t_{1/2} = 19\text{--}21$ min in St. Lawrence River water containing 3 ng/mL of
 total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3}
 with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH} = (5.4 \pm 0.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 ± 1 K, with an estimated atmospheric lifetime
 of ~ 4 d (relative rate method, Atkinson & Aschmann 1985)
 $k_{OH} = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to the $\text{C}_6\text{H}_4\text{Cl}$ ring (ring B), $k_{OH} = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1}$
 s^{-1} to ring A, and $k_{OH} = 5.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (observed ring A + ring B) with a calculated
 tropospheric lifetime of 5–11 d (Atkinson 1987)
 $k_{OH}(\text{calc}) = (2.8\text{--}5.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = (3.1\text{--}4.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1}$
 s^{-1} for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson
 1987)
 $k_{OH} = 5.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1989)

$k_{\text{OH}}(\text{exptl}) = (2.8 - 5.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = (3.2 - 4.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$,
the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegradation $t_{1/2} \approx 7 \text{ h}$ by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; selected, Pal et al. 1980);
biodegradation rate $k \sim 2.6 \text{ nmol L}^{-1} \text{ d}^{-1}$ with an initial concentration of $3.6 \text{ } \mu\text{mol L}^{-1}$ in water from Port Valdez estimated to be (data of August 1977, Reichardt et al. 1981);
biodegradation $t_{1/2} \sim 3\text{--}4 \text{ d}$ for 50% initial concentration of $1\text{--}100 \text{ } \mu\text{g L}^{-1}$ by river dieaway test (Bailey et al. 1983);
degradation rate $k = 1.6 \text{ } \mu\text{g mL}^{-1} \text{ d}^{-1}$ at $30 \text{ } \mu\text{g mL}^{-1}$ under culture conditions include river water as supportive medium and mixed bacterial cultures obtained from river sediments (Kong & Saylor 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.29 \text{ d}^{-1}$, 0.13 d^{-1} , 0.11 d^{-1} , 0.11 d^{-1} (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of $\sim 4 \text{ d}$ due to reaction with the OH radical for a 24-h average OH radical concn of $5 \times 10^5 \text{ cm}^{-3}$ (Atkinson & Aschmann 1985);
calculated tropospheric lifetime of 5–11 based on the calculated rate constant of gas-phase reaction with OH radicals for mono-chlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 2 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);
tropospheric lifetime of 2.7–5.1 d based on both the experimentally determined and calculated rate constant for reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: photolysis $t_{1/2} = 45 \text{ d}$ under sunlight in water (Mansour & Feicht 1994);

$t_{1/2} = 15\text{--}19 \text{ min}$, $8\text{--}10 \text{ min}$ and $3\text{--}4 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and $100 \text{ } \mu\text{g/mL}$ TiO_2 , respectively;
 $t_{1/2} = 16\text{--}26 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of $100 \text{ } \mu\text{g/mL}$ TiO_2 ;
 $t_{1/2} = 19\text{--}21 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of $100 \text{ } \mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 7.1.1.2.1

Reported vapor pressures of 3-chlorobiphenyl (PCB-2) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Ferro et al. 1983

torsion effusion		Knudsen	average
T/K	P/Pa	P/Pa	P/Pa
cell B			
310	1.52	2.43	1.97
313	2.29	3.62	2.96
319	3.05	4.12	3.58

(Continued)

TABLE 7.1.1.2.1 (Continued)

Reported vapor pressures of 3-chlorobiphenyl (PCB-2) at various temperatures and the coefficients for the vapor pressure equations

Ferro et al. 1983			
torsion effusion		Knudsen	average
T/K	P/Pa	P/Pa	P/Pa
323	3.81	6.23	5.02
327	8.33	8.53	6.93
332	8.38	12.9	10.6
336	11.4	18.0	14.7
341	14.5	22.5	15.4
346	19.8	30.0	24.9
350	28.2	43.2	35.7
cell C			
332	13.6	19.1	16.3
336	15.8	22.3	19.0
341	23.4	29.0	26.2
346	27.5	35.6	31.5
350	33.7	46.2	40.0
354	47.3	63.6	55.4
359	63.2	84.9	74.0
eq. 1	P/mmHg	P/mmHg	P/mmHg
	torsion	Knudsen	average
A	8.91	8.45	8.68
B	3771	3458	3614
range, K	341–402	310–359	

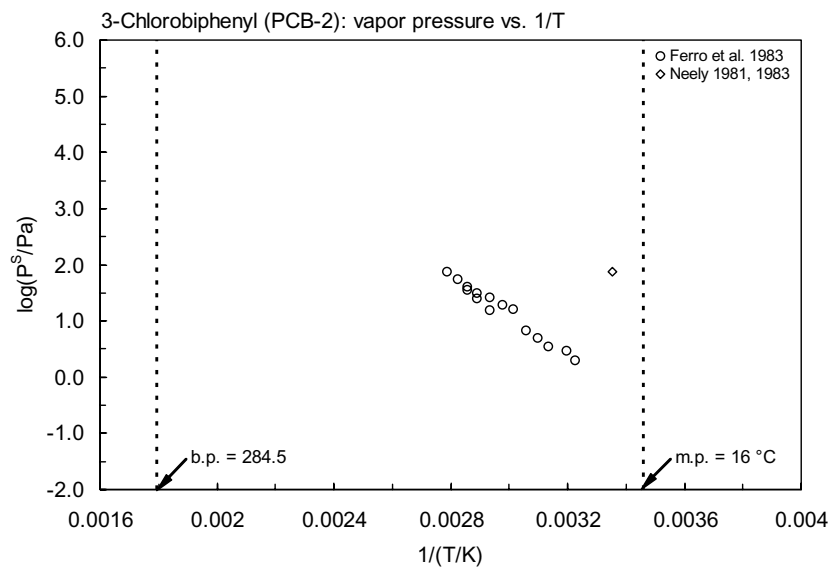
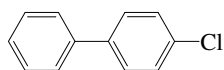


FIGURE 7.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 3-chlorobiphenyl (PCB-2).

7.1.1.3 4-Chlorobiphenyl (PCB-3)



Common Name: 4-Chlorobiphenyl

Synonym: PCB-3, *p*-chlorobiphenyl, 4-chloro-1,1'-biphenyl

Chemical Name: 4-chlorobiphenyl

CAS Registry No: 2051-62-9

Molecular Formula: C₁₂H₉Cl

Molecular Weight: 188.652

Melting Point (°C):

78.8 (Lide 2003)

Boiling Point (°C):

292.9 (Lide 2003)

Density (g/cm³ at 20°C): 0.9837

Molar Volume (cm³/mol):

205.5 (calculated-Le Bas method at normal boiling point)

172.9 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

65.94 (Geidarov et al. 1975)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

79.24 (Geidarov et al. 1975)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

13.32 (Geidarov et al. 1975; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.297 (mp at 78.8°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.0 (Webb 1970)

0.40 (Hoover, 1971)

1.19 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.90 (generator column-GC/ECD, Weil et al. 1974)

1.65 (Branson 1977)

0.0151 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)

1.478* (generator column-GC/ECD, measured range 4–32°C, Stolzenburg & Andren 1983)

$\ln x = -3428/(T/K) - 4.2786$, ΔH_{ss} = 28.5 kJ/mol (regression eq. given by Dickhut et al. 1986, based on exptl data of Stolzenburg & Andren 1983)

$\log x = -1486/(T/K) - 1.850$; ΔH_{ss} = 28.5 kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Stolzenburg & Andren 1983); or

$S/(\text{mol/L}) = 2.94 \times 10^{-8} \exp(0.041 \cdot t/^\circ\text{C})$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Stolzenburg & Andren 1983)

1.20 (selected, Shiu & Mackay 1986)

1.30, 1.38 (generator column-HPLC/UV, Billington et al. 1988)

0.82, 0.88, 0.84, 0.95 (RP- HPLC-*k'* correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

1.207 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.81 (shake flask-LSC, [¹⁴C] 4-monoCB, Eadie et al. 1990)

1.34 (shake flask-GC/ECD, Li et al. 1992; Li & Andren 1994)

1.32 (shake flask-GC/ECD, Li & Doucette 1993)

1.37* ± 0.042 (generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1997)

$\ln x = -5.9137 - 2926.22/(T/K)$, temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

3.23, 3.81 (supercooled liquid: LDV literature-derived value, FAV final-adjusted value, Li et al. 2003)

$\log S_L/(\text{mol m}^{-3}) = -631/(T/K) + 0.35$ (supercooled liquid, linear regression of literature data, Li et al. 2003)

$\log S_L/(\text{mol m}^{-3}) = -963/(T/K) + 1.53$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (96.4°C, summary of literature data, temp range 96.4–292.9°C, Stull 1947)

1.41 (supercooled liq. P_L , Weast 1972–1973)

$\log (P/\text{mmHg}) = (9.037 \pm 0.635) - (3445 \pm 18)/(T/K)$, temp range: 452–536 K (static method-quartz manometer measurements, Geidarov et al. 1975)

0.61 (Neely 1981, 1983)

0.339*; 0.253 (P_S - Knudsen effusion; P_L -torsion effusion, extrapolated from exptl. derived from Antoine eq., Ferro et al. 1983)

$\log (P_S/\text{kPa}) = - (3849 \pm 200)/(T/K) + (9.44 \pm 0.63)$; temp range 33–73°C (Knudsen effusion data, solid, Ferro et al. 1983)

$\log (P_L/\text{kPa}) = - (3541 \pm 250)/(T/K) + (8.28 \pm 0.55)$; temp range 75–136°C (torsion effusion data, liquid, Ferro et al. 1983)

1.41 (supercooled liquid P_L , converted from literature P_S , Bidleman 1984)

0.951, 0.567 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)

0.92, 0.942 (supercooled liquid P_L from P_{GC} , GC-RT correlation, different GC columns, Bidleman 1984)

0.175* (gas saturation-GC, measured range 5.2–24.9°C, Burkhard et al. 1984; Burkhard et al. 1985a)

$\log (P_S/\text{Pa}) = -4754.1/(T/K) + 15.188$; temp range: 5.2–24.9°C (gas saturation-GC, Clapeyron eq. Burkhard et al. 1984)

0.0979 (GC-RI correlation, Burkhard et al. 1985a)

0.320 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.907 (supercooled liquid P_L , GC-RT correlation, Foreman & Bidleman 1985)

0.270, 0.90 (selected P_S , supercooled P_L , Shiu & Mackay 1986)

0.593 (P_{GC} by GC-RT correlation, Hinckley et al. 1990)

0.275 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log (P_L/\text{Pa}) = -3488/(T/K) + 11.67$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

0.0677* (20°C, as saturation-GC/ECD, Wania et al. 1994)

$\log (P_S/\text{Pa}) = -4493/(T/K) + 14.15$; temp range: –20 to 30°C (gas saturation-GC, Wania et al. 1994)

0.087–0.339; 0.253–0.942 (quoted literature P_S range; literature P_L range, Delle Site 1997)

$\log P/\text{kPa} = 15.188 - 4751.1/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.468, 0.479 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log P_L/\text{Pa} = -3737/(T/K) + 12.21$ (supercooled liquid, linear regression of literature data, Li et al. 2003)

$\log P_L/\text{Pa} = -3627/(T/K) + 11.84$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

58.06 (batch stripping, Atlas et al. 1982; Dow Chemical, Neely 1982))

42.56 (calculated-P/C, Shiu & Mackay 1986)

34.14 (batch stripping-GC, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)

24.39 (wetted-wall column-GC, Fendinger & Glotfelty 1990)

23.30 (wetted-wall column-GC, Brunner et al. 1990)

5.84 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)

18.9 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 27$ kJ/mol, $\Delta S_H = 0.15 \pm 0.10$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

36.3, 23.44 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

$\log [H/(\text{Pa m}^3/\text{mol})] = -2664/(T/K) + 10.31$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.90 (Branson 1977)

4.26 (Sugiura et al. 1978)

4.80 (Hansch & Leo 1979)

4.61 ± 0.1 (shake flask-GC, Bruggeman et al. 1982)

- 4.69 (RP-TLC- k' correlation, Bruggeman et al. 1982)
- 4.34 (HPLC-RT correlation, Woodburn 1982)
- 4.49 (generator column-HPLC, Woodburn et al. 1984)
- 4.34 (HPLC-RT correlation, Woodburn et al. 1984)
- 4.40 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 4.49 (generator column-GC/ECD, Doucette & Andren 1987,1988)
- 4.55, 4.73, 4.64, 4.59 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 4.53, 4.27 (RP-HPLC- k' correlation, different stationary phases, Sherbolm & Eganhouse 1988)
- 4.61 (recommended, Sangster 1989, 1993)
- 4.72 (HPLC- k' correlation, Noegrohati & Hammers 1992)
- 4.37 (generator column-HPLC, Li & Doucette 1993)
- 4.61 (recommended, Hansch et al. 1995)
- 4.49, 4.65 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 7.01* (generator column-GC; measured range – 10 to 30°C, Harner & Mackay 1995)
- $\log K_{OA} = -6.50 + 3962/(T/K)$; temp range –10 to 20°C, (generator column-GC, Harner & Mackay 1995)
- 7.01* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
- $\log K_{OA} = -4.82 + 3470/(T/K)$; temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
- 7.86, 6.99; 6.99 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 7.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
- 6.80; 6.93 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
- 6.82, 6.78 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
- $\log K_{OA} = 3520/(T/K) - 4.97$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$:

- 2.08 (killifish, Goto et al. 1978)
- 2.68 (NAS 1979)
- 2.77 (estimated, fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 2.67 (calculated-solubility, Kenaga 1980)
- 3.88 (fish, normalized, lipid basis, Tadokoro & Tomita 1987)
- 2.77, 4.07 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.52 (calculated, Kenaga 1980)
- 4.43 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 3.90 (soil, calculated-S, Chou & Griffin 1986)
- 4.71 (Great Lake suspended matter, phase partitioning-reversed phase chromatography by Sep Pak, Eadie et al. 1990)
- 4.70 (Green Bay suspended matter, reversed phase separation, Eadie et al. 1992)
- 3.49 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Sorption Partition Coefficient, $\log K_{OM}$:

- 4.02 (Great Lakes DOC, reversed phase separation, Eadie et al. 1990)
- 4.61 (Green Bay DOC, reversed phase separation, Eadie et al. 1992)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

$k = 2.3 \times 10^{-4} \text{ d}^{-1}$ with $t_{1/2} = 8.2 \text{ yr}$ in surface water at 40°N in summer sunlight is (Dulin et al. 1986)
 $t_{1/2} = 45 \text{ d}$ in water (Mansour & Feicht 1994)

$k(\text{calc}) = 13.5 \text{ h}^{-1}$, maximum summer photolysis rate calculated under midday clear skies, experimental $k(\text{exptl}) \sim 1.0 \times 10^{-8} \text{ mol s}^{-1}$, irradiated with a low-pressure mercury lamp (Bunce et al. 1989)

$k = (0.036\text{--}0.045) \text{ min}^{-1}$ with $t_{1/2} = 15\text{--}19 \text{ min}$, $k = (0.048\text{--}0.082) \text{ min}^{-1}$ with $t_{1/2} = 8\text{--}14 \text{ min}$ and $k = (0.13\text{--}0.30) \text{ min}^{-1}$ with $t_{1/2} = 2\text{--}3 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; $k = (0.027\text{--}0.046) \text{ min}^{-1}$ with $t_{1/2} = 15\text{--}26 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ;

$k = (0.022\text{--}0.038) \text{ min}^{-1}$ with $t_{1/2} = 18\text{--}31 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (3.9 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$, with an estimated atmospheric lifetime of $\sim 6 \text{ d}$ (relative rate method, Atkinson & Aschmann 1985)

$k_{\text{OH}} = 2.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to the $\text{C}_6\text{H}_4\text{Cl}$ ring (ring B), $k_{\text{OH}} = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to ring A, and $k_{\text{OH}} = 3.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (observed ring A + ring B) with a calculated tropospheric lifetime of 5–11 d (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (2.8\text{--}5.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{exptl}) = (3.1\text{--}4.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for mono-chlorobiphenyls, the tropospheric lifetime was calculated to be 5–11 d (Atkinson 1987)

$k_{\text{OH}} = 5.28 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1989)

$k_{\text{OH}}(\text{exptl}) = (2.8\text{--}5.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = (3.2\text{--}4.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, the tropospheric lifetime is calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{1/2} = 175 \text{ h}$ biodegradation by bacteria (Wong & Kaiser 1975; quoted, Pal et al. 1980);

within 7 h by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980)

$k = 38 \text{ yr}^{-1}$ in the water column, and $k = 380 \text{ yr}^{-1}$ in the sediment, pseudo first-order rate constant for microbial degradation (Wong & Kaiser 1975; quoted, Neely 1981)

$k = 3.1 \text{ nmol L}^{-1} \text{ d}^{-1}$ with an initial concentration of 2.9 $\mu\text{mol/L}$, degradation rate in water from Port Valdez (data of Aug. 1977, Reichardt et al. 1981); $t_{1/2} = 2\text{--}5 \text{ d}$, time for 50% degradation of an initial concentration of 1–100 $\mu\text{g L}^{-1}$ by river dieaway test (Bailey et al. 1983)

$k = 2.0 \mu\text{g mL}^{-1} \text{ d}^{-1}$ at 30 $\mu\text{g mL}^{-1}$, under culture conditions include river water as supportive medium and mixed bacteria cultures obtained from river sediments (Kong & Sayler 1983)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 88 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.01 \text{ d}^{-1}$ with $t_{1/2} = 67 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: estimated atmospheric lifetime of $\sim 6 \text{ d}$ due to reaction with the OH radical for a 24-h average OH radical concn of $5 \times 10^5 \text{ cm}^{-3}$ (Atkinson & Aschmann 1985);

calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radical for mono-chlorobiphenyls (Atkinson 1987);

photolysis $t_{1/2} \sim 10\text{--}25 \text{ h}$ for noontime summer sunshine, or more realistically, several days (Bunce et al. 1989);

tropospheric lifetime of 3 d calculated based on reaction principally with OH radical and other photochemical reactions (Bunce et al. 1991);

tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for mono-chlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 4.9 \text{ d}$ in Lake Michigan (Neely 1983);

photolysis $t_{1/2} = 8.2 \text{ yr}$ in summer sunlight at 40°L in surface waters (Dulin et al. 1986);

photolysis $t_{1/2}$ = 45 d, sunlight days in water (Mansour & Feicht 1994)
 $t_{1/2}$ = 15–19 min, 8–14 min and 2–3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 respectively;
 $t_{1/2}$ = 15–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ; $t_{1/2}$ = 18–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Groundwater:
Sediment:
Soil:
Biota: depuration $t_{1/2}$ = 88 d for high-dose treatment, $t_{1/2}$ = 67 d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.3.1
Reported aqueous solubilities and octanol-air partition coefficients of 4-chlorobiphenyl (PCB-3) at various temperatures

Aqueous solubility				log K _{OA}			
Stolzenburg & Andren 1983		Shiu et al. 1997		Harner & Mackay 1995		Harner & Bidleman 1996	
generator column-GC/ECD		generator column-GC/ECD		generator column-GC		generator column-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	log K _{OA}	t/°C	log K _{OA}
4	0.661	5	0.822	−10	8.65	−10	8.34
20	1.206	15	1.07	0	8	0	7.91
25	1.478	25	1.37	10	7.48	10	7.43
32	2.128	35	2.17	20	7.01	20	7.01
		45	3.04	25	6.76	30	6.62
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 28.5$ for 5–45°C		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 24.5$ for 5–45°C		$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 75.9$		$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 75.86$	
				log K _{OA} = A + B/T		log K _{OA} = A + B/T	
				A −6.52		A −4.82	
				B 3962.2		B 3470	

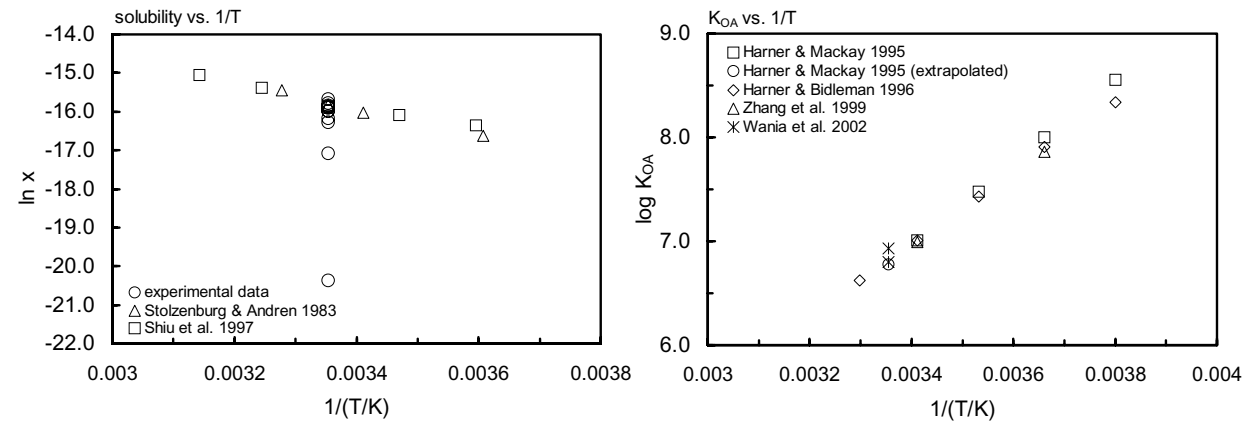


FIGURE 7.1.1.3.1 Logarithm of mole fraction solubility and K_{OA} versus reciprocal temperature for 4-chlorobiphenyl (PCB-3).

TABLE 7.1.1.3.2

Reported vapor pressures of 4-chlorobiphenyl (PCB-3) at various temperatures and the coefficients for the vapor pressure equations:

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Stull 1947		Geidarov et al. 1975		Ferro et al. 1983			
compiled literature data		static-quartz manometer		torsion-effusion		Knudsen	average
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	P/Pa	P/Pa
96.4	133.3	data presented in graph and		cell B			
129.8	666.7			33	0.762	0.697	0.729
146.0	1333	eq 1	P/mmHg	37	1.52	0.902	1.21
164.0	2666	A	9.037	50	3.05	3.57	3.31
183.8	5333	B	3445	54	3.81	4.90	4.38
196.0	7999	range: 179–263°C		59	6.10	7.41	6.75
212.6	13333			63	9.14	10.4	9.77
237.8	26664	mp/°C	74.75	73	21.3	18.3	19.8
284.5	53329	bp/°C	287	cell B			
292.9	101325			35	0.762	0.917	0.840
		$\Delta H_v/(\text{kJ mol}^{-1}) = 65.94$		41	1.62	1.41	1.47
mp/°C	75.5	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 13.32$		44	2.29	1.72	2.00
		$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 38.3$		50	3.05	2.85	2.95
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 79.24$		52	3.81	4.44	4.12
				57	5.33	6.04	5.69
				61	7.62	8.43	8.03
				62	8.38	10.9	9.66
				65	10.7	10.8	10.8
				67	12.9	11.9	12.4
				68	13.7	12.9	13.3
				69	15.2	13.9	14.6
				73	21.1	18.6	15.3
				eq. 1	P/mmHg	P/mmHg	
				A	8.28	9.44	
				B	3541	3849	
				range, °C	75–136(liq.)	33–73(solid)	
				$\Delta H_v/(\text{kJ mol}^{-1}) = 67.8$			

TABLE 7.1.1.3.2 (Continued)

2.

Burkhard et al. 1984		Wania et al. 1994	
gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
4.2	0.0111	-20	2.446×10^{-4}
15.0	0.0493	-10	1.297×10^{-3}
24.9	0.172	0	4.889×10^{-3}
25.0	0.175	10	1.883×10^{-2}
		20	6.771×10^{-2}
		30	0.2233
eq. 1	P/Pa	eq. 1	P/Pa
A	15.188	A	14.15
B	4754.1	B	4493
range: 4.2–25°C		temp range -20 to 30°C	
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.0$	

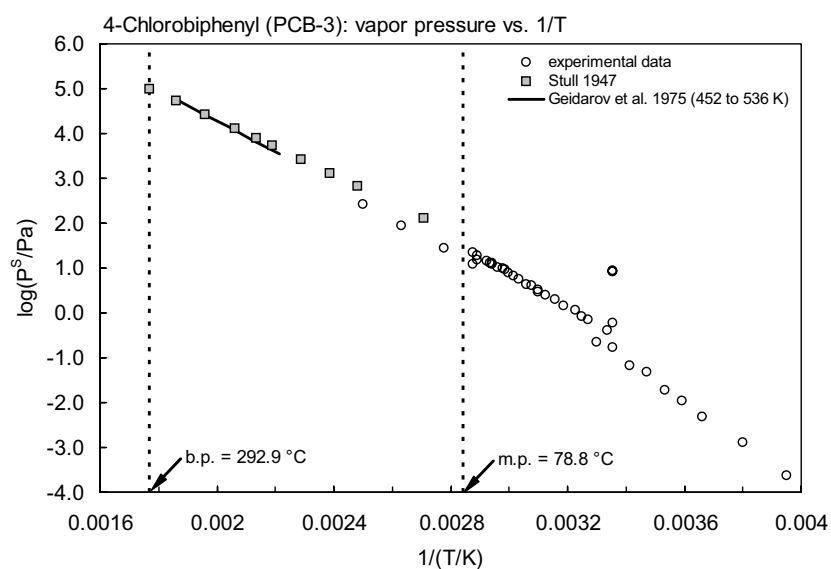
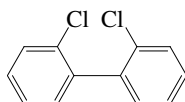


FIGURE 7.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-chlorobiphenyl (PCB-3).

7.1.1.4 2,2'-Dichlorobiphenyl (PCB-4)



Common Name: 2,2'-Dichlorobiphenyl

Synonym: PCB-4, 2,2-dichloro-1,1'-biphenyl

Chemical Name: 2,2'-dichlorobiphenyl

CAS Registry No: 13029-08-8

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

60.5 (Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

312 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)

Density (g/cm^3 at $20^{\circ}C$): 1.0536

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

185.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.448 (mp at $60.5^{\circ}C$)

0.442 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.0 (Webb 1970)

0.90 (Hoover 1971)

1.50 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.79 (generator column-GC/ECD, Weil et al. 1974)

0.0212 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)

1.86 ($20^{\circ}C$, supercooled liquid, shake flask-GC/ECD, Chiou et al. 1982,1983; Chiou 1985)

1.124 ($20^{\circ}C$, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.511, 0.322, 0.362, 0.511 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

1.207 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.133 (Knudsen-effusion technique, extrapolated from $37-54.92^{\circ}C$, Smith et al. 1964)

0.36 (quoted, Neely 1981)

0.82 (P_L calculated from P_S using F, Neely 1981)

0.189 (GC-RI correlation, Burkhard et al. 1985a)

0.424 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985a)

0.326, 0.335 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.134 (extrapolated-Antoine eq., solid, Stephenson & Malanowski 1987)

$\log(P_S/kPa) = -5019/(T/K) + 12.962$; temp range $37-55^{\circ}C$ (Antoine eq., Stephenson & Malanowski 1987)

0.152 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.275, 0.363 (supercooled liquid P_L ; GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -3462/T + 11.73$ (supercooled liquid P_L , GC-RT, Falconer & Bidleman 1994)

0.0603–0.315; 0.280–0.424 (quoted literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$ or as indicated):

30.2 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

34.14 (batch stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)

23.3 (wetted-wall column-GC, Brunner et al. 1990)

- 8.02 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
 23.0(from 11°C exptl. data and compensation point, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 50 \pm 25$ kJ/mol, $\Delta S_H = 0.13 \pm 0.09$ kJ/mol-K
 (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.04 (HPLC-RT correlation, Sugiura et al. 1978)
 5.70 (HPLC-RT correlation, Sugiura et al. 1979)
 5.51 (Hansch & Leo 1979)
 4.00 (HPLC- k' correlation, McDuffie 1981)
 5.00 \pm 0.1 (shake flask-GC, Bruggeman et al. 1982)
 3.02 (RP-TLC-retention correlation, Bruggeman et al. 1982)
 3.55 (HPLC-RT correlation, Woodburn 1982)
 4.80 (shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
 4.90; 3.55 (generator column-GC/ECD; HPLC-RT correlation, Woodburn et al. 1984)
 3.63; 4.89 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
 4.90 (generator column-GC/ECD, Doucette & Andren 1987,1988)
 4.25, 4.86, 4.65, 4.94(RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 4.965 \pm 0.013(slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 5.09 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 4.73 (recommended, Sangster 1993)
 4.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

- 7.18; 6.56 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
 $\log K_{OA} = -4.84 + 3590/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
 7.66, 6.86 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 6.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 2.04 (killifish, Goto et al. 1978)
 3.72, 2.95, 3.60, 3.26 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
 – 1.40, – 1.30, – 1.35 (adipose tissue of male, female Albino rats, rodents, Geyer et al. 1980)
 2.05, 2.45 (fish: flowing water, microcosm condition Garten & Trabalka 1983)
 3.43, 2.90 (algae, calculated, Geyer et al. 1984)
 3.43, 3.38, 3.80(algae, fish, activated sludge, Freitag et al. 1984,1985)
 3.85 (fish, normalized, lipid basis, Tadokoro & Tomita 1987)
 3.38; 3.413, 3.715(quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW} , Lu et al. 1999)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 3.68 (Woodburn silt loam soil, soil organic matter, sorption isotherm-GC, Chiou et al. 1983)
 4.76 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 3.84 (soil, calculated-S, Chou & Griffin 1986)
 3.92 (soil, calculated-MCI, Sabljic et al. 1995)
 3.96; 3.92 (soil, calculated-Characteristic Root Index CRI; quoted lit., Saçan & Balcioglu 1996)
 4.30 (soil, calculated- K_{OW} , Girvin & Scott 1997)
 4.90; 3.90 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Sorption Partition Coefficient, $\log K_{OM}$ at 25°C or as indicated:

- 3.68 (20°C, Wood burn silt loam soil, 1.9% organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
 3.68, 4.18 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 3.1$ h of evaporation with an initial concentration of 0.1 ppm from 4.5 cm depth of water solution in a glass dish at 24°C is 3.1 h and $t_{1/2} = 0.4$ h with stirring of the solution; the experimental $t_{1/2} = 3.9$ h and 0.9 h of evaporation under same condition with stirring of the solution (Chiou et al. 1979).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{OH}(\text{calc}) = (1.4 - 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the tropospheric lifetime $\tau(\text{calc}) = 8-17$ d for dichlorobiphenyls due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH} = (2.0 \pm 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} < 2.0 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 ± 2 K (relative rate method, Kwok et al. 1995)

tropospheric lifetime $\tau(\text{calc}) = 3.4-7.2$ d, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0 - 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated $k_{OH}(\text{calc}) = (1.4 - 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: Biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 but small residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

microbial degradation with pseudo first-order $k = 0.65 \text{ yr}^{-1}$ in the water column and $k = 6.5 \text{ yr}^{-1}$ in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.027 \text{ d}^{-1}$ (10°C, sandworm, Goerke & Erst 1977; quoted, Waid 1986)

$k_1 = 0.29 \text{ d}^{-1}$, 0.13 d^{-1} , 0.11 d^{-1} , 0.11 d^{-1} (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

$k_2 = 0.017 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 122 \text{ d}^{-1}$; $k_2 = 0.014 \text{ d}^{-1}$ (rainbow trout, calculated, Gobas & Mackay 1987)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 183 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 93 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 34.5$ d in Lake Michigan (Neely 1983)

Groundwater:

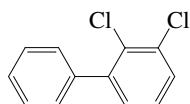
Sediment:

Soil:

Biota: $t_{1/2} = 40$ d in rainbow trout, and $t_{1/2} = 20$ d in its muscle (Niimi & Oliver 1983).

Depuration $t_{1/2} = 183$ d for high-dose treatment, $t_{1/2} = 93$ d for high-dose + enzyme treatment (juvenile rainbow trout, Buckman et al. 2004)

7.1.1.5 2,3-Dichlorobiphenyl (PCB-5)



Common Name: 2,3-Dichlorobiphenyl

Synonym: PCB-5, 2,3-dichloro-1,1'-biphenyl

Chemical Name: 2,3-dichlorobiphenyl

CAS Registry No: 16605-91-7

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$): 28.0

27.8–28.2 (Erickson 1985)

Boiling Point ($^{\circ}C$):

172 (at 4000 Pa, Erickson 1986)

Density (g/cm^3):

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.934 (mp at $28^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.70 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

1.31, 1.23, 0.756, 0.829 (quoted lit.; RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

1.00, 0.658 (quoted average of Brodsky & Ballschmiter 1988, calculated-MCI χ , Patil 1991)

1.36 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.147, 0.144, 0.114 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.151 (supercooled liquid P_L , GC-RT correlation, Burkhard et al. 1985b)

0.162 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -3769/(T/K) + 11.81$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

19.56 (calculated-P/C, Burkhard et al. 1985b)

28.57 (calculated-MCI χ , Sabljic & Güsten 1989)

23.30 (wetted-wall column-GC, Brunner et al. 1990)

24.19 (calculated-QSPR, Dunnivant et al. 1992)

8.97 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

24.5 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 48 \pm 24\ kJ/mol$, $\Delta S_H = 0.12 \pm 0.08\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.20 (RP-TLC-RT correlation, Bruggeman et al. 1982)

4.82, 4.92, 5.17, 5.05 (RP-PLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

4.99 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations:

7.40; 6.98 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)

$\log K_{OA} = -5.41 + 3820/(T/K)$; temp range 10 – $43^{\circ}C$ (fugacity meter, Kömp & McLachlan 1997a)

- 8.55, 7.59 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
 7.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

- 3.08 (oyster, Vreeland 1974)
 3.45–4.11 mean 4.11 (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
 4.41; 4.11 (rainbow trout, 15°C, kinetic BCF k_1/k_2 , steady-state BCF C_F/C_W , Oliver & Niimi 1985)
 4.11, 5.25; 3.388, 3.895 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW} , Lu et al. 1999)
 3.08, 5.33 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.11, 5.20 (rainbow trout: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} :

- 4.76 (suspended particulate matter, Burkhard 1984)
 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = (0.031\text{--}0.036) \text{ min}^{-1}$ with $t_{1/2} = 19\text{--}23 \text{ min}$, $k = (0.054\text{--}0.067) \text{ min}^{-1}$ with $t_{1/2} = 10\text{--}13 \text{ min}$ and $k = (0.22\text{--}0.25) \text{ min}^{-1}$ with $t_{1/2} = 3 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; $k = (0.022\text{--}0.028) \text{ min}^{-1}$ with $t_{1/2} = 25\text{--}32 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ; $k = (0.022\text{--}0.024) \text{ min}^{-1}$ with $t_{1/2} = 29\text{--}31 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)
 tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17 \text{ d}$, based on $k_{OH}(\text{calc.}) = (1.4\text{--}2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)
 $k_{OH}(\text{aq.}) = 7.9 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
 tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2 \text{ d}$, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0\text{--}4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated $k_{OH}(\text{calc}) = (1.4\text{--}3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_2 = 0.011 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
 $k_1 = 300 \text{ d}^{-1}$; $k_2 = 0.011 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)
 $\log 1/k_2 = 2.0, 2.2 \text{ h}$ (fish, quoted, calculated- K_{OW} , Hawker & Connell 1988b)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).
 Surface water: $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

$t_{1/2}$ = 19–23 min, 10–13 min and 3 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively;
 $t_{1/2}$ = 16–26 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ;
 $t_{1/2}$ = 29–31 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

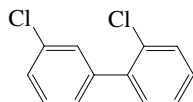
Groundwater:

Sediment:

Soil:

Biota: $t_{1/2}$ = 61 d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{1/2}$ = 26 d in its muscle (Niimi & Oliver 1983).

7.1.1.6 2,3'-Dichlorobiphenyl (PCB-6)



Common Name: 2,3'-Dichlorobiphenyl

Synonym: PCB-6

Chemical Name: 2,3'-dichlorobiphenyl

CAS Registry No: 25569-80-6

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

36 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.605 (supercooled liquid S_L , Burkhard et al. 1985a)

0.580 ($20^{\circ}C$, supercooled liquid S_L , Murphy et al. 1987)

1.226 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.928 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.165 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.157, 0.169, 0.0754 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.173, 1.208 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0799 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.141, 0.178 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -3769/(T/K) + 11.88$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

27.76 (calculated-P/C, Burkhard et al. 1985a)

30.0 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

39.42 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

25.33 (wetted-wall column-GC, Brunner et al. 1990)

33.09 (calculated-QSPR, Dunnivant et al. 1992)

4.016, 11.74 (0, $15^{\circ}C$, from modified two-film exchange model, Hornbuckle et al. 1994)

9.14 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

24.8 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 24$ kJ/mol, $\Delta S_H = 0.12 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.03 (calculated-TSA, Burkhard 1984)

5.02 (quoted and selected, Brownwell & Farrington 1985)

4.84 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.06	(calculated-TSA, Hawker & Connell 1988a)
5.02	(recommended, Hansch et al. 1995)
5.044	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

8.51; 7.55	(0; 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
7.01	(calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

4.83	(suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
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Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $k = (0.018-0.052) \text{ min}^{-1}$ with $t_{1/2} = 13-38 \text{ min}$, irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 of diCBs in St. Lawrence River water containing 3 ng/mL of total PCB (Huang et al. 1996)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8-17 \text{ d}$, based on $k_{OH}(\text{calc.}) = (1.4 - 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyl at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 8.0 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

tropospheric lifetime $\tau(\text{calc}) = 3.4-7.2 \text{ d}$, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0 - 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated $k_{OH}(\text{calc}) = (1.4 - 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.012 \text{ d}^{-1}$ with $t_{1/2} = 56 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8-17 d due to calculated rate constant of gas-phase reaction with OH radical (Atkinson 1987);

tropospheric lifetime of 3.4-7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

$t_{1/2} = 13-38 \text{ min}$ for dichlorobiphenyl in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996)

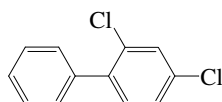
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 56 \text{ d}$ for high-dose treatment, $t_{1/2} = 53 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.7 2,4-Dichlorobiphenyl (PCB-7)



Common Name: 2,4-Dichlorobiphenyl

Synonym: PCB-7, 2,4-dichloro-1,1'-biphenyl

Chemical Name: 2,4-dichlorobiphenyl

CAS Registry No: 33284-50-3

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

24.1–24.4 (Dickerman & Weiss 1957; Weingarten 1961; Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.0536

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

185.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

1.0 (calculated, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.40 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.637 (shake flask-GC/ECD, Haque & Schmedding 1975)

1.13 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)

0.587, 0.535, 0.689, 0.659 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

1.148 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$):

0.184, 0.321 (supercooled liquid P_L , GC-RT correlation, different GC columns, Bidleman 1984)

0.175 (supercooled liquid P_L , Burkhard et al. 1984)

0.179 (GC-RI correlation, Burkhard et al. 1985a)

0.175 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.210, 0.216 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.170, 0.195 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

96.66 (gas stripping-GC, Atlas et al. 1982)

35.26 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)

28.37 (wetted-wall column.-GC/ECD, Brunner et al. 1990)

24.78 (wetted-wall column-GC, Fendinger & Glotfelty 1990)

11.5 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

28.6 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 43 \pm 22\ kJ/mol$, $\Delta S_H = 0.11 \pm 0.08\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.15 (RP-TLC-RT correlation, Bruggeman et al. 1982)

4.67 (HPLC-RT correlation, Rapaport & Eisenreich 1984)

- 5.09, 5.21, 5.20, 5.10 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.13 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 5.16 (recommended, Sangster 1993)
 5.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 8.37, 7.39; 7.25(0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 6.98 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.83 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , or Half Lives, $t_{1/2}$:

Volatilization:

Photolysis: calculated sunlight $k < 2 \times 10^{-8} \text{ s}^{-1}$ and $5.7 \times 10^{-11} \text{ s}^{-1}$, with $t_{1/2} > 400 \text{ d}$ at 40°N latitude in winter (Dulin et al. 1986);

$k = (0.30\text{--}0.036) \text{ min}^{-1}$ with $t_{1/2} = 19\text{--}23 \text{ min}$, $k = (0.054\text{--}0.067) \text{ min}^{-1}$ with $t_{1/2} = 10\text{--}13 \text{ min}$ and $k = (0.13\text{--}0.21) \text{ min}^{-1}$ with $t_{1/2} = 3\text{--}5 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; rate constants $k = (0.015\text{--}0.043) \text{ min}^{-1}$ with $t_{1/2} = 36\text{--}29 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ; rate constants $k = (0.018\text{--}0.022) \text{ min}^{-1}$ with $t_{1/2} = 31\text{--}38 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17 \text{ d}$ for dichlorobiphenyls, based on $k_{OH}(\text{calc.}) = (1.4\text{--}2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 7.1 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2 \text{ d}$ for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0\text{--}4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the $k_{OH}(\text{calc}) = (1.4\text{--}3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 from lake sediments but small amount residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 192 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 149 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for $\text{OH}\cdot$ oxidation (Sedlak & Andren 1991);
 $t_{1/2} = 19\text{--}23$ min, $10\text{--}13$ min and $3\text{--}5$ min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 respectively;
 $t_{1/2} = 36\text{--}29$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ;
 $t_{1/2} = 31\text{--}38$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

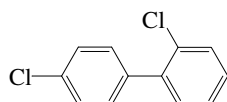
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 192$ d for high-dose treatment, $t_{1/2} = 149$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.8 2,4'-Dichlorobiphenyl (PCB-8)



Common Name: 2,4'-Dichlorobiphenyl

Synonym: PCB-8, 2,4'-dichloro-1,1'-biphenyl

Chemical Name: 2,4'-dichlorobiphenyl

CAS Registry No: 34883-43-7

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

46 (Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.0536

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

185.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.66 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.50 (Webb 1970; Hoover 1971)

1.88 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.637 (shake flask-GC, Haque & Schmedding 1975)

0.620 (generator column-GC/ECD, Weil et al. 1974)

0.139 (shake flask-GC/ECD from Aroclor 1242 mixture, Lee et al. 1979)

1.17 ($20^{\circ}C$, supercooled liquid P_L , shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985)

0.974, 0.848, 0.643, 0.658 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

1.58, 1.45 (supercooled liquid S_L : derivation of literature-derived value, final-adjusted value, Li et al. 2003)

$\log S_L/(mol m^{-3}) = -1000/(T/K) + 1.17$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0998 (GC-RI correlation, Burkhard et al. 1985a)

0.147 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.157, 0.143 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log (P/mmHg) = 9.74 - 3840/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.129, 0.158 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = -3769/(T/K) + 11.84$ (GC-RT correlation, Falconer & Bidleman 1994)

0.123, 0.148 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log P_L/Pa = -3818/(T/K) + 11.90$ (supercooled liquid, linear regression of literature data, Li et al. 2003)

$\log P_L/Pa = -3728/(T/K) + 11.68$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

96.7 (gas stripping-GC, Atlas et al. 1982)

23.30 (wetted wall column-GC/ECD, Brunner et al. 1990)

35.67 ± 2.7 (gas stripping-GC/ECD; Girvin et al. 1997)

6.01, 9.87, 15.85, $24.89^* \pm 0.29$, 36.07 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 13.2307 - 5304.31/(T/K)$; temp range $4-31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(44.1/kJ \cdot mol^{-1})/RT] + (0.110/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314 J \cdot K^{-1} \cdot mol^{-1}$ and temp range: $4-31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

25.7 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 44 \pm 3$ kJ/mol, $\Delta S_H = 0.11 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

26.3, 22.9 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

$\log H/(\text{Pa m}^3/\text{mol}) = -2428/(T/K) + 9.56$ (LDV linear regression of literature data, Li et al. 2003)

$\log H/(\text{Pa m}^3/\text{mol}) = -2728/(T/K) + 10.51$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.51 (Hansch & Leo 1979)

4.48 (HPLC-RT correlation, Woodburn 1982)

5.10 (shake flask-GC, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)

5.10 \pm 0.4 (selected, Shiu & Mackay 1986)

5.14 (generator column-GC/ECD, Woodburn et al. 1984)

4.47; 5.10 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)

5.14 (generator column-GC/ECD, Doucette & Andren 1987,1988)

4.93, 5.05, 5.24, 5.15 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.13 (HPLC- k' correlation, Noegrohati & Hammers 1992)

5.27 (average value, generator column-GC, Larsen et al. 1992)

5.09 (recommended, Sangster 1993)

5.10 (recommended, Hansch et al. 1995)

5.09, 5.12 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ as or as indicated and reported temperature dependence equations:

7.40 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)

$\log K_{OA} = -5.41 + 3820/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)

8.58, 7.61 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)

7.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

7.40, 7.34 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log K_{OA} = 3785/(T/K) - 5.35$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$:

3.83, 3.55, 3.99 (algae, fish, act. sludge, Freitag et al. 1984,1985)

2.60–4.08 (various marine species, mean dry wt. BCF, Hope et al. 1998)

4.12–5.33 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

3.83, 4.53 (algae: wet wt basis, dry wt basis, Geyer et al. 2000)

3.57, 5.76 (*Daphnia*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

3.90 (soil/sediment, sorption isotherm, Haque & Schmedding 1976)

4.16 (Woodburn silt loam soil, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

4.83 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

5.90 (Lake Michigan water column, Swackhamer & Armstrong 1987)

5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

3.99; 4.13 (soil, calculated-Characteristic Root Index CRI; quoted lit., Saçan & Balcioglu 1996)

4.54–4.56 (Catlin silt loam, $f_{OC} = 0.0226$, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.65–4.70 (Cloudland loam, $f_{OC} = 0.0024$, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.61 (Kenoma silt loam, $f_{OC} = 0.0153$, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.38–4.39 (Kenoma silt loam, $f_{OC} = 0.0092$, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.57–4.73 (Kenoma silt loam, $f_{OC} = 0.002$, depth 120–155 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.52–4.54 (Norborne silt loam, $f_{OC} = 0.0137$, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.54–4.57 (Norborne silt loam, $f_{OC} = 0.009$, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.53–4.66 (Norborne silt loam, $f_{OC} = 0.0057$, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)

4.23–4.53; 3.90–5.90 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

4.23; 3.93, 4.53, 4.46 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, $\log K_{OM}$:

3.89 (soil organic matter, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: depletion rate constant $k = 45 \text{ d}^{-1}$ from aqueous solution in a 26-cm or 67-cm purge vessel, (Girvin et al. 1997).

Photolysis: photolysis rate $k_p(\text{exptl}) < 2 \times 10^{-8} \text{ d}^{-1}$ with $t_{1/2} > 400 \text{ d}$; $k_p(\text{calc}) < 2 \times 10^{-8} \text{ d}^{-1}$ in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17 \text{ d}$ for dichlorobiphenyls, based on $k_{OH}(\text{calc.}) = (1.4 - 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2 \text{ d}$ for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0 - 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the $k_{OH}(\text{calc}) = (1.4 - 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Sorption-Desorption Rate Constants:

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 109 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 104 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: photolysis $t_{1/2} > 400 \text{ d}$ in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

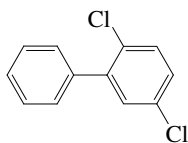
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 109 \text{ d}$ for high-dose treatment, $t_{1/2} = 104 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.9 2,5-Dichlorobiphenyl (PCB-9)



Common Name: 2,5-Dichlorobiphenyl

Synonym: PCB-9, 2,5-dichloro-1,1'-biphenyl

Chemical Name: 2,5-dichlorobiphenyl

CAS Registry No: 34883-39-1

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

22–23 (Weingarten 1962)

Boiling Point ($^{\circ}C$):

171 (15mm Hg, Erickson 1986))

Density (g/cm^3 at $20^{\circ}C$): 1.0536

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F:

1.0 (calculated, assuming $\Delta S_{fus} = 56$ J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.58 (generator column-GC/ECD, Weil et al. 1974)

2.028 (shake flask-GC, Chiou et al. 1977)

0.190 (generator column-GC/ECD, Bruggeman et al. 1981)

1.940 (generator column-GC/ECD, Miller et al. 1984; 1985)

0.0739, 0.0739, 0.0722, 0.07055 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

1.115 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0775 (Augood et al. 1953)

0.184 (supercooled liquid P_L , Yalkowsky et al. 1983)

0.184 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

0.202 (GC-RI correlation, Burkhard et al. 1985a)

0.198 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.231, 0.232 (supercooled P_L , GC-RT correlation, different GC stationary phases, Foreman & Bidleman 1985)

0.180 (selected, Shiu & Mackay 1986)

0.204 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -3862/(T/K) + 12.22$, (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.105–0.232 (quoted lit. P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations)

39.31 (batch stripping-GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)

28.37 (wetted wall column-GC/ECD, Brunner et al. 1990)

16.1, 29.6, 58.2, 82.2, 123, 165.4 (10.4, 20, 30.1, 34.9, 42.1, $47.9^{\circ}C$, gas stripping-HPLC/fluorescence, ten Hulscher et al. 1992)

30.95 ($20^{\circ}C$, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.055 - 2331/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

- 29.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW} :

- 5.18 (RP-TLC- k' correlation, Bruggeman et al. 1982; Bruggeman et al. 1984)
 5.16 (generator column-GC/ECD, Miller et al. 1984,1985)
 5.03 (calculated-TSA, Burkhard 1984)
 4.67; 5.30 (RP-HPLC-RT correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)
 5.01, 5.10, 5.19, 5.10 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.13 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 5.10 (recommended, Sangster 1993)
 5.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

- 8.37, 7.40; 7.33(0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 7.16 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 5.68 (goldfish, 3% lipid by wt., static fish-water equilibration system, 23-d exposure, Bruggeman et al. 1981)
 5.45 (goldfish, 10% lipid dry wt. in food, Bruggeman et al. 1981)
 5.72 (guppy, 3.5% lipid by wt., Bruggeman et al. 1982,1984)
 4.14; 3.90 (goldfish, exptl.; correlated, Mackay & Hughes 1984)
 3.38–4.11 mean 4.00 (rainbow trout, 15°C, steady-state BCF, 7- to 96-d study, Oliver & Niimi 1985)
 4.0 (rainbow trout, mean of 7–96 d exposure, Oliver & Niimi 1985)
 4.53, 4.00 (rainbow trout: kinetic BCF; steady state BCF, Oliver & Niimi 1985)
 4.26 (guppy, Gobas et al. 1987)
 5.68 (goldfish, Noegrohati & Hammers 1992)
 3.89; 3.42 (zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
 4.0, 5.09 (rainbow trout, flow through 96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.89, 5.43 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.00; 4.13 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 4.83 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.01 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constants $k = (0.024\text{--}0.038)$ min⁻¹ with $t_{1/2} = 18\text{--}29$ min, $k = (0.033\text{--}0.048)$ min⁻¹ with $t_{1/2} = 14\text{--}21$ min and $k = (0.13\text{--}0.14)$ min⁻¹ with $t_{1/2} = 5$ min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 µg/mL TiO₂, respectively; rate constant $k = (0.056\text{--}0.064)$ min⁻¹ with $t_{1/2} = 11\text{--}12$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO₂; rate constant $k = (0.015\text{--}0.027)$ min⁻¹ with $t_{1/2} = 26\text{--}47$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 µg/mL TiO₂ (Huang et al. 1996)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = 1.8 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17$ d for dichlorobiphenyls, based on $k_{\text{OH}}(\text{calc.}) = (1.4 - 2.9) \times 10^{-12}$ $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2$ d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{\text{OH}}(\text{exptl}) = (2.0 - 4.2) \times 10^{-12}$ $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the $k_{\text{OH}}(\text{calc}) = (1.4 - 3.1) \times 10^{-12}$ $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 95% degradation at 24 h in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 920 \text{ d}^{-1}$; $k_2 = 0.066 \text{ d}^{-1}$ (23°C, goldfish, 3% lipid, Bruggeman et al. 1981; quoted, Waid 1986)

$k_2 = 0.008 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 190 \text{ d}^{-1}$; $k_2 = 0.11 \text{ d}^{-1}$ (guppy, Bruggeman et al. 1984; quoted, Clark et al. 1990)

$k_2 = 0.066, 0.0523 \text{ d}^{-1}$ (goldfish, exptl., calculated, Mackay & Hughes 1984)

$k_1 = 280 \text{ d}^{-1}$; $k_2 = 0.0082 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1 = 38.3, 49.2 \text{ h}^{-1}$; $1/k_2 = 360, 220 \text{ h}$ (goldfish, guppy, quoted, Hawker & Connell 1985)

$k_1 = 1200 \text{ d}^{-1}$ (guppy, Opperhuizen 1986)

$k_1 = 122 \text{ d}^{-1}$; $k_2 = 0.0089 \text{ d}^{-1}$ (rainbow trout, calculated, Gobas & Mackay 1987)

$\log k_1 = 2.96, 3.07 \text{ d}^{-1}$; $\log 1/k_2 = 0.96, 1.18 \text{ d}$ (fish, quoted, Connell & Hawker 1988)

$\log 1/k_2 = 2.1, 2.3 \text{ h}$ (fish, quoted, calculated- K_{OW} , Hawker & Connell 1988b)

$\log k_2 = -0.96, -1.17 \text{ d}^{-1}$ (fish, quoted, Thomann 1989)

$k_1 = 2760 \text{ d}^{-1}$; $k_2 = 0.368 \text{ d}^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 192 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 149 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 18\text{--}29$ min, 14–21 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; $t_{1/2} = 11\text{--}12$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ; $t_{1/2} = 26\text{--}47$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

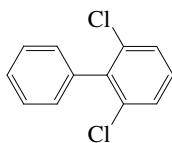
Biota: clearance $t_{1/2} = 10$ d in goldfish (Bruggeman et al. 1981)

$t_{1/2} = 6.5$ d in guppy (Bruggeman et al. 1984);

$t_{1/2} = 85$ d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and its muscle, $t_{1/2} = 56$ d (Niimi & Oliver 1983).

depuration $t_{1/2} = 192$ d for high-dose treatment, $t_{1/2} = 149$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.10 2,6-Dichlorobiphenyl (PCB-10)



Common Name: 2,6-Dichlorobiphenyl

Synonym: PCB-10, 2,6-dichloro-1,1'-biphenyl

Chemical Name: 2,6-dichlorobiphenyl

CAS Registry No: 33146-45-1

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

35.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

185.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.6 (differential scanning calorimetry, Miller et al. 1984)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

41.0 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.789 (mp at $35.5^{\circ}C$)

0.801 Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.452 (shake flask-GC, Chiou et al. 1977)

1.390 (generator column-GC/ECD, Miller et al. 1984,1985)

0.294, 0.435, 0.245, 0.406 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

2.41 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.540 (generator column-GC/ECD, Opperhuizen et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.288 (GC-RI correlation, Burkhard et al. 1985a)

0.365 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.336, 0.371 (supercooled P_L , GC-RT correlation, different GC stationary phases, Foreman & Bidleman 1985)

0.347 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -3642/(T/K) + 11.74$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

47.83 (calculated-P/C, Burkhard et al. 1985b)

47.61 (calculated-MCI χ , Sabljic & Güsten 1989)

23.30 (wetted wall column-GC, Brunner et al. 1990)

42.86 (calculated-QSPR, Dunnivant et al. 1992)

27.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6\ kJ/mol$, $\Delta S_H = 0.10 \pm 0.01\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.30 (quoted, Kaiser 1983)
- 4.96 (calculated-TSA, Burkhard 1984)
- 5.31 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 4.93 (generator column-GC/ECD, Miller et al. 1984,1985)
- 4.97, 5.00, 4.97, 5.01 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 4.982 \pm 0.013 (shake flask/slow stripping-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 4.99 (recommended, Sangster 1993)
- 4.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

- 7.18 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
- $\log K_{OA} = -4.84 + 3590/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 6.18 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:Sorption Partition Coefficient, $\log K_{OC}$:

- 4.76 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 3.99 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $k = 0.043 \text{ min}^{-1}$ with $t_{1/2} = 16 \text{ min}$, $k = 0.082 \text{ min}^{-1}$ with $t_{1/2} = 8 \text{ min}$ and $k = 0.30 \text{ min}^{-1}$ with $t_{1/2} = 2 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; rate constants $k = 0.034 \text{ min}^{-1}$ with $t_{1/2} = 20 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are: irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ; rate constants $k = 0.052 \text{ min}^{-1}$ with $t_{1/2} = 13 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)
 tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17 \text{ d}$ for dichlorobiphenyls, based on $k_{OH}(\text{calc.}) = (1.4\text{--}2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)
 tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2 \text{ d}$ for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0\text{--}4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the $k_{OH}(\text{calc}) = (1.4\text{--}3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 183 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 93 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2}$ = 16 min, 8 min and 2 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; $t_{1/2}$ = 20 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ; $t_{1/2}$ = 13 min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

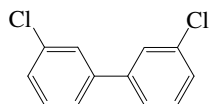
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 56 d for high-dose treatment, $t_{1/2}$ = 53 d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.11 3,3'-Dichlorobiphenyl (PCB-11)



Common Name: 3,3'-Dichlorobiphenyl

Synonym: PCB-11, 3,3'-dichloro-1,1'-biphenyl

Chemical Name: 3,3'-dichlorobiphenyl

CAS Registry No: 2050-67-1

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

29 (Weast 1972–73, 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

320 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

185.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.912 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.057 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.0406, 0.102, 0.093, 0.0974 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.354 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0267 (P_s from GC-RT correlation, Westcott & Bidleman 1981; Westcott et al. 1981)

0.0865, 0.0952 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Bidleman 1984)

0.0645 (supercooled liquid P_L , GC-RT correlation, Burkhard 1984)

0.0612 (GC-RI correlation, Burkhard et al. 1985a)

0.0646 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.091, 0.076 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.090 (selected P_L , supercooled liquid, Shiu & Mackay 1986)

$\log(P_L/Pa) = -3936/(T/K) + 12.14$; (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.0306–0.143; 0.0646–0.0953 (literature. P_s range; literature P_L range, Delle & Site 1997)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

13.58 (calculated-P/C, Burkhard et al. 1985b)

23.61 (batch stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)

23.61; 38.69 (quoted exptl.; calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

23.61; 29.42 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)

20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.30 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)

5.34 (RP-TLC- k' correlation, Bruggeman et al. 1982)

- 5.30, 5.39, 5.22, 5.18 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.17 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 5.27 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 7.86, 7.90; 7.93 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.90 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.00 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 2.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17 \text{ d}$ for dichlorobiphenyls, based on $k_{OH}(\text{calc.}) = (1.4\text{--}2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

$k_{OH} = (4.1 \pm 1.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ (relative rate method, Kwok et al. 1995)

tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2 \text{ d}$ for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0\text{--}4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated $k_{OH}(\text{calc}) = (1.4\text{--}3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 : 0.1385 d^{-1} (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995)

Surface water:

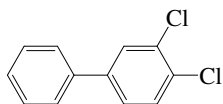
Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 5 \text{ d}$ in rainbow trout, and $t_{1/2} < 5 \text{ d}$ in its muscle (Niimi & Oliver 1983)

7.1.1.12 3,4-Dichlorobiphenyl (PCB-12)



Common Name: 3,4-Dichlorobiphenyl

Synonym: PCB-12, 3,4-dichloro-1,1'-biphenyl

Chemical Name: 3,4-dichlorobiphenyl

CAS Registry No: 2974-92-7

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

49–50 (Weingarten 1961)

Boiling Point ($^{\circ}C$):

195–200 (Weast 1972–73)

Density (g/cm^3):

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

185.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.566 (calculated, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.233 (calculated-TSA, supercooled liquid P_L , Burkhard et al. 1985b)

0.0523, 0.112, 0.0888, 0.128 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00791 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.0138 (supercooled liquid P_L , calculated-mp, Dunnivant & Elzerman 1988)

0.280 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.091; 0.658 (quoted average of Brodsky & Ballschmiter 1988; calculated- χ , Patil 1991)

0.4004 (calculated-QSPR, Dunnivant et al. 1992)

0.930 (calculated-group contribution, Kühne et al. 1995)

0.268, 0.722 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

2.373 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0532 (supercooled liquid P_L , GT-RT correlation, Burkhard 1984)

0.0313 (GC-RI correlation, Burkhard et al. 1985a)

0.0532 (supercooled liquid P_L , GC-RT correlation, Burkhard et al. 1985b)

0.078, 0.062 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.741 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -3885/(T/K) + 11.92$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.000736–0.0888; 0.0128–0.0783 (literature P_s range; literature P_L range, Delle Site 1997)

0.259 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioğlu 1998)

20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Henry's Law Constant (Pa m³/mol at 25°C):

- 20.77 (batch stripping/GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
 14.18 (wetted-wall column-GC, Brunner et al. 1990)

Octanol/Water Partition Coefficient, log K_{OW}:

- 5.51 (Hansch & Leo 1979)
 5.10, 5.51 (HPLC-RT correlation, calculated- π , Woodburn 1982; Woodburn et al. 1984)
 5.29 (generator column-GC, Woodburn et al. 1984)
 5.29 (generator column-GC/ECD, Doucette & Andren 1987)
 5.26, 5.39, 5.22, 5.18 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.12 (HPLC-k' correlation, Noegrohati & Hammers 1992)
 5.29 (recommended, Sangster 1993)
 5.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

- 8.71, 7.80; 8.06(0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
 8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

- 4.85 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
 3.98 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: rate constants $k = (0.019\text{--}0.034) \text{ min}^{-1}$ with $t_{1/2} = 21\text{--}36 \text{ min}$, $k = (0.041\text{--}0.064) \text{ min}^{-1}$ with $t_{1/2} = 11\text{--}17 \text{ min}$ and $k = (0.12\text{--}0.16) \text{ min}^{-1}$ with $t_{1/2} = 4\text{--}6 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO₂, respectively; rate constants $k = (0.013\text{--}0.029) \text{ min}^{-1}$ with $t_{1/2} = 26\text{--}52 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO₂ (Huang et al. 1996).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated, *data at other temperatures see reference:
 $k_{\text{OH}}(\text{calc}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)
 tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17 \text{ d}$ for dichlorobiphenyls, based on $k_{\text{OH}}(\text{calc.}) = (1.4\text{--}2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)
 tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2 \text{ d}$ for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{\text{OH}}(\text{exptl}) = (2.0\text{--}4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated $k_{\text{OH}}(\text{calc}) = (1.4\text{--}3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 100% degraded by Nocardia strain NCIB 10603 within one week (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 88 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 67 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the

experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2}$ = 21–36 min, 11–17 min and 4–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; $t_{1/2}$ = 26–52 min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

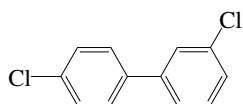
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2}$ = 88 d for high-dose treatment, $t_{1/2}$ = 67 d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.13 3,4'-Dichlorobiphenyl (PCB-13)



Common Name: 3,4'-Dichlorobiphenyl

Synonym: PCB-13, 3,4'-dichloro-1,1'-biphenyl

Chemical Name: 3,4'-dichlorobiphenyl

CAS Registry No: 2974-90-5

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 233.1

Melting Point ($^{\circ}C$):

51 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.084 (supercooled liquid S_L , Burkhard et al. 1985a)

0.093 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.369 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0572 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0595 (GC-RI correlation, Burkhard et al. 1985b)

0.083, 0.067 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -3885/(T/K) + 11.92$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\cdot m^3/mol$):

12.36 (calculated-P/C, Burkhard et al. 1985b)

31.92 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

25.75 (calculated-QSPR, Dunnivant et al. 1992)

49.63 (calculated-QSPR, Achman et al. 1993)

7.44 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

21.9 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 51 \pm 25\ kJ/mol$, $\Delta S_H = 0.13 \pm 0.09\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.10 (calculated-TSA, Burkhard 1984)

5.15 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.29 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.15 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

4.90 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 2.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17 \text{ d}$ for dichlorobiphenyls, based on $k_{OH}(\text{calc.}) = (1.4\text{--}2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2 \text{ d}$ for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0\text{--}4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated $k_{OH}(\text{calc}) = (1.4\text{--}3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water:

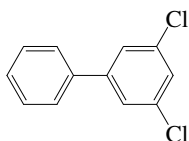
Ground water:

Sediment:

Soil:

Biota:

7.1.1.14 3,5-Dichlorobiphenyl (PCB-14)



Common Name: 3,5-Dichlorobiphenyl

Synonym: PCB-14, 3,5-dichloro-1,1'-biphenyl

Chemical Name: 3,5-dichlorobiphenyl

CAS Registry No: 34883-41-5

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

36 (Hinkel & Hay 1928)

31–32 (Weingarten 1961; Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.872 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.05 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.00792, 0.0425, 0.0722, 0.109 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.128, 0.0662, 0.114 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.0785 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.126, 0.117 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -3885/(T/K) + 12.13$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

16.72 (calculated-P/C, Burkhard et al. 1985b)

49.55 (calculated- QSAR-MCI χ , Sabljic & Güsten 1989)

42.63 (calculated-QSPR, Dunnivant et al. 1992)

20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3\ kJ/mol$, $\Delta S_H = 0.14 \pm 0.01\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.37 ± 0.1 (shake flask-GC/ECD, Bruggeman et al. 1982)

5.63, 5.56, 5.29, 5.16 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.28 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.17 (HPLC- k' correlation, Noegrohati & Hammers 1992)

5.41 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

8.82, 7.78 (0, $20^{\circ}C$, multi-column GC- k' correlation, Zhang et al. 1999)

7.53 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.38–3.83 mean 3.79 (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
3.82; 3.79 (rainbow trout: kinetic BCF, steady-state BCF, Oliver & Niimi 1985)

Sorption Partition Coefficient, log K_{OC} :

4.90 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17 \text{ d}$ for dichlorobiphenyls, based on $k_{OH}(\text{calc.}) = (1.4 - 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)

$k_{OH} = (4.2 \pm 1.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $297 \pm 2 \text{ K}$ (relative rate method, Kwok et al. 1995)

tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2 \text{ d}$ for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0 - 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated $k_{OH}(\text{calc}) = (1.4 - 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 310 \text{ d}^{-1}$; $k_2 = 0.046 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$\log 1/k_2 = 1.3, 2.5 \text{ h}$ (fish, selected, calculated- K_{OW} , Hawker & Connell 1988)

$1/k_2 = 21.7 \text{ d}$ (rainbow trout, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

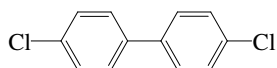
Sediment:

Soil:

Biota: $t_{1/2} = 15 \text{ d}$ in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985),

$t_{1/2} = 14 \text{ d}$ in its muscle (Niimi & Oliver 1983).

7.1.1.15 4,4'-Dichlorobiphenyl (PCB-15)



Common Name: 4,4'-Dichlorobiphenyl

Synonym: PCB-15, 4,4'-dichloro-1,1'-biphenyl

Chemical Name: 4,4'-dichlorobiphenyl

CAS Registry No: 2050-68-2

Molecular Formula: $C_{12}H_8Cl_2$

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

149.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

317 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$): 1.0536Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point)

185.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} ($J/mol K$):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.059 (Shiu & Mackay 1986)

0.0546 (Gobas et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

0.050 (Webb 1970)

0.060 (Hoover 1971)

0.080 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.056 (generator column-GC/ECD, Weil et al. 1974)

0.062 ($20^{\circ}C$, shake flask-GC, Chiou et al. 1977; Freed et al. 1977)

0.046 (generator column-HPLC/UV, Billington 1982)

0.065 (generator column-HPLC/UV, Huang 1983)

0.058 (generator column-HPLC/UV, Billington et al. 1988)

0.151, 0.0774, 0.0952, 0.07055 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0363 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.057 \pm 0.0021*(generator column-GC/ECD, measured range $5-45^{\circ}C$, Shiu et al. 1997) $\ln x = -2.8677 - 4839.46/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

1.116, 0.959 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

 $\log S_L/(mol m^{-3}) = -807/(T/K) + 0.41$ (supercooled liquid, linear regression of literature data, Li et al. 2003) $\log S_L/(mol m^{-3}) = -909/(T/K) + 0.68$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00253* (Knudsen-effusion technique, extrapolated, Smith et al. 1964)

0.043 (P_L calculated from P_s using fugacity ratio F, Smith et al. 1964)0.071, 0.084 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Bidleman 1984)0.0508 (supercooled liquid P_L , Burkhard 1984)0.075, 0.059 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00313 (GC-RI correlation, Burkhard et al. 1985a)

0.0508 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0263 (extrapolated Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = -5416/(T/\text{K}) + 12.585$; temp range 50–87°C (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 10.10 - 4090/(T/\text{K})$ (GC-RT correlation, Tateya et al. 1988)
 0.0603, 0.0776 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/\text{Pa}) = -3971/(T/\text{K}) + 12.18$; (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)
 0.00197* (gas saturation-GC/ECD, Wania et al. 1994)
 $\log (P_s/\text{Pa}) = -4977/(T/\text{K}) + 14.10$; temp range –20 to 30°C (gas saturation-GC, solid, Wania et al. 1994)
 0.0426 (supercooled liquid P_L , 20°C, from Falconer & Bidleman, Harner & Bidleman 1996)
 0.00313–0.0219; 0.018–0.0837 (literature P_s range; literature P_L range, Delle Site 1997)
 0.223; 0.084 (P_L , calculated-MCI χ and Characteristic Root Index [CRI]; quoted lit., Saçan & Balcioglu 1998)
 $\log P/\text{Pa} = 14.10 - 4977/(T/\text{K})$ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 0.0589, 0.0575 (supercooled liquid P_L ; LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log P_L/\text{Pa} = -3931/(T/\text{K}) + 11.89$ (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
 $\log P_L/\text{Pa} = -3829/(T/\text{K}) + 11.60$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

30.4 (calculated-P/C, Murphy et al. 1983)
 11.04 (calculated-P/C, Burkhard et al. 1985b)
 14.69 (calculated, Coates & Elzerman 1986)
 17.0 (calculated-P/C, Shiu & Mackay 1986)
 20.16 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988)
 9.66 (wetted-wall column-GC/ECD, Fendinger & Glotfelty 1990)
 18.95; 22.70 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)
 20.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3 \text{ kJ/mol}$, $\Delta S_H = 0.14 \pm 0.01 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004
 14.12, 13.49 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -2921/(T/\text{K}) + 10.92$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.58 (shake flask-GC, Chiou et al. 1977)
 5.17 (HPLC-RT correlation, Sugiura et al. 1978)
 5.51 (Hansch & Leo 1979)
 5.50 (shake flask-GC, Platford 1982)
 5.36 \pm 0.1; 5.28 (shake flask-GC; RP-TLC- k' correlation, Bruggeman et al. 1982)
 4.92 (HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)
 5.33 (generator column-GC/ECD; Woodburn et al. 1984)
 4.82 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
 5.30 (selected, Shiu & Mackay 1986)
 5.33 (generator column-GC/ECD, Doucette & Andren 1987)
 5.03, 5.39, 5.22, 5.28 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.17 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 5.23 (recommended, Sangster 1993)
 5.58 (recommended, Hansch et al. 1995)
 5.35, 5.36 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.67* (generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)
 $\log K_{OA} = -5.10 + 3791.7/(T/\text{K})$, temp range: –10 to 20°C (generator column-GC, Harner & Mackay 1995)
 7.88 (20°C, generator column-GC, Harner & Bidleman 1996)
 $\log K_{OA} = -5.06 + 3792/(T/\text{K})$; (temp range –10 to +20°C, Harner & Bidleman 1996)
 8.87, 7.88; 7.89 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)

8.12 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
 7.73; 7.77 (calibrated GC-RT correlation, GC-RT correlation, Wania et al. 2002)
 7.65, 7.85 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log K_{OA} = 4078/(T/K) - 5.83$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

2.97 (killifish, Goto et al. 1978)
 2.33 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
 3.47 (calculated-S, Kenaga 1980)
 3.58 (rainbow trout, highest value-non-equilibrated, Oliver & Niimi 1984)
 4.27 (*pecea omorika*, Reischl et al. 1989 from Reischl 1988)
 4.06, 5.36 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} :

4.30 (calculated-solubility, Kenaga 1980)
 4.91 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.65 (EPA-B2 river sediment, Coates & Elzerman 1986)
 4.03 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated evaporation $t_{1/2} = 4.5$ h for an initial concentration of 0.03 ppm in a 4.5 cm depth of water solution in a glass dish and $t_{1/2} = 1.7$ h with stirring of the solution; while experimental observed $t_{1/2} = 4.0$ h and 1.5 h under the same condition with stirring of the solution (Chiou et al. 1979).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)
 tropospheric lifetime $\tau(\text{calc}) = 8\text{--}17$ d for dichlorobiphenyls, based on $k_{OH}(\text{calc.}) = (1.4 - 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for dichlorobiphenyls at room temp. (Atkinson 1987)
 tropospheric lifetime $\tau(\text{calc}) = 3.4\text{--}7.2$ d for dichlorobiphenyls, based on the experimentally determined gas-phase reaction $k_{OH}(\text{exptl}) = (2.0 - 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and the calculated $k_{OH}(\text{calc}) = (1.4 - 3.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50–80% biodegraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);
 $t_{1/2} = 72$ h for 50% degradation in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, and 55% degradation at 24 h in another PCB mixture by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986);
 aerobic biodegradation $t_{1/2} = 1.42$ d without the addition of polymer chitin, $t_{1/2} = 0.98$ d with chitin and $t_{1/2} = 0.46$ d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 81$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 99$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radical for dichlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 3.4–7.2 d based on the experimentally determined rate constant for gas-phase reaction with OH radical for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 57.5$ d in Lake Michigan, 57.5 d (Neely 1983);

aerobic biodegradation $t_{1/2} = 1.42$ d without the addition of polymer chitin, $t_{1/2} = 0.98$ d with chitin and $t_{1/2} = 0.46$ d with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 27$ d in *Picea omorika* (Reischl et al. 1989).

depuration $t_{1/2} = 81$ d for high-dose treatment, $t_{1/2} = 99$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.15.1

Reported aqueous solubilities, vapor pressure and octanol-air partition coefficients of 4,4'-dichlorobiphenyl (PCB-15) at various temperatures

Aqueous solubility		Vapor pressure				log K_{OA}	
Shiu et al. 1997		Smith et al. 1964		Wania et al. 1994		Harner & Mackay 1995	
generator column-GC/ECD		Knudsen effusion		gas saturation-GC/ECD		generator column-GC	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	log K_{OA}
5	0.021	29.88	0.149	-10	1.206×10^{-5}	-10	9.36
15	0.0346	29.88	0.152	0	8.303×10^{-5}	0	8.83
25	0.0570	66.58	0.504	10	4.159×10^{-4}	10	8.35
35	0.106	66.58	0.432	20	1.197×10^{-3}	20	7.88
45	0.186	76.78	1.26	30	4.475×10^{-3}	25	7.67
		76.78	1.27				
		87.0	3.55	log P/Pa = A - B/(T/K)		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 72.6$	
$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 40.2$ at 5–45°C		87.0	3.57	A	14.10	log $K_{OA} = A + B/T$	
				B	4977	A	-5.1
		log P/mmHg = A - B/(T/K)		temp range -10 to 30°C		B	3791.7
		A	13.460	$\Delta H_{subl}/(\text{kJ mol}^{-1}) = 95.3$			
		B	5416				

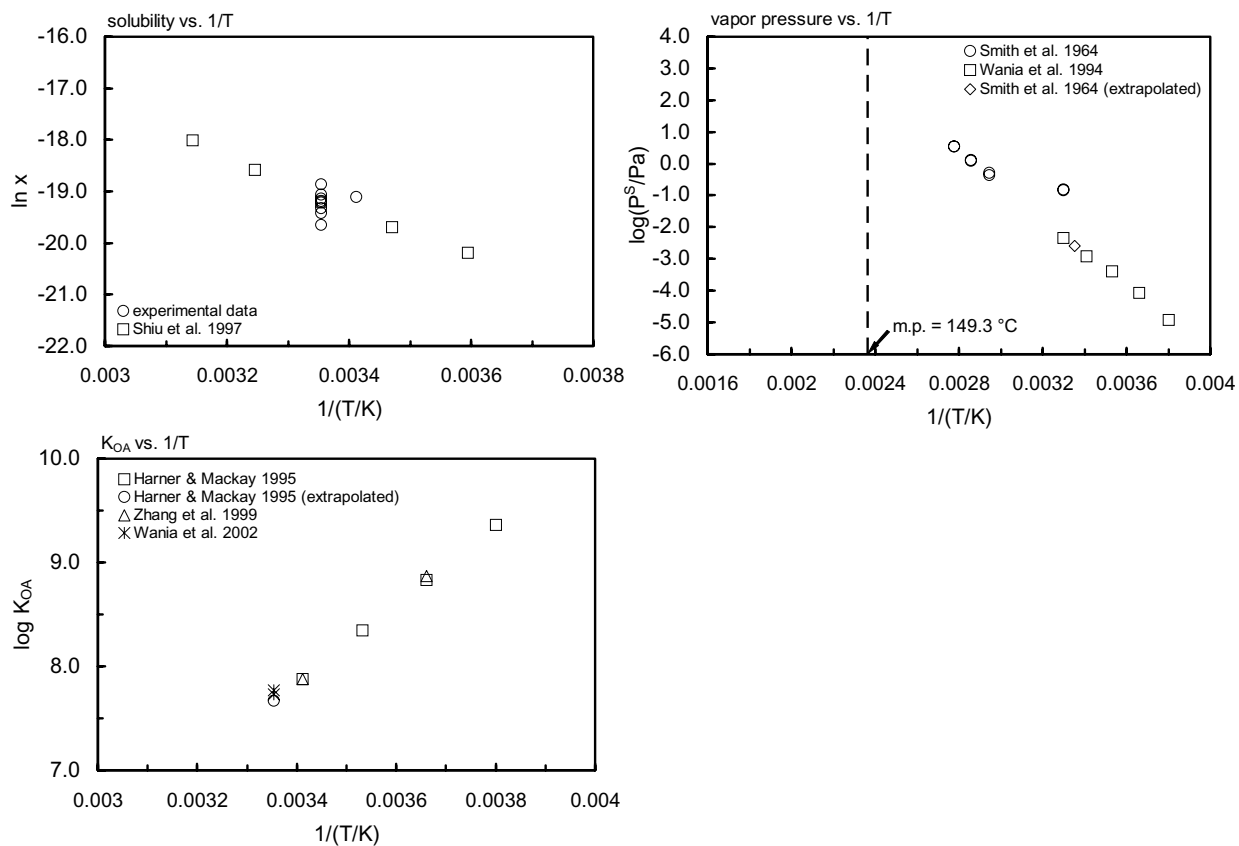
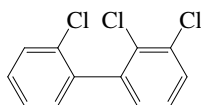


FIGURE 7.1.15.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 4,4'-dichlorobiphenyl (PCB-15).

7.1.1.16 2,2',3-Trichlorobiphenyl (PCB-16)



Common Name: 2,2',3-Trichlorobiphenyl

Synonym: PCB-16, 2,2',3-trichloro-1,1'-biphenyl

Chemical Name: 2,2',3-trichlorobiphenyl

CAS Registry No: 38444-78-9

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

28.1–28.8 (Weingarten 1961; Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.934 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.505 (supercooled liquid, calculated-TSA, Burkhard et al. 1985b)

0.293 ($20^{\circ}C$, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.205 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.814 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.174 (calculated-MCI χ , Patil 1991)

0.674 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0522, 0.066, 0.033 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.069 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)

0.0538, 0.060 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0275 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 10.10 - 4100/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0427; 0.0427 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -3935/(T/K) + 11.93$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.0506; 0.0427 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI; quoted lit., Saçan & Balcioglu 1998)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated):

35.16 (calculated-P/C, Burkhard et al. 1985b)

80.0 (calculated-P/C, Shiu & Mackay 1986)

24.11 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

81.77 (batch stripping, Atlas et al. 1982)

28.07 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)

25.45 (calculated-QSPR, Dunnivant et al. 1992)

4.02, 11.74 (0, $15^{\circ}C$, from modified two-film exchange model, Hornbuckle et al. 1994)

9.36 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

25.2 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 24$ kJ/mol, $\Delta S_H = 0.12 \pm 0.08$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.36 (calculated-TSA, Burkhard 1984)
- 4.15 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 5.31 (calculated- π const., Rapaport & Eisenreich 1984)
- 5.12 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
- 5.12 (recommended, Sangster 1993)
- 5.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations.:

- 7.22; 7.18 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -6.50 + 4240/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 8.87, 7.98 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
- 7.32 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.16 (suspended particulate matter, Burkhard 1984)
- 6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 5.00 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 7.2 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50% degraded by Nocardia strain NCIB 10603 within 7 d (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 90$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 72$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for $\text{OH}\cdot$ oxidation (Sedlak & Andren 1991)

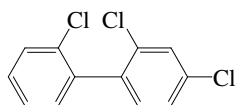
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 90$ d for high-dose treatment, $t_{1/2} = 72$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.17 2,2',4-Trichlorobiphenyl (PCB-17)



Common Name: 2,2',4-Trichlorobiphenyl

Synonym: PCB-17, 2,2',4-trichloro-1,1'-biphenyl

Chemical Name: 2,2',4-trichlorobiphenyl

CAS Registry No: 37680-66-3

Molecular Formula: $C_{12}H_8Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

35 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.292 (supercooled liquid S_L , Burkhard et al. 1985a)

0.259 (supercooled liquid S_L , Murphy et al. 1987)

0.103 (RP-HLC- k' correlation, Brodsky & Ballschmiter 1988)

0.647 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.080 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0566, 0.0828, 0.0219 (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.0705, 0.0739 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0335 (supercooled liquid P_L , Murphy et al. 1987)

0.0692; 0.0526 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -3935/(T/K) + 12.05$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.0692; 0.526 (P_L , quoted lit.; calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

52.18 (calculated-P/C, Burkhard et al. 1985b)

33.03 (calculated-P/C, Murphy et al. 1987)

40.63 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

37.82 (calculated-QSPR, Dunnivant et al. 1992)

26.04 (calculated-QSPR, Achman et al. 1993)

13.9 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

32.1 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.60, 5.76 (RP-HPLC-RT correlation: uncorrected, with ortho correction, Rapaport & Eisenrich 1984)

5.39 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.50 (generator column-GC, Larsen et al. 1992)

- 5.50 (recommended, Sangster 1993)
 5.76 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 8.06; 7.74 (0; 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
 7.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.24 (suspended particulate matter, Burkhard 1984)
 6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 4.84 (calculated-QSAR-MCI χ , Sabljic et al. 1995)
 5.20; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14-30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 7.5 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9-15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 81 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 99 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14-30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9-17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

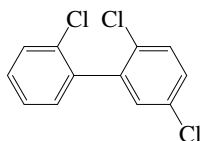
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 81 \text{ d}$ for high-dose treatment, $t_{1/2} = 99 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.18 2,2',5-Trichlorobiphenyl (PCB-18)



Common Name: 2,2',5-Trichlorobiphenyl

Synonym: PCB-18, 2,2',5-trichloro-1,1'-biphenyl

Chemical Name: 2,2',5-trichlorobiphenyl

CAS Registry No: 37680-65-2

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

43–44 (Hutzinger et al. 1974; Erickson 1986)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.1485

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.648 (Mackay et al. 1980)

0.651 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.640 (shake flask-GC/ECD, Weil et al. 1974)

0.248 (shake flask-GC/ECD, Haque & Schmedding 1975)

0.016 (radioactive isotope- ^{14}C labeled, Metcalf et al. 1975)

0.0614 (shake flask-GC/ECD from Aroclor 1242, Lee et al. 1979)

0.085 (Kenaga & Goring 1980; Kenaga 1980)

0.110 (shake flask GC/ECD, Bruggeman et al. 1981)

0.299 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.203, 0.135, 0.100, 0.112 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.510; 0.780 (generator column-GC/ECD, supercooled liquid S_L , Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.267 (Neely 1981)

0.412 (P_L calculated from P_S using fugacity ratio F, Neely 1981)

0.012 (Neely 1983)

0.0904 (supercooled liquid P_L , Burkhard 1984)

0.0605 (GC-RI correlation, Burkhard et al. 1985a)

0.0904 (supercooled liquid P_L , GC-RT correlation, Burkhard et al. 1985b)

0.0776, 0.0833 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.143; 0.220 (selected: solid P_S ; supercooled liquid P_L , Shiu & Mackay 1986)

0.0352 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log (P/mmHg) = 10.10 - 4090/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0603, 0.0851 (supercooled liquid P_L ; GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = -3935/(T/K) + 12.09$; (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.033–0.0762; 0.035–0.116 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 101.53 (23°C, gas stripping-GC, Atlas et al. 1982)
 20.26 (20°C, gas stripping-GC, Oliver 1985)
 38.5 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988)
 25.33 (wetted-wall column-GC/ECD, Brunner et al. 1990)
 8.11, 12.07, 17.64, 25.358* ± 0.34, 34.14 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
 $\ln K_{AW} = 9.5020 - 4197.74/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(34.9/kJ\cdot mol^{-1})/RT] + (0.079/kJ\cdot mol^{-1}\cdot K^{-1})/R]$; where $R = 8.314 J\cdot K^{-1}\cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
 25.3 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 35 \pm 3 kJ/mol$, $\Delta S_H = 0.08 \pm 0.01 kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW} :

- 3.89 (radiolabeled-¹⁴C, Metcalf et al. 1975)
 6.22 (shake flask, Hansch & Leo 1979)
 5.88 (calculated after Rekker 1977, Könemann 1981)
 5.64 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 5.59; 4.34 (generator column-GC/ECD; HPLC-RT correlation, Woodburn 1982)
 4.39, 5.55 (RP-HPLC-RT correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
 5.60; 4.34 (generator column-GC/ECD; HPLC-RT correlation, Woodburn et al. 1984)
 4.97 (HPLC-RT correlation, DeVoe et al. 1987)
 4.97, 5.68 (HPLC- k' correlation, De Kock & Lord, 1987)
 5.60 (generator column-GC/ECD, Doucette & Andren 1987,1988)
 5.31, 5.37, 5.29, 5.37 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.55 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 5.44 (generator column-GC, Larsen et al. 1992)
 5.44 (recommended, Sangster 1993)
 5.60 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations:

- 7.60; 7.12 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
 $\log K_{OA} = -6.00 + 4060/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
 8.39 (10°C, estimated, Thomas et al. 1998)
 8.70, 7.79 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 7.48 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 3.86, 3.76, 2.91, 3.81 (algae, snail, mosquito, fish, ¹⁴C-labeled, Metcalf et al. 1975)
 1.72 (green sunfish, 15 d in static water, Sanborn et al. 1975)
 3.39 (calculated-S, Kenaga 1980)
 5.52; 5.83 (goldfish: 10% lipid by wt. in food; 3% lipid, static equilibration system-GC/ECD, 23-d exposure studies, Bruggeman et al. 1981)
 3.43–4.23 highest value 4.23 not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
 4.91, 4.23; 5.77 (rainbow trout, laboratory data: kinetic BCF(k_1/k_2), steady-state BCF (C_F/C_W); Lake Ontario field BCF, Oliver & Niimi 1985)
 4.30 (fish, calculated- C_B/C_W or k_1/k_2 , Connell & Hawker 1988; Hawker 1990)
 3.75 (*Picea omorika*, Reischl et al. 1989 from Reischl 1988)
 4.23 (fish, Isnard & Lambert 1989)
 5.82; 5.87 (goldfish; rainbow trout, Noegrohati & Hammers 1992)
 4.11; 5.64 (zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

- 2.60–4.19 (various marine species, mean dry wt. BCF, Hope et al. 1998)
 4.08–6.01 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
 4.23, 5.32 (rainbow trout, flow through-96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.30, 5.60 (goldfish: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.11, 5.64 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} :

- 4.50, 4.50, 5.0 (sediments: offshore Grand Haven 2.0% OC, nearshore Grand Haven 3.4% OC, Benton Harbor sediment 3.8% OC, batch equilibrium-sorption isotherm, Voice et al. 1983; Voice & Weber, Jr., 1985)
 5.24 (suspended particulate matter, Burkhard 1984)
 5.40; 5.50; 5.20 (field data of sediment trap material; Niagara River-organic matter; calculated- K_{OW} , Oliver & Charlton 1984)
 5.1–6.3, 5.5; 7.0 (suspended sediment, average; algae > 50 μ m, Oliver 1987a)
 4.57, 4.85 (natural solids, Aldrich humic acid, equilibrium dialysis, Chin & Weber 1989, Chin et al. 1990)
 5.34 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
 4.49 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
 4.85, 4.15 (Aldrich humic acid substrate with methyl salicylate, organic polymers present in Huron River water, Chin et al. 1990)
 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 4.23 (soil, calculated-MCI, Sabljic et al. 1995)
 4.53; 4.57 (soil, calculated-Characteristic Root Index [CRI]; quoted lit., Saçan & Balcioglu 1996)
 5.20; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
 4.85 (sediment: organic carbon OC \geq 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 6.9 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 50–80% being degraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 950 \text{ d}^{-1}$; $k_2 = 0.048 \text{ d}^{-1}$ (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986; Clark et al. 1990)

$k_2 = 0.0037 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark 1990)

$k_2 = 0.048, 0.0372 \text{ d}^{-1}$ (goldfish, exptl., correlated, Mackay & Hughes 1984)

$k_1 = 300 \text{ d}^{-1}$; $k_2 = 0.0037 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1 = 39.6 \text{ h}^{-1}$; $1/k_2 = 500 \text{ h}$ (goldfish, quoted, Hawker & Connell 1985)

$\log k_1 = 2.98 \text{ d}^{-1}$; $\log 1/k_2 = 1.32 \text{ d}$ (goldfish, quoted, Connell & Hawker 1988b)

$\log 1/k_2 = 2.4, 2.4 \text{ d}$ (fish, quoted, calculated- K_{OW} , Hawker & Connell 1988b).

$\log 1/k_2 = 1.32 \text{ d}$ (goldfish, quoted, Connell & Hawker 1988b; Thomann 1989)

$k_1 = 3760 \text{ d}^{-1}$; $k_2 = 0.292 \text{ d}^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.020 \text{ d}^{-1}$ with $t_{1/2} = 36 \text{ d}$ and $k_2 = 0.029 \text{ d}^{-1}$ with $t_{1/2} = 24 \text{ d}$ for food concn of 29 ng/g and 182 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 79 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 96 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 43.1 \text{ d}$ in Lake Michigan (Neely 1983); $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991).

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: 0.47 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 1.16 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 1.21 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.17 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: 0.00838 d^{-1} from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 0.00368 d^{-1} from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 0.00357 d^{-1} from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.00062 d^{-1} from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{1/2} = 190 \text{ d}$ in rainbow trout, 190 d and its muscle 86 d (Niimi & Oliver 1983);

$t_{1/2} = 190 \text{ d}$ in fish (rainbow trout, Niimi & Oliver 1983; Oliver & Niimi 1985);

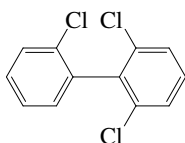
$t_{1/2} = 26 \text{ d}$ in worms at 8°C (Oliver 1987c);

$t_{1/2} = 25 \text{ d}$ in omorika (Reischl et al. 1989)

Depuration $t_{1/2} = 32\text{--}42 \text{ d}$ for a 32-d dietary exposure followed by a 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 79 \text{ d}$ for high-dose treatment, $t_{1/2} = 96 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.19 2,2',6-Trichlorobiphenyl (PCB-19)



Common Name: 2,2',6-Trichlorobiphenyl

Synonym: PCB-19, 2,2',6,-trichloro-1,1'-biphenyl

Chemical Name: 2,2',6-trichlorobiphenyl

CAS Registry No: 38444-73-4

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

46 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.345 (supercooled liquid S_L , Burkhard et al. 1985a)

0.448 (supercooled liquid S_L , Murphy et al. 1987)

0.447, 0.408, 0.235, 0.246 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.814 (calculated-TSA, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.167 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.171 (GC-RI correlation, Burkhard et al. 1985b)

0.113, 0.131 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0529 (supercooled liquid P_L , Murphy et al. 1987)

$\log(P/mmHg) = 9.86 - 3970/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0933, 0.138 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -3836/T + 11.93$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

124.6 (calculated-P/C, Burkhard et al. 1985b)

30.70 (calculated-P/C, Murphy et al. 1987)

45.09 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

23.30 (wetted-wall column-GC, Brunner et al. 1990)

44.74 (calculated-QSPR, Dunnivant et al. 1992)

13.9 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

32.2 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.75, 5.48 (RP-HPLC correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

4.88, 5.06, 5.03, 5.19 (RP-HPLC- k' correction, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

- 5.04 (recommended, Sangster 1993)
 5.48 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 6.72 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.28 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14-30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9-15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 155 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 84 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–15 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

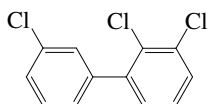
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 155 \text{ d}$ for high-dose treatment, $t_{1/2} = 84 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.20 2,3,3'-Trichlorobiphenyl (PCB-20)



Common Name: 2,3,3'-Trichlorobiphenyl

Synonym: PCB-20, 2,3,3'-trichloro-1,1'-biphenyl

Chemical Name: 2,3,3'-trichlorobiphenyl

CAS Registry No: 38444-84-7

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

58 (calculated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

337 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.402 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985a)

0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.174 (calculated-MCI χ , Patil 1991)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.033 (supercooled liquid P_L , GC-RT correlation, Burkhard et al. 1985a)

0.0283 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0269 (supercooled liquid P_L , GC-RT correlation, Foreman & Bidleman 1985)

$\log(P/mmHg) = 10.40 - 4310/(T/K)$, (GC-RT correlation, Tateya et al. 1988)

0.0302 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4075/(T/K) + 12.12$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry' Law Constant (Pa m^3/mol at $25^{\circ}C$):

81.77 (batch stripping-GC, Atlas et al. 1982)

17.23 (calculated-P/C, Burkhard et al. 1985b)

30.7 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

16.21 (wetted-wall column-GC/ECD, Brunner et al. 1990)

22.01 (calculated-QSPR, Dunnivant et al. 1992)

29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.99, 5.57 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)

5.57 (calculated-TSA, Hawker & Connell 1988a)

5.68 (generator column-GC, Larsen et al. 1992)

5.62 (recommended, Sangster 1993)

5.57 (recommended, Hansch et al. 1995)

5.4846 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated:

9.51, 8.49 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)

7.95 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

5.23 (suspended particulate matter, Burkhard 1984)

4.01–4.88; 5.20 (range, calculated from sequential desorption of 11 urban soils; lit. value, Krauss & Wilcke 2001)

5.13; 5.01, 4.88, 5.45 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 88 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

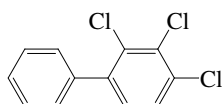
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 91 \text{ d}$ for high-dose treatment, $t_{1/2} = 88 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.21 2,3,4-Trichlorobiphenyl (PCB-21)



Common Name: 2,3,4-Trichlorobiphenyl

Synonym: PCB-21, 2,3,4-trichloro-1,1'-biphenyl

Chemical Name: 2,3,4-trichlorobiphenyl

CAS Registry No: 55702-46-0

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

101–102 (Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.176 (mp at $102^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.469 (calculated-TSA, Burkhard et al. 1985b)

0.224, 0.195, 0.142; 0.132 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.174 (calculated-MCI χ , Patil 1991)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00489 (GC-RI correlation, Burkhard et al. 1985a)

0.0269 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)

0.0295 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4075/(T/K) + 12.11$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

14.79 (calculated-P/C, Burkhard et al. 1985b)

21.38 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

23.0 (calculated-QSPR, Dunnivant et al. 1992)

29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.88 (calculated after Rekker 1977, Könnemann 1981)

5.77 (RP-TLC- k' correlation, Bruggeman et al. 1982)

5.51, 5.61, 5.87, 5.73 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.860 ± 0.017 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990;)

5.68 (recommended, Sangster 1993)

5.86 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.16 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}

5.19 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constants $k = 0.021 \text{ min}^{-1}$ with $t_{1/2} = 33 \text{ min}$, $k = 0.059 \text{ min}^{-1}$ with $t_{1/2} = 12 \text{ min}$ and $t_{1/2} = 0.14 \text{ min}^{-1}$ with $t_{1/2} = 5 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; rate constants $k = 0.0050 \text{ min}^{-1}$ with $t_{1/2} = 139 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 33 \text{ min}$, 12 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; $t_{1/2} = 139 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

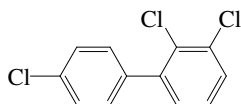
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.22 2,3,4'-Trichlorobiphenyl (PCB-22)



Common Name: 2,3,4'-Trichlorobiphenyl

Synonym: PCB-22, 2,3,4'-trichloro-1,1'-biphenyl

Chemical Name: 2,3,4'-trichlorobiphenyl

CAS Registry No: 38444-85-8

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

73 (Burkhard et al. 1985a; Shiu & Mackay 1986; Brodsky & Ballschmiter 1988)

69.0 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):Density (g/cm^3):Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at 25 $^{\circ}C$, F:0.335 (calculated-assuming $\Delta S_{fus} = 56$ J/mol K, Shiu & Mackay 1986)Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):0.397 (supercooled liquid S_L , Burkhard et al. 1985b)0.142 (supercooled liquid S_L , Murphy et al. 1987)0.408 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0696 (calculated-QSPR, Dunnivant et al. 1992)

0.187 (calculated-group contribution method, Kühne et al. 1995)

0.0677, 0.178 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.469 (calculated-mp and K_{ow} , Ran et al. 2002)Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations):0.0239 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0084 (GC-RI correlation, Burkhard et al. 1985b)

0.026, 0.023 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)0.0111 (supercooled liquid P_L , Murphy et al. 1987)0.0191, 0.0263 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992) $\log(P_L/Pa) = -4075/(T/K) + 12.08$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)0.0478 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Sağan & Balcıoğlu 1998)Henry's Law Constant (Pa·m 3 /mol at 25 $^{\circ}C$):

15.40 (calculated-P/C, Burkhard et al. 1985b)

20.16 (calculated-P/C, Murphy et al. 1987)

14.18 (wetted-wall column-GC/ECD, Brunner et al. 1990)

22.60 (calculated-molecular connectivity indices χ , Sabljic & Güsten 1989)

25.03; 19.35 (quoted exptl.; calculated-QSPR, Dunnivant et al. 1992)

13.2 (11 $^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)31.1 (from 11 $^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002) $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 31 \pm 1$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW} :

- 4.84, 5.42 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
 5.29 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
 5.63 (generator column-GC, Larsen et al. 1992)
 5.45 (recommended, Sangster 1993)
 5.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

- 9.60; 8.58 (0; 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 8.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :Partition Coefficient between particulate and dissolved contaminant concentrations, log K_p or log K_d

- 5.70, 4.90 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, log K_{OC} :

- 5.24 (suspended particulate matter, Burkhard 1984)
 6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 4.90 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14-30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 7.4 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0-2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9-15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.012 \text{ d}^{-1}$ with $t_{1/2} = 56 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.011 \text{ d}^{-1}$ with $t_{1/2} = 64 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

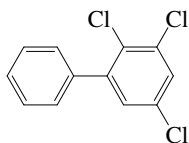
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 56 \text{ d}$ for high-dose treatment, $t_{1/2} = 64 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.23 2,3,5-Trichlorobiphenyl (PCB-23)



Common Name: 2,3,5-Trichlorobiphenyl

Synonym: PCB-23, 2,3,5-trichloro-1,1'-biphenyl

Chemical Name: 2,3,5-trichlorobiphenyl

CAS Registry No: 55720-44-0

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

41 (Burkhard et al. 1985a)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F:

0.694 (calculated-assuming $\Delta S_{fus} = 56$ J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.402 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.223 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0402 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0291 (GC-RI correlation, Burkhard et al. 1985b)

0.0447 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4075/(T/K) + 12.36$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

25.74 (calculated-P/C, Burkhard et al. 1985a)

35.6 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

32.26 (calculated-QSPR, Dunnivant et al. 1992)

29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.44 (calculated-TSA, Burkhard 1984)

5.53 (calculated, Miertus & Jakus 1990; quoted, Sangster 1993)

5.57 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.6729 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.23 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

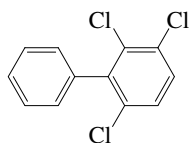
Ground water:

Sediment:

Soil:

Biota:

7.1.1.24 2,3,6-Trichlorobiphenyl (PCB-24)



Common Name: 2,3,6-Trichlorobiphenyl

Synonym: PCB-24, 2,3,6-trichloro-1,1'-biphenyl

Chemical Name: 2,3,6-trichlorobiphenyl

CAS Registry No: 55702-45-9

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

49 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.581 (mp at $49^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.507 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.132 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0677, 0.118, 0.0604, 0.098 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.514 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.167; 0.136, 0.358 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.132; 0.853 (quoted exptl., calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.087 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0899 (GC-RI correlation, Burkhard et al. 1985b)

0.0166 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log (P/mmHg) = 10.6 - 4090/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0708 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log (P_L/Pa) = -3935/(T/K) + 12.02$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

44.18 (calculated-P/C, Burkhard et al. 1985a)

32.12 ($20^{\circ}C$, Murphy et al. 1987)

34.35 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

22.3 (wetted-wall column-GC, Brunner et al. 1990)

31.53 (calculated-QSPR, Dunnivant et al. 1992)

14.1 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

32.4 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21 kJ/mol$, $\Delta S_H = 0.10 \pm 0.07 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.52, 5.67 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
 5.45, 5.42, 5.44, 5.46 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.44 (recommended, Sangster 1993)
 5.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 7.75 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:Sorption Partition Coefficient, $\log K_{OC}$:

- 5.16 (suspended particulate matter, Burkhard 1984)
 6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $k = (0.019\text{--}0.029) \text{ min}^{-1}$ with $t_{1/2} = 24\text{--}36 \text{ min}$, $k = (0.041\text{--}0.059) \text{ min}^{-1}$ with $t_{1/2} = 12\text{--}17 \text{ min}$ and $k = (0.12\text{--}0.22) \text{ min}^{-1}$ with $t_{1/2} = 3\text{--}6 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; rate constants, $k = (0.0066\text{--}0.030) \text{ min}^{-1}$ with $t_{1/2} = 23\text{--}105 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are: irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ; rate constant $k = 0.022 \text{ min}^{-1}$ with $t_{1/2} = 31 \text{ min}$ in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 7.6 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 81 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime $\tau = 14\text{--}30 \text{ d}$ due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime $\tau = 6.9\text{--}17 \text{ d}$ based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
 $t_{1/2} = 24\text{--}36$ min, 12–17 min and 3–6 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively;
 $t_{1/2} = 23\text{--}105$ min in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB are irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 ; $t_{1/2} = 31$ min in St. Lawrence River water containing 3 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

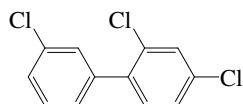
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 91$ d for high-dose treatment, $t_{1/2} = 81$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.25 2,3',4-Trichlorobiphenyl (PCB-25)



Common Name: 2,3',4-Trichlorobiphenyl

Synonym: PCB-25, 2,3',4-trichloro-1,1'-biphenyl

Chemical Name: 2,3',4-trichlorobiphenyl

CAS Registry No: 55712-37-3

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

61 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.317 (supercooled liquid S_L , Burkhard et al. 1985a)

0.025 (supercooled liquid S_L , Murphy et al. 1987)

0.20 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.1025 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0313 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0327 (GC-RI correlation, Burkhard et al. 1985b)

0.0373, 0.0366 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.24×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0295, 0.0372 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4075/(T/K) + 12.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

25.53 (calculated-P/C, Burkhard et al. 1985a)

43.27 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

32.04 (calculated-QSPR, Dunnivant et al. 1992)

17.20 (calculated-QSPR, Achman et al. 1993)

14.0 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

32.3 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 39 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.51 (calculated-TSA, Burkhard 1984)

5.67 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.54 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.63 (calculated, Miertus & Jakus 1990)

5.54 (recommended, Sangster 1993)

5.6793 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

9.31; 8.28; 8.23(0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
7.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.31 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 14-30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(aq.) = 7.2 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(calc) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 6.9-5 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 87 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 102 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

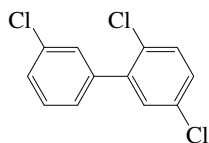
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 87 \text{ d}$ for high-dose treatment, $t_{1/2} = 102 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.26 2,3',5-Trichlorobiphenyl (PCB-26)



Common Name: 2,3',5-Trichlorobiphenyl

Synonym: PCB-26, 2,3',5-trichloro-1,1'-biphenyl

Chemical Name: 2,3',5-trichlorobiphenyl

CAS Registry No: 38444-81-4

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

40.0–40.5 (Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.705 (mp at $40.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.219, 0.166, 0.205, 0.155 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.253 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.138 ($20^{\circ}C$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0353 (supercooled liquid P_L , Burkhard et al. 1984)

0.0262 (GC-RI correlation, Burkhard et al. 1985a)

0.0363 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0411, 0.0412 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0182 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0316, 0.389 (supercooled liquid P_L , GC-RI correlation, different stationary phases Fischer et al. 1992)

$\log(P_L/Pa) = -4075/(T/K) + 12.28$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.0112–0.0402; 0.0182–0.0449 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

32.93 (gas stripping, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)

20.27 (wetted-wall column-GC, Brunner et al. 1990)

12.6 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

30.2 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.08$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.76 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)

5.52, 5.68, 5.72, 5.68 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.65 (recommended, Sangster 1993)

5.76 (recommended, Hansch et al. 1995):

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

9.30, 8.27; 8.24(0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)

8.57 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.31 (suspended particulate matter, Burkhard 1984)

6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 6.3 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegraded fairly quickly by *Alcaligenes* sp. strain Y-42 from lake sediments but small residue was detected after 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 105 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 135 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

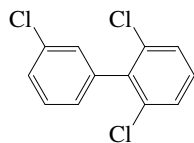
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 105 \text{ d}$ for high-dose treatment, $t_{1/2} = 135 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.27 2,3',6-Trichlorobiphenyl (PCB-27)



Common Name: 2,3',6-Trichlorobiphenyl

Synonym: PCB-27, 2,3',6-trichloro-1,1'-biphenyl

Chemical Name: 2,3',6-trichlorobiphenyl

CAS Registry No: 38444-81-4

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

45 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.404 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985a)

0.039 (supercooled liquid S_L , Murphy et al. 1987)

0.256 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0653 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0676 (GC-RI correlation, Burkhard et al. 1985b)

0.0598, 0.0628 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

4.26×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0490, 0.0708 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -3935/(T/K) + 11.97$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

41.64 (calculated-P/C, Burkhard et al. 1985a)

49.95 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

41.0 (calculated-QSPR, Dunnivant et al. 1992)

22.17 (quoted as PCB-24 and 27, Achman et al. 1993)

27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6 kJ/mol$, $\Delta S_H = 0.10 \pm 0.02 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.43 (calculated-TSA, Burkhard 1984)

5.44 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.52 (calculated, Miertsus & Jakus 1990; quoted, Sangster 1993)

5.50 (quoted as PCB-24 and 27, Murray & Andren 1992)

5.2417 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

5.23 (suspended particulate matter, Burkhard 1984)

6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7-1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14-30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 7.6 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4-11 d in freshwater systems, 0.1-10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0-2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9-15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 81 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14-30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9-17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

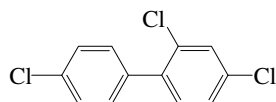
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 91 \text{ d}$ for high-dose treatment, $t_{1/2} = 81 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.28 2,4,4'-Trichlorobiphenyl (PCB-28)



Common Name: 2,4,4'-Trichlorobiphenyl

Synonym: PCB-28, 2,4,4'-trichloro-1,1'-biphenyl

Chemical Name: 2,4,4'-trichlorobiphenyl

CAS Registry No: 7012-37-5

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

57–58 (Hutzinger et al. 1971, 1974)

Boiling Point ($^{\circ}C$):

206–207 (Sengupta 1966)

Density (g/cm^3 at $20^{\circ}C$): 1.1485Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.6 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.482 (Mackay et al. 1980; Shiu & Mackay 1986)

0.482 (Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.085 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.260 (generator column-GC/ECD, Weil et al. 1974)

0.119 (Dexter & Pavlou 1978)

0.270 ($20^{\circ}C$, supercooled liquid S_L , shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985)

0.142 (generator column-HPLC/UV, Huang 1983)

0.163 (generator column-GC/ECD, Miller et al. 1984)

0.312 (supercooled liquid P_L , calculated-TSA, Burkhard et al. 1985b)

0.116 (shake flask-GC/ECD, Chiou et al. 1986)

0.143 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixture, Murphy et al. 1987)0.177, 0.107, 0.144, 0.117 (RP-HPLC- k' correlation, different stationary and mobile Brodsky & Ballschmiter 1988)0.067 ($22^{\circ}C$, generator column-GC, Opperhuizen et al. 1988)

0.117 (generator column-GC, Dunnivant & Elzerman 1988)

 $\log [S_L/(mol/L)] = 0.232 - 975.5/(T/K)$; (supercooled liquid, Passivirta et al. 1999)

0.260, 0.228 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

 $\log [S_L/(mol m^{-3})] = -1147/(T/K) + 0.79$ (supercooled liquid, final adjusted eq., Li et al. 2003)Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):0.0277 (supercooled liquid P_L , Burkhard 1984)

0.014 (GC-RI correlation, Burkhard et al. 1985a)

0.0277 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)0.0339, 0.0340 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)0.0149 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0277, 0.0335 (supercooled liquid, Dunnivant & Elzerman 1988)

 $\log (P/mmHg) = 10.40 - 4270/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.257, 0.0324 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/Pa) = -4075/(T/K) + 12.20$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)
 0.0210; 0.0436 (solid, supercooled liquid, Passivirta et al. 1999)
 $\log (P_S/Pa) = 15.15 - 5049/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/Pa) = 12.20 - 4075/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 0.0234, 0.0269 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log (P_L/Pa) = -4157/(T/K) + 12.31$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
 $\log (P_L/Pa) = -4007/(T/K) + 11.87$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^\circ C$ or as indicated and reported temperature dependence equations

32.02 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988)
 20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
 8.7, 21.2, 47.4, 50.3, 70.8, 120.6, 122.2 (10.4, 20, 30.1, 34.9, 42.1, 47.9, $48.4^\circ C$, gas stripping-HPLC/fluorescence, ten Hulscher et al. 1992)
 $\log [H/(Pa\cdot m^3/mol)] = 11.97 - 3100/(T/K)$; (Passivirta et al. 1999)
 13.13, 19.06, 27.18, 38.14 ± 0.37 , 50.39 (4, 11, 18, 25, $31^\circ C$, gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(32.5/kJ\cdot mol^{-1})/RT] + (0.074/kJ\cdot mol^{-1}\cdot K^{-1})/R$; where $R = 8.314\ J\cdot K^{-1}\cdot mol^{-1}$ and temp range: $4-31^\circ C$, (gas stripping-GC, Bamford et al. 2000)
 19.72 ($20^\circ C$, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 6.324 - 2467/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 36.5 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 33 \pm 2\ kJ/mol$, $\Delta S_H = 0.07 \pm 0.01\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004
 33.11, 30.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
 $\log [H/(Pa\ m^3/mol)] = -2010/(T/K) + 857$ (LDV linear regression of literature data, Li et al. 2003)
 $\log [H/(Pa\ m^3/mol)] = -2860/(T/K) + 11.08$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.38 (shake flask-GC, Paris et al. 1978)
 5.74 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 5.62 (shake flask-GC/ECD, Chiou et al. 1983; Chiou 1985; Chiou & Block 1986)
 5.69 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
 5.51, 5.77, 5.81, 5.74 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.68 (generator column-GC, Larsen et al. 1992)
 5.59 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 5.71 (recommended, Sangster 1993)
 5.62 (recommended, Hansch et al. 1995)
 5.55, 5.66 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^\circ C$ or as indicated and reported temperature dependence equations:

7.92 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
 $\log K_{OA} = -6.12 + 4190/(T/K)$ (fugacity meter, temp range $10-43^\circ C$, Kömp & McLachlan 1997a)
 8.76 ($10^\circ C$, estimated, Thomas et al. 1997)
 9.43, 8.40 ($0, 20^\circ C$, multi-column GC- k' correlation, Zhang et al. 1999)
 8.03 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
 7.93, 7.85 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log K_{OA} = 4102/(T/K) - 5.91$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$:

2.60–3.82 (various marine species, mean dry wt. BCF, Hope et al. 1998)
 3.82–4.93 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
 4.32, 5.62 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.74, 5.66 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

5.50, 4.70 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 4.23 (calculated, Kenaga 1980)
- 4.38 ($\log K_{OM}$ soil organic matter, Wood burn soil, equilibrium sorption isotherm-GC/ECD, Chiou et al. 1983)
- 5.31 (suspended particulate matter, Burkhard 1984)
- 5.28 (sediment: suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
- 5.30; 4.59 (suspended solids-Lake Superior: calculated- K_{OW} , Baker et al. 1986)
- 4.40; 3.54 (Sanhedron soil-Suwannee River; humic acid, shake flask-GC, Chiou et al. 1986, 1987)
- 3.89; 3.57 (Sanhedron soil-Suwannee River; fulvic acid, shake flask-GC, Chiou et al. 1986, 1987)
- 4.84; 4.24 (Fluka-Tridom humic acid; Calcasieu River humic extract, Chiou et al. 1987)
- 3.53; 3.27 (Suwannee River water sample; Sopchoppy River water sample, Chiou et al. 1987)
- 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.03–4.91; 5.30–5.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.25; 5.27, 4.91, 5.32 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolysis rate k_p (exptl) = $6 \times 10^{-8} \text{ d}^{-1}$ with $t_{1/2} = 133 \text{ d}$; k_p (calc) = $2.2 \times 10^{-8} \text{ d}^{-1}$ in winter sunlight at 40°L in surface waters (Dulin et al. 1986)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k_{OH} (calc) = $(0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime τ (calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH} (aq.) = $7.2 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

k_{OH} (calc) = $(1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime τ (calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: $t_{1/2} = 7 \text{ h}$ of biodegradation by *Alcaligenes* sp. strain Y-42 from lake sediments (Furukawa & Matsumura 1976; quoted, Pal et al. 1980);

49% degradation at 72 h in one of the defined PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.016 \text{ d}^{-1}$ with $t_{1/2} = 44 \text{ d}$ and $k_2 = 0.015 \text{ d}^{-1}$ with $t_{1/2} = 46 \text{ d}$ for food concn of 16 ng/g and 108 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_1 = 0.00054 \text{ h}^{-1}$; $k_2 = 0.089 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

k_1 (calc) = 11 (food lipid (mg)/(g worm lipid-d); k_2 (calc) = 0.14 d^{-1} (earthworm, Wågman et al. 2001)

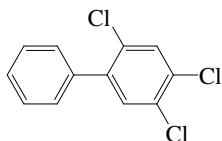
$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 88 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

- Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995);
 $t_{1/2} = 72$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
- Surface water: photolysis $t_{1/2} = 133$ d in winter sunlight at 40°L in surface waters (Dulin et al. 1986);
half-lives range from $t_{1/2} \sim 4$ –11 d in freshwater systems, $t_{1/2} = 0.1$ –10 d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);
 $t_{1/2} = 1450$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
- Groundwater:
- Sediment: $t_{1/2} = 26000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
- Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: 0.47 d⁻¹ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 1.15 d⁻¹ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 1.34 d⁻¹ from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.53 d⁻¹ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; 0.00378 d⁻¹ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, 0.00183 d⁻¹ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, 0.0016 d⁻¹ from Tarehee surface soil consist of sand and silt with 0.02% OC and 0.00044 d⁻¹ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).
 $t_{1/2} = 26000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
- Biota: depuration $t_{1/2} = 44$ –46 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
 $t_{1/2} = 7.8$ h in blood plasma (ring doves, Drouillard & Norstrom 2000);
elimination $t_{1/2} = 5$ d in earthworm given contaminated food (predicted, Wågman et al. 2001)
depuration $t_{1/2} = 91$ d for high-dose treatment, $t_{1/2} = 88$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.29 2,4,5-Trichlorobiphenyl (PCB-29)



Common Name: 2,4,5-Trichlorobiphenyl

Synonym: PCB-29, 2,4,5-trichloro-1,1'-biphenyl

Chemical Name: 2,4,5-trichlorobiphenyl

CAS Registry No: 15862-07-4

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

78.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.1485

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.8 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

65.27 (Miller et al. 1984)

65.24, 63.0 (literature exptl. value, calculated, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.30 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.092 (generator column-GC/ECD, Weil et al. 1974)

0.119 (Dexter & Pavlou 1978)

0.140 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)

0.142 (generator column-HPLC/UV, Huang 1983)

0.162 (generator column-GC/ECD, Miller et al. 1984, 1985)

0.0098, 0.107, 0.138, 0.120 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.106* \pm 0.0045 (generator column-GC/ECD, Shiu et al. 1997)

0.0413, 0.0682, 0.106, 0.203, 0.33 (5, 15, 25, 35, $45^{\circ}C$, generator column-GC, Shiu et al. 1997)

$\ln x = -3.06175 - 4633.86/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.479, 0.389 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

$\log S_L/(mol m^{-3}) = -824/(T/K) + 0.03$ (supercooled liquid, linear regression of literature data, Li et al. 2003)

$\log S_L/(mol m^{-3}) = -977/(T/K) + 0.46$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0443 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

0.0112 (GC-RI correlation, Burkhard et al. 1985a)

0.0320 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0453, 0.0464 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log (P_L/Pa) = -4075/(T/K) + 12.20$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.0263 ($20^{\circ}C$, supercooled liquid P_L , from Falconer & Bidleman 1994; Harner & Bidleman 1996)

0.0447, 0.0457 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log P_L/Pa = -3904/(T/K) + 11.75$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

20.27 (wetted-wall column-GC, Brunner et al. 1990; quoted, Achman et al. 1993)

37.89* ± 0.53 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)

$\ln K_{AW} = 9.863 - 4197.74/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(34.9/\text{kJ}\cdot\text{mol}^{-1})/RT + (0.082/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R]$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)

36.3 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 35 \pm 3 \text{ kJ/mol}$, $\Delta S_H = 0.08 \pm 0.01 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

32.36, 30.20 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

$\log [H/(\text{Pa m}^3/\text{mol})] = -1674/(T/K) + 7.13$ (LDV linear regression of literature data, Li et al. 2003)

$\log [H/(\text{Pa m}^3/\text{mol})] = -2927/(T/K) + 11.30$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$ or as indicated and reported temperature dependence equations:

6.22 (Hansch & Leo 1979)

5.77 (RP-TLC- k' correlation, Bruggeman et al. 1982)

5.86 (HPLC-RT correlation, Woodburn 1982)

5.51 (generator column-GC/ECD, Miller et al. 1984)

5.81 (generator column-GC, Woodburn et al. 1984)

5.86 (HPLC-RT correlation, Woodburn et al. 1984)

6.25 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)

5.66 (HPLC-RP/MS, Burkhard & Kuehl 1986)

5.81 (generator column-GC/ECD, Doucette & Andren 1987)

5.78, 5.82, 5.88, 5.76 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.86 (shake flask/slow stirring-GC, De Bruijn et al. 1989)

5.901 ± 0.007 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)

5.54 (HPLC- k' correlation, Noegrohati & Hammers 1992)

5.81 (recommended, Sangster 1993)

5.90 (recommended, Hansch et al. 1995)

5.74, 5.60 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.96* (generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)

$\log K_{OA} = -4.80 + 3791.7/(T/K)$; temp range –10 to +20°C (generator column-GC, Harner & Mackay 1995)

8.03 (20°C, generator column-GC, Harner & Bidleman 1996)

$\log K_{OA} = -4.77 + 3792/(T/K)$; temp range –10 to +20°C (generator column-GC, Harner & Bidleman 1996)

9.15, 8.05 (0, 20°C, multi-column GC- k' correlation; Zhang et al. 1999)

8.21 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

8.01; 8.03 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

7.80, 7.78 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log K_{OA} = 4175/(T/K) - 6.22$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$:

4.97 (guppy, lipid wt. based, Gobas et al. 1989)

5.41 (guppy, corr. lipid wt. based, Gobas et al. 1989)

4.36, 5.53 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

5.26 (suspended particulate matter, Burkhard 1984)

4.51 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constants $k = (0.019\text{--}0.022) \text{ min}^{-1}$ with $t_{1/2} = 31\text{--}36 \text{ min}$, $k = (0.033\text{--}0.048) \text{ min}^{-1}$ with $t_{1/2} = 14\text{--}21 \text{ min}$ and $k = (0.13\text{--}0.14) \text{ min}^{-1}$ with $t_{1/2} = 5 \text{ min}$ in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; rate constants $k = (0.0056\text{--}0.020) \text{ min}^{-1}$ with $t_{1/2} = 35\text{--}123 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: half-life of biodegradation by *Alcaligenes* sp. strain Y-42 from lake sediments estimated to be less than 7 h (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$\log k_2 = -1.68 \text{ d}^{-1}$ (fish, quoted, Hawker & Connell 1985; Thomann 1989)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 190 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 100 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 31\text{--}36 \text{ min}$, 14–21 min and 5 min in aqueous Aroclor 1248 solution containing 45 ng/mL of total PCB irradiated by UVA-340 in the presence of 25, 50 and 100 $\mu\text{g/mL}$ TiO_2 , respectively; $t_{1/2} = 35\text{--}123 \text{ min}$ in aqueous Aroclor mixtures (Aroclor 1221, 1016, 1254, 1260) solution containing 450 ng/mL of total PCB irradiated by sunlight in the presence of 100 $\mu\text{g/mL}$ TiO_2 (Huang et al. 1996).

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 190 \text{ d}$ for high-dose treatment, $t_{1/2} = 100 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.29.1
Reported aqueous solubilities, Henry’s law constants and octanol-air partition coefficient log of 2,4,5-trichlorobiphenyl (PCB-29) at various temperatures

Solubility		Henry’s law constant		log K _{OA}	
Shiu et al. 1997		Bamford et al. 2000		Harner & Mackay 1995	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
5	0.0413	4	12.12	−10	9.5
15	0.0682	11	18.04	0	8.97
25	0.106	18	28.37	10	8.51
35	0.203	25	37.89	20	8.03
45	0.330	31	51.03	25	7.96

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 36.9$
at 5–45°C

$\ln K_{\text{AW}} = -\Delta H/RT + \Delta S/R$
 K_{AW}
A 9.8629
B 4197.74
enthalpy, entropy change:
 $\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 34.9 \pm 2.8$
 $\Delta S/(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) = 82 \pm 10$

$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 72.6$
 $\log K_{\text{OA}} = A + B/T$
A −4.8
B 3791.7

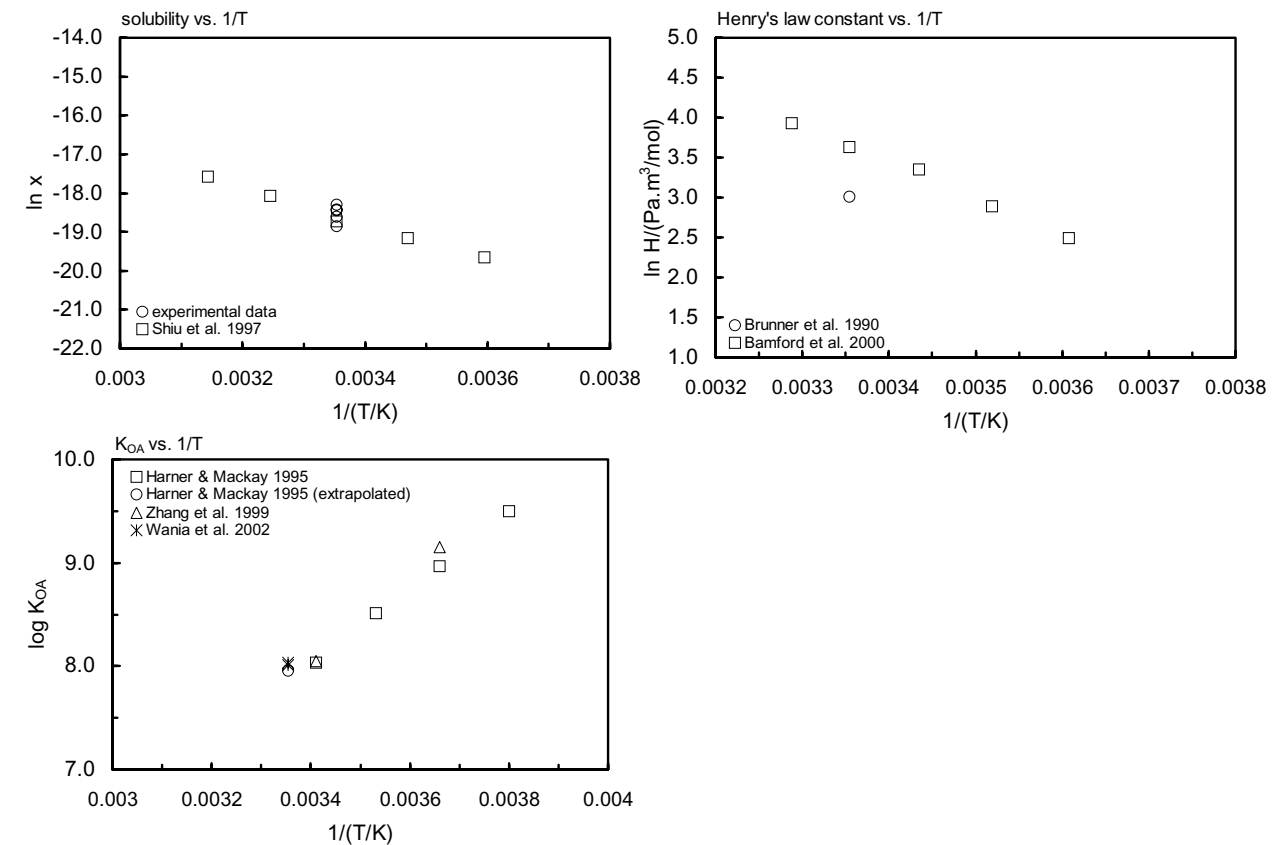
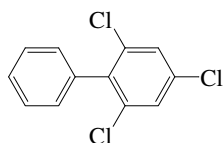


FIGURE 7.1.1.29.1 Logarithm of mole fraction solubility, Henry’s law constant and K_{OA} versus reciprocal temperature for 2,4,5-trichlorobiphenyl (PCB-29).

7.1.1.30 2,4,6-Trichlorobiphenyl (PCB-30)



Common Name: 2,4,6-Trichlorobiphenyl

Synonym: PCB-30

Chemical Name: 2,4,6-trichlorobiphenyl

CAS Registry No: 35693-92-6

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

62.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

16.5 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

49.37 (Miller et al. 1984)

49.36, 63.0 (literature exptl. value, calculated, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F :

0.427 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.226 (generator column/ECD, Miller et al. 1984,1985)

0.024, 0.0468, 0.0491, 0.0893 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.187* (generator column-GC/ECD, measured range $4-40^{\circ}C$, Doucette & Andren 1988)

0.0803, 0.187, 0.435 (4, 25, $40^{\circ}C$, generator column-GC/ECD, Doucette & Andren 1988)

$S/(mol/L) = 2.49 \times 10^{-7} \exp(0.047 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range $4-40^{\circ}C$, Doucette & Andren 1988a); or

$\log x = -1742/(T/K) - 1.983$, temp range $4-40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

0.252, 0.243 (generator column-GC, Dunnivant & Elzerman 1988)

0.236 (generator column-GC, Li et al. 1992)

0.235 (generator column-GC/ECD, Li et al. 1993)

0.217 (shake flask-GC/ECD, Li & Andren 1994)

$\ln x = -4.5969 - 4004.7/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.031 (Augood 1953; quoted, Bidleman 1984)

0.0865, 0.0948(P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)

0.030 (supercooled liquid P_L , converted from literature P_s with ΔS_{fus} Bidleman 1984)

0.0955, 0.144(supercooled liquid P_L calculated from P_{GC} , GC-RT correlation, different stationary phases, Bidleman 1984)

0.0421 (GC-RI correlation, Burkhard et al. 1985a)

0.111, 0.135(supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0946 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.110; 0.0851(supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = -3886/(T/K) + 12.02$; (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.0130–0.0637; 0.085–0.146 (literature P_s range; literature P_L range, Delle Site 1997)

Henry's Law Constant (Pa m³/mol at 25°C):

- 61.40 (calculated-P/C, Burkhard et al. 1985b)
- 49.51 (calculated-P/C, Shiu & Mackay 1986)
- 65.76 (batch stripping, Dunnivant et al. 1988 Dunnivant & Elzerman 1988)
- 47.51 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
- 58.04 (calculated-QSPR, Dunnivant et al. 1992)
- 27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
- $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

- 5.47 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 5.57 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
- 5.77, 5.70, 5.51, 5.48 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.33, 5.57 (RP-HPLC-k' correlation, different stationary phases, Sherblom & Eganhouse 1988)
- 5.711 \pm 0.014 (shake flask/slow stirring, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 5.75 (generator column-GC, Li et al. 1993)
- 5.62 (recommended, Sangster 1993)
- 5.71 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

- 7.28 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

- 5.24 (suspended particulates matter, Burkhard 1984)
- 4.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.7–1.6) \times 10⁻¹² cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime τ (calc) = 14–30 d, due to gas-phase loss process at room temp. (Atkinson 1987)

k_{OH}(calc) = (1.0–2.1) \times 10⁻¹² cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime τ (calc) = 6.9–15 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 30% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

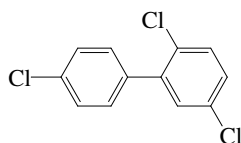
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.31 2,4',5-Trichlorobiphenyl (PCB-31)



Common Name: 2,4',5-Trichlorobiphenyl

Synonym: PCB-31, 2,4',5-trichloro-1,1'-biphenyl

Chemical Name: 2,4',5-trichlorobiphenyl

CAS Registry No: 16606-02-3

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

67 (Bellavita 1935; Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.384 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.11 (Kilzer et al. 1979)

0.075 (shake flask-GC/ECD, Bruggeman et al. 1981)

0.265, 0.155, 0.179, 0.120 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.090 (generator column-GC/ECD, Opperhuizen et al. 1988)

0.143 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.220, 0.194 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

$\log S_L/(mol m^{-3}) = -1123/(T/K) + 0.64$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0341, 0.0474 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Bidleman 1984)

0.0132 (GC-RI correlation, Burkhard et al. 1985a)

0.0313 (supercooled liquid P_L , calculated-GC-RI correlation, Burkhard et al. 1985b)

0.0373, 0.0346 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0149 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log (P/mmHg) = 10.40 - 4270/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0263, 0.0347 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = -4058/(T/K) + 12.14$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.024, 0.0257 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log (P_L/Pa) = -4149/(T/K) + 12.29$ (supercooled liquid, linear regression of literature data, Li et al. 2003)

$\log (P_L/Pa) = -4010/(T/K) + 11.86$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

94.13 (gas-stripping-GC, Atlas et al. 1982)

20.26 (calculated, Murphy et al. 1983)

25.43 (calculated-P/C, Burkhard et al. 1985b)

26.75 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

- 28.47 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
 19.25 (wetted-wall column-GC/ECD, Brunner et al. 1990)
 27.78 (calculated-QSPR, Dunnivant et al. 1992)
 20.21 (calculated-QSPR, Achman et al. 1993)
 12.9 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
 30.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 21$ kJ/mol, $\Delta S_H = 0.10 \pm 0.08$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
 37.15, 33.88 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -2887/(T/K) + 11.22$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.22 (Hansch & Leo 1979)
 5.30 (HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)
 5.77 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 5.69 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
 5.79 (generator column-GC/ECD, Woodburn et al. 1984)
 5.70 (selected, Shiu & Mackay 1986)
 5.99, 6.22, 6.18, 6.33 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.79 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
 5.59 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 5.68 (recommended, Sangster 1993)
 5.79 (recommended, Hansch et al. 1995)
 5.79, 5.78 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

- 7.92 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
 $\log K_{OA} = -6.12 + 4190/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
 9.43, 8.40; 8.23 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 8.13 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
 7.93, 7.94 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log K_{OA} = 4110/(T/K) - 5.84$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$:

- 3.45 (fish, Korte et al. 1978)
 -0.30, -0.22 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
 6.15 (goldfish, 3% lipid, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
 5.98 (goldfish, 10% lipid content in food, Bruggeman et al. 1981)
 3.95, 3.95, 4.51 (algae, fish, activated sludge, Freitag et al. 1984, 1985)
 3.66 (salmon fry in humic water-steady state, Carlberg et al. 1986)
 3.83 (salmon fry in lake water-steady state, Carlberg et al. 1986)
 4.62 (fish, calculated- C_B/C_W or k_1/k_2 Connell & Hawker 1988; Hawker 1990)
 4.66; 6.19 (zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)
 4/09 (algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)
 5.04 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
 3.95, 4.65 (algae: wet wt basis, dry wt basis, Geyer et al. 2000)
 4.23, 5.23 (*Daphna*: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.08, 6.04 (mussel: wet wt basis, dry wt basis, Geyer et al. 2000)
 4.63, 5.93 (goldfish: wet wt basis, dry wt basis, Geyer et al. 2000)
 4.67, 6.19 (zebrafish: wet wt basis, dry wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.90, 4.80 (Lake Superior suspended sediment, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.31 (suspended particulates, Burkhard 1984)
- 5.5–6.3, 5.9; 6.80 (suspended sediment, average; algae > 50 μm , Oliver 1987a)
- 5.48 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 4.63 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.51 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioglu 1996)
- 5.10 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 7.2 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation: 50–80% being degraded by *Alcaligenes* sp. strain Y-42 from lake sediments within 7-h period (Furukawa & Matsumura 1976; quoted, Pal et al. 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 890 \text{ d}^{-1}$; $k_2 = 0.021 \text{ d}^{-1}$ (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986)

$k_2 = 0.0035 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 37.1 \text{ h}^{-1}$; $1/k_2 = 1142 \text{ h}$ (goldfish, quoted, Hawker & Connell 1985)

$\log k_1 = 2.95 \text{ d}^{-1}$; $\log 1/k_2 = 1.68 \text{ d}$ (fish, quoted, Connell & Hawker 1988; Thomann 1989)

$k_1 = 3950 \text{ d}^{-1}$; $k_2 = 0.0867 \text{ d}^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)

$k_1 = 5044 \text{ h}^{-1}$, $k_2 = 0.411 \text{ h}^{-1}$ (algae *Chlorella fusca*, Wang et al. 1996)

$k_1 = 0.00447 \text{ h}^{-1}$; $k_2 = 0.100 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_1 = 14 \text{ L d}^{-1} \text{ g}^{-1} \text{ dry wt.}$; $k_2 = 0.129 \text{ d}^{-1}$ (Baltic Sea blue mussels, flow-through expt. Gustafsson et al. 1999)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 88 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from, $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2}$ = 196 d in rainbow trout, and $t_{1/2}$ = 81d in its muscle, (Niimi & Oliver 1983);

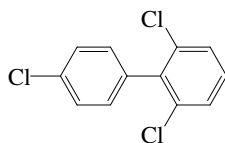
$t_{1/2}$ = 30 d in worms at 8°C (Oliver 1987c);

theoretical half-life to reach 90% steady-state tissue concn 5.4 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);

$t_{1/2}$ = 6.9 h in blood plasma (ring doves, Drouillard & Norstrom 2000).

depuration $t_{1/2}$ = 91 d for high-dose treatment, $t_{1/2}$ = 88 d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.32 2,4',6-Trichlorobiphenyl (PCB-32)



Common Name: 2,4',6-Trichlorobiphenyl

Synonym: PCB-32, 2,4',6-trichloro-1,1'-biphenyl

Chemical Name: 2,4',6-trichlorobiphenyl

CAS Registry No: 38444-77-8

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

70 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.399 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.355, 0.182, 0.129, 0.0778 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0578 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.060 (GC-RI correlation, Burkhard et al. 1985b)

0.0543, 0.0562 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P/mmHg) = 16.10 - 4100/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0427, 0.0589 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -3935/(T/K) + 11.93$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

37.29 (calculated-P/C, Burkhard 1984)

41.75 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)

39.69 (calculated-QSPR, Dunnivant et al. 1990)

27.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 6$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.60, 5.75 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

5.80 (selected, Shiu & Mackay 1986)

4.95, 5.29, 5.21, 5.52 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.47 (generator column-GC, Larsen et al. 1992)

5.49 (recommended, Sangster 1993)

5.75 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

- 7.72 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
 $\log K_{OA} = -6.50 + 4240/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
 8.89, 7.97; 7.92 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al 1999)
 7.49 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.23 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 8.0 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 85 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 111 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

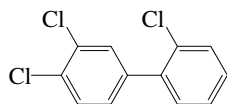
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 85 \text{ d}$ for high-dose treatment, $t_{1/2} = 111 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.33 2,3',4'-Trichlorobiphenyl (PCB-33)



Common Name: 2,3',4'-Trichlorobiphenyl

Synonym: PCB-33, 2,3',4'-trichlorobiphenyl, 2',3,4-trichloro-1,1'-biphenyl

Chemical Name: 2,3',4'-trichlorobiphenyl

CAS Registry No: 38444-86-9

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

60–60.5 (Wallnöfer et al. 1973)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.1485

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.452 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.078 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.291 (calculated-TSA, Mackay et al. 1980)

0.0796 (quoted lit. average, Yalkowsky et al. 1983)

0.371 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b;)

0.246, 0.170, 0.103, 0.142 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0814 (calculated-MCI χ , Nirmalakhandan & Speece 1989)

0.133 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.103 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.174 (calculated-MCI χ , Patil 1991)

0.152 (calculated-QSPR, Dunnivant et al. 1992)

0.209 (calculated-group contribution, Kühne et al. 1995)

0.0833, 0.219 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.576 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0107 (P_s from GC-RT correlation, Westcott & Bidleman 1981)

0.0133, 0.0160 (solid P_s , 25, $30^{\circ}C$, gas saturation-GC/ECD, Westcott et al. 1981)

$\log(P_s/mmHg) = 1.09 - 1510/(T/K)$, temp range $30-40^{\circ}C$ (gas saturation-GC/ECD, Westcott et al. 1981)

0.030 (P_L calculated from P_s using fugacity ratio F, Westcott et al. 1981)

0.0115 (GC-RI correlation, Burkhard et al. 1985a)

0.0243 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0264, 0.0219 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0136, 0.030 (selected P_s , P_L , Shiu & Mackay 1986)

0.0119 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P_L/mmHg) = 10.40 - 4330/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0137; 0.0272 (quoted; calculated-UNIFAC, Banerjee et al. 1990)

0.0214, 0.0295 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/P_a) = -4075/(T/K) + 12.09$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)
 0.00484–0.0270; 0.0119–0.030 (quoted lit. P_S range; lit. P_L range, Delle Site 1997)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

15.20 (calculated, Murphy et al. 1983)
 16.92 (calculated-P/C, Burkhard et al. 1985b)
 43.67 (calculated-P/C, Shiu & Mackay 1986)
 22.70 (20°C , calculated-P/C, Murphy et al. 1987)
 21.99 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
 16.21 (wetted wall column-GC/ECD, Brunner et al. 1990)
 24.31 (calculated-QSPR, Dunnivant et al. 1992)
 11.9 (11°C , gas stripping-GC/ECD, Bamford et al. 2002)
 29.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 22 \text{ kJ/mol}$, $\Delta S_H = 0.11 \pm 0.08 \text{ kJ/mol-K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.48, 5.66, 5.98, 5.71 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.872 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 5.71 (recommended, Sangster 1993)
 5.87 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

9.52, 8.52 ($0, 20^\circ\text{C}$, multi-column GC- k' correlation; Zhang et al. 1999)
 8.03 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log \text{BCF}$:

3.79 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)
 3.79, 6.04 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.57, 5.87 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

5.26 (suspended particulate matter, Burkhard 1984)
 4.64 (soil, calculated-S, Chou & Griffin 1986)
 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 5.20 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{aq.}) = 7.2 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C , half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
 $k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 88 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

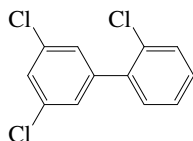
Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 1.90 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.88 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.37 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00413 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00099 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00052 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: depuration $t_{1/2} = 91 \text{ d}$ for high-dose treatment, $t_{1/2} = 88 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.34 2,3',5'-Trichlorobiphenyl (PCB-34)



Common Name: 2,3',5'-Trichlorobiphenyl

Synonym: PCB-34, 2,3',5'-trichlorobiphenyl, 2,3',5'-trichloro-1,1'-biphenyl

Chemical Name: 2,3',5'-trichlorobiphenyl

CAS Registry No: 37680-68-5

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

58.0 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.474 (mp at $58^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.319 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.129 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.162 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.205 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.036 (P_L supercooled liquid, Burkhard et al. 1985a)

0.0177 (GC-RI correlation, Burkhard et al. 1985b)

0.0447 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log (P_L/Pa) = -4075/(T/K) + 12.37$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

29.08 (calculated-P/C, Burkhard 1984)

51.17 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

42.73 (calculated-QSPR, Dunnivant et al. 1992)

29.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 41 \pm 4$ kJ/mol, $\Delta S_H = 0.10 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.51 (calculated-TSA, Burkhard 1984)

5.66 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.71 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988; recommended, Sangster 1993)

5.6522 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.72 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.31 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

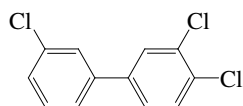
Ground water:

Sediment:

Soil:

Biota:

7.1.1.35 3,3',4-Trichlorobiphenyl (PCB-35)



Common Name: 3,3',4-Trichlorobiphenyl

Synonym: PCB-35

Chemical Name: 3,3',4-trichlorobiphenyl

CAS Registry No: 37680-69-6

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

87.0 (Burkhard et al. 1985a)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.246 (mp at $87^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.301 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.0152 (quoted-3,4,4'-trichlorobiphenyl from Weil et al. 1974; Opperhuizen et al. 1988)

0.0814 (calculated-MCI χ , Nirmalakhandan & Speece 1989)

0.0514 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00246 (GC-RI correlation, Burkhard et al. 1985a)

0.00949 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.014, 0.0105 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0129 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4242/(T/K) + 12.37$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

8.13 (calculated-P/C, Burkhard et al. 1985b)

22.49 (calculated-MCI χ , Sabljic & Güsten 1989)

18.23 (calculated-QSPR, Dunnivant et al. 1992)

20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.53 (calculated-TSA, Burkhard 1984)

5.82 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.7151 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.85 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.33 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

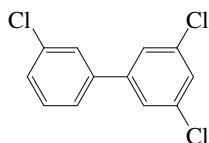
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.36 3,3',5-Trichlorobiphenyl (PCB-36)



Common Name: 3,3',5-Trichlorobiphenyl

Synonym: PCB-36, 3,3',5-trichloro-1,1'-biphenyl

Chemical Name: 3,3',5-trichlorobiphenyl

CAS Registry No: 38444-87-0

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

46 (estimated, Abramowitz & Yalkowsky)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.260 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985a)

0.00469, 0.0155, 0.010 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0814 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0141 (P_L supercooled liquid, Burkhard et al. 1985a)

0.0149 (GC-RI correlation, Burkhard et al. 1985b)

0.0191 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4242/(T/K) + 2.48$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

13.98 (calculated-P/C, Burkhard et al. 1985a)

51.47 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

17.40 (wetted-wall column-GC/ECD, Brunner et al. 1990)

34.10 (calculated-QSPR, Dunnivant et al. 1992)

20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.57 (calculated-TSA, Burkhard 1984)

4.15 (RP-HPLC- k' correlation, Rapaport & Eisenreich 1984)

5.70 (selected, Shiu & Mackay 1986)

5.88 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.76, 5.86, 5.80 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.81 (recommended, Sangster 1993)

5.8293 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

5.37 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

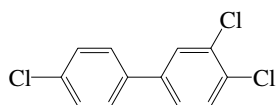
Ground water:

Sediment:

Soil:

Biota:

7.1.1.37 3,4,4'-Trichlorobiphenyl (PCB-37)



Common Name: 3,4,4'-Trichlorobiphenyl

Synonym: PCB-37

Chemical Name: 3,4,4'-trichlorobiphenyl

CAS Registry No: 38444-90-5

Molecular Formula: $C_{12}H_7Cl_3$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

86.8–87.8 (Weingarten 1961)

Boiling Point ($^{\circ}C$):Density (g/cm^3 at $20^{\circ}C$): 1.2024Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

198.7 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.244 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0152 (generator column-GC/ECD, Weil et al. 1974)

0.135 (calculated-TSA, Mackay et al. 1980)

0.296 (supercooled liquid, calculated-TSA, Burkhard et al. 1985b)

0.0853 (calculated-fragment solubility constants, Wakita et al. 1986)

0.072 ($20^{\circ}C$, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)0.0110, 0.0142, 0.00853, 0.853 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0408 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.0287 (calculated-QSPR, Dunnivant et al. 1992)

0.0437, 0.115 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.170 (calculated-mp and K_{ow} , Ran et al. 2002)Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):0.0566, 0.00897, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.0084 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)

0.0127, 0.0094 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)0.00454 ($20^{\circ}C$, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)0.00912, 0.0115 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992) $\log(P_L/Pa) = -4242/(T/K) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)0.0612 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioğlu 1998)Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated):

84.21 (batch stripping, Atlas et al. 1982)

7.34 (calculated-P/C, Burkhard et al. 1985b)

15.40 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)14.59 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)

15.41 (calculated-QSPR, Dunnivant et al. 1992)

20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.90 (RP-TLC- k' correlation, Bruggeman et al. 1982)

6.00 (calculated-fragment const., Yalkowsky et al. 1983)

5.53 (calculated-TSA, Burkhard 1984)

4.94 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)

5.58, 5.86, 5.84, 5.85 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.83 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.78 (recommended, Sangster 1993)

5.7373 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.97 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

4.58, 5.90 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

5.70, 4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

5.33 (suspended particulate matter, Burkhard 1984)

4.81 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)

4.81 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)

4.46 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7-1.6) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14-30$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0-2.1) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9-15$ d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

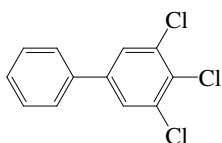
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.38 3,4,5-Trichlorobiphenyl (PCB-38)



Common Name: 3,4,5-Trichlorobiphenyl

Synonym: PCB-38, 3,4,5-trichloro-1,1'-biphenyl

Chemical Name: 3,4,5-trichlorobiphenyl

CAS Registry No: 53555-66-1

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

114 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.353 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0258 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0104 (P_L supercooled liquid, Burkhard et al. 1985a)

0.0566, 0.0111, 0.0219 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

Henry's Law Constant (Pa-m³/mol at $25^{\circ}C$ or as indicated):

7.62 (calculated-P/C, Burkhard 1984)

20.97 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

2.027 (wetted-wall column-GC/ECD, Brunner et al. 1990)

23.54 (calculated-QSPR, Dunnivant et al. 1992)

19.30 (calculated-QSPR, Achman et al. 1993)

20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.48 (calculated-TSA, Burkhard 1984)

5.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.7298 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.92 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.28 (suspended particulate matter, cal- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

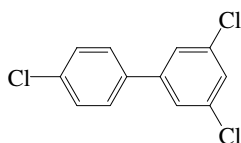
Ground water:

Sediment:

Soil:

Biota:

7.1.1.39 3,4',5-Trichlorobiphenyl (PCB-39)



Common Name: 3,4',5-Trichlorobiphenyl

Synonym: PCB-39, 3,4',5-trichloro-1,1'-biphenyl

Chemical Name: 3,4',5-trichlorobiphenyl

CAS Registry No: 38444-88-1

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

88 (Burkhard et al. 1985b)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.241 (mp at $88^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.353 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985a)

0.0258 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0310 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0125 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0135, 0.00314, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.0203, 0.0174 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4242/(T/K) + 12.53$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

12.56 (calculated-P/C, Burkhard et al. 1985a)

43.57 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

30.32 (calculated-QSPR, Dunnivant et al. 1992)

20.3 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 54 \pm 3$ kJ/mol, $\Delta S_H = 0.14 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.58 (calculated-TSA, Burkhard 1984)

5.89 (calculated-TSA, Hawker & Connell 1988a quoted, Hansch et al. 1995)

5.8173 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.79 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.38 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.7\text{--}1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 14\text{--}30 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (1.0\text{--}2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for trichlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 6.9\text{--}15 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

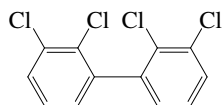
Ground water:

Sediment:

Soil:

Biota:

7.1.1.40 2,2',3,3'-Tetrachlorobiphenyl (PCB-40)



Common Name: 2,2',3,3'-Tetrachlorobiphenyl

Synonym: PCB-40

Chemical Name: 2,2',3,3'-tetrachlorobiphenyl

CAS Registry No: 38444-93-8

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

119.5–121.5 (Wallnöfer et al. 1973; Hutzinger et al. 1974; Erickson 1986)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2024

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.113 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.034 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.070, 0.0583, 0.0232, 0.0385 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0156 (generator column-GC/ECD; Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0098 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

0.00134 (GC-RI correlation, Burkhard et al. 1985a)

0.0112 (supercooled liquid P_L , GC-RI correlation, Burkhard et al.)

0.00887, 0.00861 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00255; 0.0020 (selected solid P_S ; supercooled liquid P_L , Shiu & Mackay 1986)

0.00452 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 10.70 - 4480/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00676, 0.012 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4271/(T/K) + 12.32$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.000473–0.00957; 0.00450–0.0120 (literature P_S range; literature P_L range, Delle Site 1997)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated):

20.27 (calculated- P/C , Burkhard et al. 1985b;)

12.16 ($20^{\circ}C$, batch stripping-GC, Oliver 1985)

21.94 (calculated- P/C , Shiu & Mackay 1986)

16.31 ($20^{\circ}C$, calculated- P/C , Murphy et al. 1987)

20.47 (batch stripping-GC, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)

45.14 (calculated-QSAR- χ , Sabljic & Güsten 1989)

10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)

18.52 (calculated-QSPR, Dunnivant et al. 1992)

15.4 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

29.7 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.63 (HPLC-RT correlation, Sugiura et al. 1978)
 5.56 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
 5.80 (shake flask-GC, Chiou 1985)
 5.48, 5.66, 5.84, 5.85 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.55 (generator column-GC/ECD, Hawker & Connell 1988a)
 6.178 (slow stirring-GC; De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 5.67 (recommended, Sangster 1993)
 6.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.05 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

3.08 (killifish, Goto et al. 1978)
 3.36–4.23 highest value 4.23 not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
 4.69, 4.23; 5.38 (rainbow trout: laboratory data: kinetic BCF; steady state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
 4.38, 4.23 (worms, fish, Oliver 1987c)
 4.23 (fish, quoted, Isnard & Lambert 1988, 1989)

Bioaccumulation Factor, $\log BAF$:

6.48 (rainbow trout, L/kg(Ip), quoted, Thomann 1989)

Biota Sediment Accumulation Factor, BSAF:

10 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

5.57 (suspended particulate matter, Burkhard 1984)
 5.50; 5.50 (field data of sediment trap material; Niagara River organic matter; Oliver & Charlton 1984)
 5.00 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioglu 1996)
 5.00 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{aq.}) = 6.1 \times 10^9$ dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)
 $k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-40$ d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0065 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 320 \text{ d}^{-1}$; $k_2 = 0.0065 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$\log 1/k_2 = 2.2, 2.9 \text{ h}$ (fish, quoted, calculated- K_{OW} , Hawker & Connell 1988b)

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 107 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 112 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4$ –11 d in freshwater systems, $t_{1/2} = 0.1$ –10 d in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.20 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.95 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.36 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.39 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00155 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00285 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00258 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00119 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

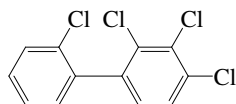
Biota: half-life in rainbow trout, $t_{1/2} = 107 \text{ d}$ and $t_{1/2} = 61 \text{ d}$ its muscle (Niimi & Oliver 1983);

$t_{1/2} = 107 \text{ d}$ in rainbow trout (Oliver & Niimi 1985);

$t_{1/2} = 29 \text{ d}$ in worms at 8°C (Oliver 1987c).

depuration $t_{1/2} = 107 \text{ d}$ for high-dose treatment, $t_{1/2} = 112 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.41 2,2',3,4-Tetrachlorobiphenyl (PCB-41)



Common Name: 2,2',3,4-Tetrachlorobiphenyl

Synonym: PCB-41, 2,2',3,4-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4-tetrachlorobiphenyl

CAS Registry No: 52663-59-9

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

63 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.150 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985a)

0.0648 ($20^{\circ}C$, supercooled liquid S_L , Murphy et al. 1987)

0.0306, 0.0328, 0.0197, 0.0351 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.116 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0124 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0131 (GC-RI correlation, Burkhard et al. 1985b)

0.0110, 0.0098 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

4.59×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0776, 0.0120 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.22$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

23.91 (calculated-P/C, Burkhard et al. 1984)

20.37 (calculated-P/C, Murphy et al. 1987)

20.87 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

14.19 (wetted-wall column-GC, Brunner et al. 1990; quoted, Achman et al. 1993)

24.76 (calculated-QSPR, Dunnivant et al. 1992)

35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2\ kJ/mol$, $\Delta S_H = 0.05 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.09, 6.11 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

5.73, 5.83, 5.82, 5.78 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.79 (recommended, Sangster 1993)

6.11 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

9.79, 8.82 (0, 20°C, RP-HPLC-RT, Zhang et al. 1999)

8.46 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

5.80, 4.80 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

5.59 (suspended particulate matter, Burkhard 1984)

5.01 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioglu 1996)

5.40 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 6.4 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 147 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 162 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

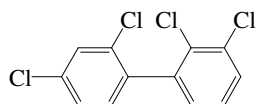
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 147 \text{ d}$ for high-dose treatment, $t_{1/2} = 162 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.42 2,2',3,4'-Tetrachlorobiphenyl (PCB-42)



Common Name: 2,2',3,4'-Tetrachlorobiphenyl

Synonym: PCB-42, 2,2',3,4'-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4'-tetrachlorobiphenyl

CAS Registry No: 36559-22-5

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

69.0 (Burkhard et al. 1985; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.370 (mp at $69^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.150 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985a)

0.0608 ($20^{\circ}C$, supercooled liquid S_L , Murphy et al. 1987)

0.032 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0334 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0131 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00507 (GC-RI correlation, Burkhard et al. 1985b)

0.0116, 0.0116 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

4.19×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 10.70 - 4480/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00912, 0.0135 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.25$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

29.49 (calculated-P/C, Burkhard et al. 1985a)

32.02 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

14.19 (wetted-wall column-GC, Brunner et al. 1990)

25.92 (calculated-QSPR, Dunnivant et al. 1995)

10.13 (calculated-QSPR, Achman et al. 1993)

21.4 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

38.0 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 3$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.84 (calculated-TSA, Burkhard 1984)

5.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.72 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.72 (quoted values; recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.19 (10°C, estimated, Thomas et al. 1998)
- 8.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.64 (suspended particulate matter, Burkhard 1984)
- 5.30 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 123 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 140 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

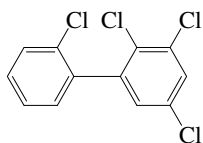
Ground water:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.20 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.89 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.23 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.35 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00066 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00309 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.0016 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00101 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: depuration $t_{1/2} = 123 \text{ d}$ for high-dose treatment, $t_{1/2} = 140 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.43 2,2',3,5-Tetrachlorobiphenyl (PCB-43)



Common Name: 2,2',3,5-Tetrachlorobiphenyl

Synonym: PCB-43

Chemical Name: 2,2',3,5-tetrachlorobiphenyl

CAS Registry No: 70362-46-8

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

42 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.130 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.146 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0183 (P_L supercooled liquid, Burkhard et al. 1985a)

0.0194 (GC-RI correlation, Burkhard et al. 1985b)

0.0166, 0.0191 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0123, 0.0191 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.40$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

41.14 (calculated-P/C, Burkhard 1984)

35.26 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

33.94 (calculated-QSPR, Dunnivant et al. 1992)

35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2\ kJ/mol$, $\Delta S_H = 0.05 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.84 (calculated-TSA, Burkhard 1984)

5.75 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.8627 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.64 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2): $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 155 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004) $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 188 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

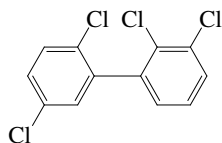
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 155 \text{ d}$ for high-dose treatment, $t_{1/2} = 188 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.44 2,2',3,5'-Tetrachlorobiphenyl (PCB-44)



Common Name: 2,2',3,5'-Tetrachlorobiphenyl

Synonym: PCB-44

Chemical Name: 2,2',3,5'-tetrachlorobiphenyl

CAS Registry No: 41464-39-5

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

46.5–47 (Hutzinger et al. 1974; Erickson 1986)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2024

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.608 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.170 (shake flask-GC, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.080 (generator column-HPLC/UV, Billington 1982)

0.10 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.08 (generator column-HPLC/UV, Billington et al. 1988)

0.0463, 0.0394, 0.0254, 0.0343 (RP-HPLC- k' correlation correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00943 (GC-RI correlation, Burkhard et al. 1985a)

0.0147 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0128, 0.013 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0152 (quoted, Eisenreich 1987)

0.0064 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00955, 0.0151 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.29$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

79.28 (batch stripping, Atlas et al. 1982)

24.32 (calculated, Murphy et al. 1983)

32.83 (calculated-P/C, Burkhard et al. 1985b)

19.15 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

25.43 (calculated-QSPR-MCI χ , Sabljic & Gusten 1989)

14.19 (wetted-wall column-GC, Brunner et al. 1990)

23.32 (calculated-QSPR, Dunnivant et al. 1992)

11.86, 16.02, 21.33, 28.05* \pm 0.27, 35.13 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 5.8937 - 3103.2/(T/K)$; temp range 4 – $31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(25.8/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.049/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)—see Comment by Goss et al. 2004
 27.0 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 2 \text{ kJ/mol}$, $\Delta S_H = 0.05 \pm 0.01 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.67 (calculated-fragment const., Yalkowsky et al. 1983)
 5.84 (calculated-TSA, Burkhard 1984)
 5.81 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
 5.29 (calculated-S, Chou & Griffin 1986)
 5.61, 5.78, 5.74, 5.79 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.75 (calculated-TSA, Hawker & Connell 1988b)
 5.88 (calculated-MCI χ , Patil 1991)
 5.73 (recommended, Sangster 1993)
 5.81 (recommended, Hansch et al. 1995)
 6.20, 4.79–6.67 (calculated-Characteristic Root Index [CRI]; minimum-maximum range, Saçan & Inel 1995)
 5.6625 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
 6.26 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

8.36 (fugacity meter/generator column-GC; Kömp & McLachlan 1997a)
 $\log K_{OA} = -6.20 + 4340/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
 9.19 (10°C, estimated, Thomas et al. 1998)
 9.67, 8.71; 8.41 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 8.58 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

4.04 (oyster, Vreeland 1974)
 4.84; 6.37 (zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)
 4.04, 6.29 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.84, 5.37 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

5.60, 4.70 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

5.64 (suspended particulate matter, Burkhard 1984)
 4.43 (soil, calculated-S, Chou & Griffin 1986)
 5.60 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
 4.67 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
 5.05 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balcioglu 1996)
 5.40 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{aq.}) = 5.5 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{\text{OH}}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation: 99% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 200 \text{ d}^{-1}$; $k_2 = .0461 \text{ d}^{-1}$ (Zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.014 \text{ d}^{-1}$ with $t_{1/2} = 49 \text{ d}$ and $k_2 = 0.018 \text{ d}^{-1}$ with $t_{1/2} = 38 \text{ d}$ for food concn of 18 ng/g and 129 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 146 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 175 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Groundwater:

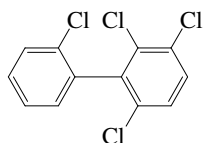
Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.23 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.98 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.32 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.38 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are; $k = 0.00090 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00253 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00161 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00122 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

Biota: depuration $t_{1/2} = 38\text{--}49 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 146 \text{ d}$ for high-dose treatment, $t_{1/2} = 175 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.45 2,2',3,6-Tetrachlorobiphenyl (PCB-45)



Common Name: 2,2',3,6-Tetrachlorobiphenyl

Synonym: PCB-45, 2,2',3,6-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',3,6-tetrachlorobiphenyl

CAS Registry No: 70362-45-7

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

42 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.115 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.146 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.292 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0398 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0416 (GC-RI correlation, Burkhard et al. 1985b)

0.0226, 0.0268 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0295 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4117/(T/K) + 12.16$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

101.1 (calculated-P/C, Burkhard 1984)

31.92 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

35.95 (calculated-QSPR, Dunnivant et al. 1992)

12.47 (calculated-QSPR, Achman et al. 1993)

25.1 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

43.0 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.88 (calculated-TSA, Burkhard 1984)

5.53 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

4.84 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

4.84 (recommended, Sangster 1993)

5.4616 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.28 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

5.68 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 6.7 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 7 \text{ food lipid (mg)/(g worm lipid-d)}$; $k_2 = 0.12 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 175 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 128 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991)

Ground water:

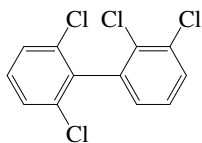
Sediment:

Soil:

Biota: elimination $t_{1/2} = 6 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2} = 175 \text{ d}$ for high-dose treatment, $t_{1/2} = 128 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.46 2,2',3,6'-Tetrachlorobiphenyl (PCB-46)



Common Name: 2,2',3,6'-Tetrachlorobiphenyl

Synonym: PCB-46, 2,2',3,6'-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',3,6'-tetrachlorobiphenyl

CAS Registry No: 41464-47-5

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

42 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.114 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.106 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.149 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0280 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0272 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0285 (GC-RI correlation, Burkhard et al. 1985b)

0.0186, 0.0206 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

9.04×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0155 (supercooled liquid P_L ; GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.37$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

69.81 (calculated-P/C, Burkhard 1984)

26.04 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

36.68 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

34.33 (calculated-QSPR, Dunnivant et al. 1992)

18.87 (calculated-QSAR, Achman et al. 1993)

18.8 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

34.5 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3 kJ/mol$, $\Delta S_H = 0.06 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.89 (calculated-TSA, Burkhard 1984)

5.53 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

4.84 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.86 (calculated, Miertus & Jakus 1990)

- 4.84 (recommended, Sangster 1993)
5.2787 (calculated-molecular properties MNDO-AM1 method, Makino 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 9.49, 8.56 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1998)
7.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.69 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 112 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 907 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

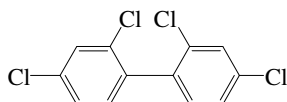
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 112 \text{ d}$ for high-dose treatment, $t_{1/2} = 107 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.47 2,2',4,4'-Tetrachlorobiphenyl (PCB-47)



Common Name: 2,2',4,4'-Tetrachlorobiphenyl

Synonym: PCB-47

Chemical Name: 2,2',4,4'-tetrachlorobiphenyl

CAS Registry No: 2437-79-8

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

83 (Fichter & Adler 1926; Kühne et al. 1995; Ruelle & Kesselring 1997)

41–42 (Hall & Minhaj 1957; Wallnöfer et al. 1973)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2024

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.268 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.068 (shake flask-GC, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.990 (supercooled liquid S_L , Johnstone et al. 1974)

0.0160, 0.0157, 0.0172, 0.0202 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0541 ($22^{\circ}C$, generator column-GC, Opperhuizen et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0115 (Neely 1983)

0.0111 (GC-RI correlation, Burkhard et al. 1985a)

0.0151 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0152, 0.0156 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0115, 0.0162 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.37$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

42.86 (calculated-P/C, Burkhard et al. 1985b)

17.38 (calculated-P/C, Shiu & Mackay 1986)

44.48 (calculated-QSAR- χ , Sabljic & Güsten 1989)

19.25 (wetted-wall column-GC/ECD, Brunner et al. 1990)

37.30 (calculated-QSPR, Dunnivant et al. 1992)

3.05, 8.91 (0, $15^{\circ}C$, from modified two-film exchange model, Hornbuckle et al. 1994)

12.67 (estimated-bond method, EPIWIN v3.04, Hardy 2002)

35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2\ kJ/mol$, $\Delta S_H = 0.05 \pm 0.01\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.68 (shake flask, Tulp & Hutzinger 1978)

5.20 (HPLC- k' correlation, McDuffie 1981)

- 6.29 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 6.17 (HPLC- k' correlation, De Kock & Lord 1987)
- 5.93, 6.04, 5.86, 5.94 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.94 (recommended, Sangster 1993)
- 6.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 9.55, 8.56 (0, 20°C, multi-column GC- k' correlation; Zhang et al. 1999)
- 8.01 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 3.98 (rainbow trout muscle, steady state, Branson et al. 1975; quoted, Waid 1986)
- 4.09 (rainbow trout, Neely et al. 1974)
- 3.95 (rainbow trout, Branson et al. 1975)
- 4.85; 4.782, 4.717 (quoted-whole fish; calculated-molecular connectivity indices, K_{OW} , Lu et al. 1999)
- 2.97, 2.71 (phytoplankton *Nanochloropsis oculata*, PCB concn at 50 ppb, after 4-d culture, Wang et al. 1998)
- 2.19, 2.11 (phytoplankton *Isochrysis galbana*, PCB concn at 500 ppb, after 4-d culture, Wang et al. 1998)
- 4.00, 5.52 (rainbow trout 8–10 g, muscle 3% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 4.46, 5.56 (rainbow trout 10–15 g, whole fish: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 4.76 (estimated-EPIWIN v3.04, Hardy 2002)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.30, 4.70 (Lake Superior suspended solid, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.61 (soil, calculated-solubility, Kenaga 1980)
- 5.72 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 4.68 (soil, calculated-S, Chou & Griffin 1986)
- 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.04 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 5.70 (soil, calculated- K_{OW} , Girvin & Scott 1997)
- 4.65 (estimated-EPIWIN v3.04, Hardy 2002)

Sorption Partition Coefficient, $\log K_p$:

- 5.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.18–5.64 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 0.2921$ d from river, $t_{1/2} = 9.256$ d from lake (estimated-EPIWIN v3.04, Hardy 2002).

Photolysis: photolysis rate $k_p = 0.553$ d⁻¹ with $t_{1/2} = 13$ d in summer sunlight; $k_p(\text{exptl}) = 6 \times 10^{-8}$ d⁻¹ with $t_{1/2} = 133$ d, and $k_p(\text{calc}) = 2.2 \times 10^{-8}$ d⁻¹ in winter sunlight, at 40°L in surface waters (Dulin et al. 1986)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 6.4 \times 10^9$ dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4-11$ d in freshwater systems, $t_{1/2} = 0.1-10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-0$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: no degradation observed after 98 d incubation by river dieaway test (Bailey et al. 1983).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 286 \text{ d}^{-1}$; $k_2 = 0.030 \text{ d}^{-1}$ (10–12°C, rainbow trout muscle, Branson et al. 1975; quoted, Waid 1986)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 160 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 177 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radical for trichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 49.2 \text{ d}$ in Lake Michigan (Neely 1983);

photolysis $t_{1/2} = 13 \text{ d}$ in summer sunlight and $t_{1/2} = 170 \text{ d}$ in winter sunlight at 40°L in surface waters (Dulin et al. 1986);

half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);

half-life of volatilization: $t_{1/2} = 0.2021 \text{ d}$ from river, and $t_{1/2} = 9.156 \text{ d}$ from lake, (estimated-EPIWIN v3.04, Hardy 2002).

Groundwater:

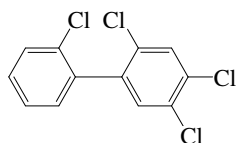
Sediment:

Soil:

Biota: $t_{1/2} = 28 \text{ d}$ in rainbow trout muscle (Branson et al. 1975; selected, Waid 1986).

depuration $t_{1/2} = 160 \text{ d}$ for high-dose treatment, $t_{1/2} = 177 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.48 2,2',4,5-Tetrachlorobiphenyl (PCB-48)



Common Name: 2,2',4,5-Tetrachlorobiphenyl

Synonym: PCB-48, 2,2',4,5-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',4,5-tetrachlorobiphenyl

CAS Registry No: 70362-47-9

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

65.9 (Miller et al. 1984; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.4 (Miller et al. 1984; Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

69.04 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$, F:

0.393 (calculated-assuming $\Delta S_{fus} = 56\ J/mol\ K$, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.121 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.030 (supercooled liquid S_L , Murphy et al. 1987)

0.0328, 0.0376, 0.0467, 0.0452 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0222, 0.0596 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0167 (supercooled liquid P_L , GC-RT correlation, Burkhard et al. 1985a)

0.0177 (ΔG_v and GC- k' correlation, Burkhard et al. 1985b)

0.0157, 0.016 (supercooled P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0265 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0115, 0.0170 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.37$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

0.010 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI; Saçan & Balcioglu 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

42.71 (calculated-P/C, Burkhard et al. 1985b)

26.64 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)

30.67 (calculated-QSPR, Dunnivant et al. 1992)

19.30 (calculated-QSPR, Achman et al. 1993)

3.05, 8.91 (0, $15^{\circ}C$, from modified two-film exchange model, Hornbuckle et al. 1994)

22.8 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

39.8 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2\ kJ/mol$, $\Delta S_H = 0.05 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.86 (calculated-TSA, Burkhard 1984)
- 5.78 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 5.71, 5.79, 5.56 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.95 (calculated-solvatochromic parameters and intrinsic molar volume V_i , Kamlet et al. 1988)
- 5.69 (recommended, Sangster 1993)
- 5.9108 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 9.49, 8.50 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
- 8.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.41, 5.71 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.66 (suspended particulate matter, Burkhard 1984)
- 5.80 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 6.4 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 160 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 177 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

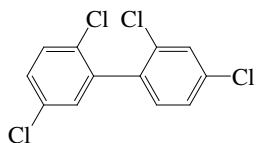
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 160 \text{ d}$ for high-dose treatment, $t_{1/2} = 177 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.49 2,2',4,5'-Tetrachlorobiphenyl (PCB-49)



Common Name: 2,2',4,5'-Tetrachlorobiphenyl

Synonym: PCB-49, 2,2',4',5-tetrachlorobiphenyl, 2,2',4,5'-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',4,5'-tetrachlorobiphenyl

CAS Registry No: 41464-40-8

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

66.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.4 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

69.04 (Miller et al. 1984)

69.01, 64.3 (exptl., calculated, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.392 (mp at $66.5^{\circ}C$)

0.411 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0164 (generator column-GC/ECD, Miller et al. 1984,1985)

0.0202, 0.0193, 0.0232, 0.0266 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00708 (GC-RI correlation, Burkhard et al. 1985a)

0.0170 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0167, 0.0162 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00742 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 10.60 - 4440/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0123, 0.0182 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.41$ (supercooled liquid P_L GC-RT correlation, Falconer & Bidleman 1994)

0.00955 ($20^{\circ}C$, supercooled liquid P_L , from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ as indicated):

20.27 (calculated, Murphy et al. 1983)

47.72 (calculated-P/C, Burkhard et al. 1985b)

27.96 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

37.90 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

21.28 (wetted-wall column-GC/ECD, Brunner et al. 1990)

35.79 (calculated-QSPR, Dunnivant et al. 1992)

22.8 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

39.9 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW} :

- 6.23 (calculated- π constant, Bruggeman et al. 1982)
- 5.73 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 6.22 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 5.86, 5.98, 5.77, 5.86 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.361 ± 0.046 ; 6.23 (slow stirring-GC, calculated- π const., De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 5.87 (recommended, Sangster 1993)
- 6.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

- 8.57 (20°C, generator column-GC, measured range -10 to 20°C, Harner & Bidleman 1996)
- 9.64, 9.08, 8.57, 8.21 (-10, 0, 10, 20, 30°C, generator column-GC, Harner & Bidleman 1996)
- $\log K_{OA} = -4.96 + 3981/(T/K)$; temp range -10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
- 9.08 (10°C, estimated, Thomas et al. 1998)
- 9.50, 8.63; 8.48 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 8.34 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 4.84; 6.37 (zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
- 4.84, 6.38 (zebrafish, kinetic approach: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} :

- 5.71 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.50 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 6.2 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 3200 \text{ d}^{-1}$; $k_2 = 0.0458 \text{ d}^{-1}$ (zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 158 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 196 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25-60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5-40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

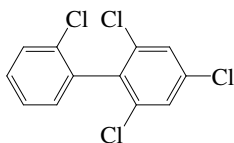
Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.25\text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.99\text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.31\text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.39\text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00094\text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00243\text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00168\text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00147\text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: depuration $t_{1/2} = 158$ d for high-dose treatment, $t_{1/2} = 196$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.50 2,2',4,6-Tetrachlorobiphenyl (PCB-50)



Common Name: 2,2',4,6-Tetrachlorobiphenyl

Synonym: PCB-50, 2,2',4,6-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',4,6-tetrachlorobiphenyl

CAS Registry No: 62796-65-8

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

45.0 (calculated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.092 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.0320, 0.032, 0.030, 0.0412 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.1842 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.044 (calculated-MCI χ , Patil 1991)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0451 (GC-RI correlation, Burkhard et al. 1985a)

0.0433 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

76.80 (gas stripping-GC, Atlas et al. 1982)

137.8 (calculated-P/C, Burkhard et al. 1985b)

58.57 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

61.76 (calculated-QSPR, Dunnivant et al. 1992)

28.68, 38.18, 49.84, 64.30 ± 1.4 , 70.30 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 5.8937 - 2862.64/(T/K)$; temp range $4-31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(23.8/kJ\cdot mol^{-1})/RT] + (0.049/kJ\cdot mol^{-1}\cdot K^{-1})/R$; where $R = 8.314\ J\cdot K^{-1}\cdot mol^{-1}$ and temp range: $4-31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

60.5 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 4\ kJ/mol$, $\Delta S_H = 0.05 \pm 0.01\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.96 (calculated-TSA, Burkhard 1984)

5.72, 5.84, 5.70, 5.74 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.63 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.87 (calculated-MCI χ , Patil 1991)

5.75 (recommended, Sangster 1993)

5.6545 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.89 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

4.26, 3.50, 3.81 (algae, fish, activated sludge, Freitag et al. 1984, 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

5.76 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

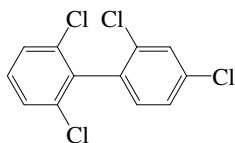
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.51 2,2',4,6'-Tetrachlorobiphenyl (PCB-51)



Common Name: 2,2',4,6'-Tetrachlorobiphenyl

Synonym: PCB-51

Chemical Name: 2,2',4,6'-tetrachlorobiphenyl

CAS Registry No: 68194-04-7

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

66 (Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.396 (mp at $66^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0911 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.065 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.1842 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.044 (calculated-MCI χ , Patil 1991)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.033 (GC-RI correlation, Burkhard et al. 1985a)

0.0315 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

$\log(P/mmHg) = 10.40 - 4330/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0263 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4117/(T/K) + 12.20$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

76.80 (gas stripping-GC, Atlas et al. 1982)

101.2 (calculated-P/C, Burkhard et al. 1985b)

49.04 (calculated-molecular connectivity indices χ , Sabljic & Güsten 1989)

51.73 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.96 (calculated-TSA, Burkhard 1984)

5.86, 5.98, 5.77, 5.86 (RP-HPLC- k' correlation, different stationary phases, Brodsky & Ballschmiter 1988)

5.63 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.88 (calculated-MCI χ , Patil 1991)

5.51 (recommended, Sangster 1993)

5.4591 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.62 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

5.76 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 10 \text{ food lipid (mg)/(g worm lipid-d)}$; $k_2 = 0.11 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 126 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 150 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

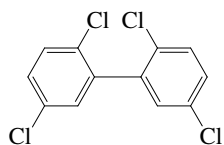
Sediment:

Soil:

Biota: elimination $t_{1/2} = 6 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2} = 126 \text{ d}$ for high-dose treatment, $t_{1/2} = 150 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.52 2,2',5,5'-Tetrachlorobiphenyl (PCB-52)



Common Name: 2,2',5,5'-Tetrachlorobiphenyl

Synonym: PCB-52

Chemical Name: 2,2',5,5'-tetrachlorobiphenyl

CAS Registry No: 35693-99-3

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

87–89 (Webb & McCall 1972; Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2024

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point,)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

46.02 (Hinckley et al. 1990)

46.1 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.243 (calculated, assuming $\Delta S_{fus} = 56$ J/mol K, Mackay et al. 1980)

0.316 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.046 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.0265 (shake flask-GC/ECD, Haque & Schmedding 1975)

0.016 (shake flask-LSC, Metcalf et al. 1975)

0.0060 ($16.5^{\circ}C$, shake flask-GC/ECD, Wiese & Griffin 1978)

0.0223 (shake flask-GC/ECD from Aroclor 1242 mixture, Lee et al. 1979)

0.055 (generator column-GC/ECD, Bruggeman et al. 1981)

0.0365 (generator column-HPLC/UV, Huang 1983)

0.027 (generator column-GC/ECD, Miller et al. 1984; 1985)

0.0237, 0.0279, 0.0335, 0.0335 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.170 (generator column-HPLC/UV, Billington et al. 1988)

0.110; 0.461 (generator column-GC; supercooled liquid S_L , calculated-mp, Dunnivant & Elzerman 1988)

0.0153 ($22^{\circ}C$, generator column-GC/ECD, Opperhuizen et al. 1988)

0.0161 (shake flask-LSC, Eadie et al. 1990)

$\log (S_L/(mol/L)) = -0.790 - 3352/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

0.0923 (calculated-mp and K_{ow} , Ran et al. 2002)

0.199, 0.140 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

$\log S_L/(mol\ m^{-3}) = -1103/(T/K) + 0.37$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00733 (solid P_s from GC-RT correlation, Westcott & Bidleman 1981)

0.00253, 0.0048 (solid P_s , 25, $30^{\circ}C$, gas saturation-GC/ECD, Westcott et al. 1981)

$\log (P_s/mmHg) = 11.8 - 4920/(T/K)$, temp range 30 – $40^{\circ}C$ (gas saturation-GC, Westcott et al. 1981)

0.104; 0.428 (solid P_s ; supercooled liq. P_L calculated from P_s using fugacity ratio F, Neely 1981)

0.0188, 0.0165 (P_{GC} by GC-RT correlation, different GC stationary phases, Bidleman 1984)

- 0.0104 (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)
 0.0159, 0.0229 (supercooled liquid P_L calculated from P_{GC} , GC-RT correlation, different stationary phases, Bidleman 1984)
 0.00492 (GC-RI correlation, Burkhard et al. 1985a)
 0.00497; 0.0193 (selected exptl. P_S ; supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985)
 0.0184, 0.0173 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 0.0049; 0.0020 (selected solid P_S ; supercooled liquid P_L , Shiu & Mackay 1986)
 0.00904 (20°C, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
 0.0127; 0.0546 (calculated-S \times HLC; solid P_S ; supercooled liquid P_L , Dunnivant & Elzerman 1988)
 $\log (P/\text{mmHg}) = 10.60 - 4430/(T/K)$ (GC-RT correlation, supercooled liquid, Tateya et al. 1988)
 0.0104, 0.008 (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 0.0188, 0.012 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log (P_L/Pa) = 11.74 - 4127/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
 0.0132, 0.020 (supercooled liquid P_L ; GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/Pa) = -4220/(T/K) + 12.36$ (supercooled liq. P_L , GC-RT correlation, Falconer & Bidleman 1994)
 0.00690; 0.00218 (solid P_S ; supercooled liq. P_L , Passivirta et al. 1999)
 $\log (P_S/Pa) = 14.77 - 5087/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/Pa) = 12.36 - 4220/(T/K)$ (liquid, Passivirta et al. 1999)
 0.0033–0.013; 0.00901–0.0512 (literature P_S range; literature P_L range, Delle Site 1997)
 0.00904 (supercooled liquid P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)
 0.0107, 0.0120 (supercooled liquid P_L ; LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log (P_L/Pa) = -4190/(T/K) + 12.08$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
 $\log (P_L/Pa) = -4059/(T/K) + 11.69$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 31.41–53.7 (calculated-P/C, Westcott et al. 1981)
 14.1–53.7 (calculated-P/C, Westcott & Bidleman 1981)
 94.15 (gas stripping-GC/ECD, Atlas et al. 1982)
 22.29 (calculated-P/C, Murphy et al. 1983)
 26.34 (calculated-P/C, Murphy 1984)
 31.41–53.70 (calculated-P/C, Bidleman 1984)
 53.20 (calculated-P/C, Burkhard et al. 1985b)
 2.53 (batch stripping-GC, Hassett & Milicic 1985)
 12.16 (20°C, gas stripping-GC, Oliver 1985)
 47.59 (calculated-P/C, Shiu & Mackay 1986)
 24.11 (20°C, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
 34.65 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988)
 44.04 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
 20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)
 32.34 (calculated-QSPR, Dunnivant et al. 1992)
 16.4* (20°C, gas stripping-HPLC/fluorescence, measured range 10–48°C, ten Hulscher et al. 1992)
 17.0 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 28.78 \pm 3.4 (gas stripping-GC/ECD, Girvin et al. 1997)
 $\log [H/(Pa \text{ m}^3/\text{mol})] = 13.15 - 3552/(T/K)$ (Passivirta et al. 1999)
 31.07* \pm 0.42 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
 $K_{AW} = \exp[-(30.5/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.066/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C
 (gas stripping-GC, Bamford et al. 2000)
 28.27 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 2001)
 $\log K_{AW} = 6.427 - 2530/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)
 31.3 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 31 \pm 3 \text{ kJ/mol}$, $\Delta S_H = 0.07 \pm 0.01 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004
 28.18, 25.12 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

$\log [H/(\text{Pa m}^3/\text{mol})] = -2189/(T/K) + 8.79$ (LDV linear regression of literature data, Li et al. 2003)

$\log [H/(\text{Pa m}^3/\text{mol})] = -2956/(T/K) + 11.32$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.91 (shake flask-radiolabeled- ^{14}C -LSC, Metcalf et al. 1975)
- 5.81 (Hansch & Leo 1979)
- 6.26 (RP-TLC- k' correlation, Bruggeman et al. 1982)
- 6.09 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 5.81, 5.87, 5.43, 5.80 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.02 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
- 5.81 (generator column-GC, Larsen et al. 1992)
- 6.00 (HPLC- k' correlation, Noegrohati & Hammers 1992)
- 5.79 (recommended, Sangster 1993)
- 6.09 (recommended, Hansch et al. 1995)
- 6.10 (calculated, Passivirta et al. 1999)
- 6.00, 5.91 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ as or as indicated and reported temperature dependence equations:

- 7.90 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
- 8.22; 7.73 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -6.20 + 4340/(T/K)$; temp range: 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
- 9.10 (10°C, estimated, Thomas et al. 1998)
- 9.46, 8.49; 8.56 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 8.33 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
- 8.47; 8.44 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
- 8.22, 8.22 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
- $\log K_{OA} = 4251/(T/K) - 6.04$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log \text{BCF}$:

- 3.87 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)
- 4.26, 4.60, 4.02, 4.07 (algae, snail, mosquito, fish, Metcalf et al. 1975)
- 2.66 (green sunfish, 15 d in static water, Sanborn et al. 1975)
- 6.21; 6.07 (goldfish, 3% lipid; 10% lipid dry wet in food, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
- 6.38 (guppy, 3.5% lipid, Bruggeman et al. 1982, 1984; quoted, Gobas et al. 1987)
- 4.69, 4.98 (goldfish, exptl., correlated, Mackay & Hughes 1984)
- 3.49–4.26 highest value 4.26, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)
- 5.30, 4.26; 6.28 (rainbow trout, laboratory data: kinetic BCF (k_1/k_2), steady state BCF (C_F/C_W); Lake Ontario field BCF, Oliver & Niimi 1985)
- 4.26, 4.69 (guppy, goldfish, calculated- C_B/C_W , or k_1/k_2 , Connell & Hawker 1988; Hawker 1990)
- 4.26 (fish, quoted, Isnard & Lambert 1988, 1989)
- 6.38; 5.76 (guppy, lipid wt. based, corrected lipid wt. based, Gobas et al. 1989)
- 4.25 (guppy, estimated, Banerjee & Baughman 1991)
- 6.21; 6.32 (lipid basis: goldfish; rainbow trout, Noegrohati & Hammers 1992)
- 4.54, 6.02; 4.782, 4.708 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW} , Lu et al. 1999)
- 3.08–4.58 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 4.86–6.31 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
- 5.23 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
- 5.03, 4.67; 3.57, 4.76, 4.17, 5.39 (oligochaetes; chironomid larvae, Bott & Standley 2000)
- 3.36, 5.60 (*Daphnia*, 21-d renewal: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 3.87, 6.12 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)

- 4.28, 6.23 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.42, 6.34 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.63, 5.93 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.69, 5.99 (goldfish: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.92, 6.46 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.01; 3.89 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Bioaccumulation Factor, log BAF at 25°C or as indicated:

- 7.38 (rainbow trout, lipid based-L/kg(Ip), quoted, Thomann 1989)
 4.92; 6.43 (22°C, zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_p or log K_d

- 5.60, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
 5.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 4.73–5.15 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 4.67 (Woodburn soil silt loam, sorption isotherm measurement, Haque & Schmedding 1976)
 5.91 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
 5.60; 5.50; 5.70 (field data of sediment trap material; Niagara River-organic matter; calculated-K_{OW}, Oliver & Charlton 1984)
 4.54, 4.42 (Aldrich humic acid with 9.4 mg/L DOC: reversed-phase separation, equilibrium dialysis, Landrum et al. 1984)
 3.87, 4.36 (Huron River water with 7.8 mg/L DOC: reversed-phase separation, equilibrium dialysis, Landrum et al. 1984)
 4.87 (dissolved humic acid, gas purging-LSC, Hassett & Milicic 1985)
 5.35 (suspended solids-Lake Superior; field measurement-GC/ECD, Baker et al. 1986)
 5.70, 4.87 (Lake Superior suspended solids: calculated-K_{OW}, Baker et al. 1986)
 6.15 (Composite Condie silt soil 0.36% OC, batch sorption equilibrium, Anderson & Pankow 1986)
 5.0–6.4, 5.9 (suspended sediment, range, average, Oliver 1987a)
 6.12 (Lake Michigan water column, Swackhamer & Armstrong 1987)
 4.65 (calculated, Bahnick & Doucette 1988)
 3.48 (12 lakes/streams in southern Ontario at 1.6–26.5 mg/L DOC, Evans 1988)
 4.35 (calculated-polymaleic acid, Chin & Weber 1989)
 5.88 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
 4.88 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
 5.83 (organic carbon from total suspended matter of raw water from Lake Michigan, Eadie et al. 1990)
 5.00, 3.88 (Aldrich humic acid, natural DOC, reversed-phase separation, Eadie et al. 1990)
 5.00; 4.38–4.81; 2.89–3.93 (Aldrich humic acid; humic acid from soil & water samples; fulvic acid & dissolved organic matter samples, Jota & Hassett 1991)
 6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 5.41 (soil, batch sorption equilibration-GC, Paya-Perez et al. 1991)
 6.04, 4.80 (Hamlet City lake sediment, WES reference soil, batch sorption equilibrium, Brannon et al. 1995)
 4.73 (Ispra oil, calculated-MCI 'χ, Sabljic et al. 1995)
 5.02, 6.04; 4.80 (sediments from Brown's Lake, Hamlet City Lake; WES reference soil, shake flask-HPLC/fluorescence, Brannon et al. 1995)
 4.97; 5.09 (soil, quoted lit.; calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioglu 1996)
 5.30–5.41 (soil-Catlin silt loam, f_{OC} = 0.0226, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
 5.61–5.65 (Cloudland loam, f_{OC} = 0.0024, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997)
 5.30–5.31 (Kenoma silt loam, f_{OC} = 0.0153, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
 5.38 (Kenoma silt loam, f_{OC} = 0.0092, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
 5.43–5.53 (Kenoma silt loam, f_{OC} = 0.002, depth 120–155 cm, batch equilibrium-GC, Girvin & Scott 1997)
 5.26–5.44 (Norborne silt loam, f_{OC} = 0.0137, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)

- 5.24–5.36 (Norborne silt loam, $f_{OC} = 0.009$, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
 5.39–5.40 (Norborne silt loam, $f_{OC} = 0.0057$, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
 5.50 (soil, calculated- K_{OW} , Girvin & Scott 1997)
 5.50; 4.90 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
 4.98 (sediment, Bott & Standley 2000)
 5.02, 4.55 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)
 5.58 (sediment: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)
 3.79–6.07; 4.40–6.40 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
 5.32; 5.52, 5.38, 5.60 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, $\log K_{OM}$:

- 4.67 (Haque & Schmedding 1976; Chou & Griffin 1986)
 4.67, 4.62 (quoted, calculated-MCI χ , Sabljic 1984)
 3.88 (Great Lake DOC, reversed-phase separation, Eadie et al. 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ (exptl) = 2.8 h of evaporation from an initial concentration of 0.005 ppm in a glass dish of 4.5 cm depth of water solution at 24°C and $t_{1/2} = 0.68$ h with stirring of the solution (Chiou et al. 1979); depletion $k = 34$ d⁻¹ from a 26-cm or 67-cm height purge vessels. from aqueous solution (Girvin et al. 1997).

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40$ d at room temp. (Kwok et al. 1995)

Biodegradation: microbial degradation with pseudo first-order rate constant $k = 0.1$ yr⁻¹ in the water column and $k = 1.0$ yr⁻¹ in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_2 = 0.008$ d⁻¹ (11°C, rainbow trout, Guiney et al. 1977; quoted, Waid 1986)
 $k_2 = 0.003$ d⁻¹ (10–11°C, rainbow trout eggs and sac fry, Guiney et al. 1980; quoted, Waid 1986)
 $k_1 = 740$ d⁻¹; $k_2 = 0.015$ d⁻¹ (23°C, goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986; Clark et al. 1990)
 $k_1 = 280$ d⁻¹; $k_2 = 0.0014$ d⁻¹ (rainbow trout, Oliver & Niimi 1985)
 $k_1 = 1200$ d⁻¹; $k_2 = 0.015$ d⁻¹ (guppy, Bruggeman et al. 1984)
 $k_2 = 0.015, 0.0134$ d⁻¹ (goldfish, exptl., correlated, Mackay & Hughes 1984)
 $k_1 = 2800$ d⁻¹; $k_2 = 0.0014$ d⁻¹ (rainbow trout, Oliver & Niimi 1985)
 $k_1 = 30.8$ h⁻¹; $1/k_2 = 1600$ h (goldfish, quoted, Hawker & Connell 1985)
 $k_1 = 50.0$ h⁻¹; $1/k_2 = 1600$ h (guppy, quoted, Hawker & Connell 1985)
 $k_1 = 1100$ d⁻¹ (guppy, Opperhuizen 1986)
 $\log k_1 = 2.87$ d⁻¹; $\log 1/k_2 = 1.82$ d (fish, quoted, Connell & Hawker 1988)
 $\log 1/k_2 = 2.9, 3.0$ h (fish, quoted, calculated- K_{OW} , Hawker & Connell 1988b).
 $1/k_2 = 30.3$ d (guppy, quoted, Clark et al. 1990)
 $1/k_2 = 61.7, 102$ d (guppy, Gobas et al. 1989; quoted, Clark et al. 1990)
 $k_1 = 3230$ d⁻¹; $k_2 = 0.0387$ d⁻¹ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 $k_2 = 0.011$ d⁻¹ with $t_{1/2} = 65$ d and $k_2 = 0.018$ d⁻¹ with $t_{1/2} = 39$ d for food concn of 22 ng/g and 125 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
 $k_1 = 20$ L d⁻¹ g⁻¹ dry wt.; $k_2 = 0.118$ d⁻¹ (Baltic Sea blue mussels, flow-through experiment., Gustafsson et al. 1999)

$k_1 = 0.00061 \text{ h}^{-1}$; $k_2 = 0.0115 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
 $k_1(\text{calc}) = 9 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2(\text{calc}) = 0.09 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 158 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 196 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
 $k_2 = 0.015 \text{ d}^{-1}$ with $t_{1/2} = 46.2 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1996);

$t_{1/2} = 1500 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 19.7 \text{ d}$ in Lake Michigan (Neely 1983);

$t_{1/2} = 30000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{1/2} = 87600 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.27 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.99 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.30 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.39 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00112 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00251 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00174 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00127 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

$t_{1/2} = 87600 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} = 1.76 \text{ yr}$ in female rainbow trouts, $t_{1/2} = 1.43 \text{ yr}$ in males (Guiney et al. 1980);

$t_{1/2} = 500 \text{ d}$ in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985); and $t_{1/2} = 99 \text{ d}$ in its muscle, (Niimi & Oliver 1983);

$t_{1/2} = 46 \text{ d}$ in guppy (Bruggeman et al. 1984);

$t_{1/2} = 43 \text{ d}$ in worms at 8°C , 43 d (Oliver 1987c)

depuration $t_{1/2} = 39\text{--}65 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

theoretical half-life to reach 90% steady-state tissue concn 5.9 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);

$t_{1/2} = 6.0 \text{ h}$ in blood plasma (ring doves, Drouillard & Norstrom 2000)

elimination $t_{1/2} = 8 \text{ d}$ in earthworm given contaminated food (predicted, Wågman et al. 2001).

depuration $t_{1/2} = 158 \text{ d}$ for high-dose treatment, $t_{1/2} = 196 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

depuration $t_{1/2} = 46.2 \text{ d}$ for juvenile carp in 100-d experiment (Stapleton et al. 2004)

TABLE 7.1.1.52.1
Reported vapor pressures and Henry's law constants of 2,2',5,5'-tetrachlorobiphenyl (PCB-52) at various temperatures and temperature dependence equations

Vapor pressure		Henry's law constant			
Westcott et al. 1981		ten Hulscher et al. 1992		Bamford et al. 2000	
gas saturation-GC/ECD		gas stripping-GC		gas stripping-GC/MS	
t/°C	P/Pa	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
25	0.00253	10.4	8.6	4	11.34
30	0.0048	20.0	16.4	11	16.13
		30.1	37.4	18	22.56
		34.9	38.8	25	31.07
		42.1	68.7	31	40.43
		47.9	109.2		
		48.4	120.6		
log P = A – B/(T/K)		ln K _{AW} = A – B/(T/K)		ln K _{AW} = –ΔH/RT + ΔS/R	
	P/mmHg			A	7.9384
A	11.8	A	23.387	B	3668.5
B	4920	B	6254.5		
temp range 30–40°C		enthalpy of volatilization:		enthalpy, entropy change:	
		ΔH _{vol} /(kJ·mol ^{–1}) = 52.0 ± 5		ΔH/(kJ·mol ^{–1}) = 30.5 ± 2.8	
		entropy of volatilization, ΔS:		ΔS/(J·K ^{–1} mol ^{–1}) = 66 ± 10	
		TΔS _{vol} /(kJ·mol ^{–1}) = 57.0 ± 6			
		at 20°C			

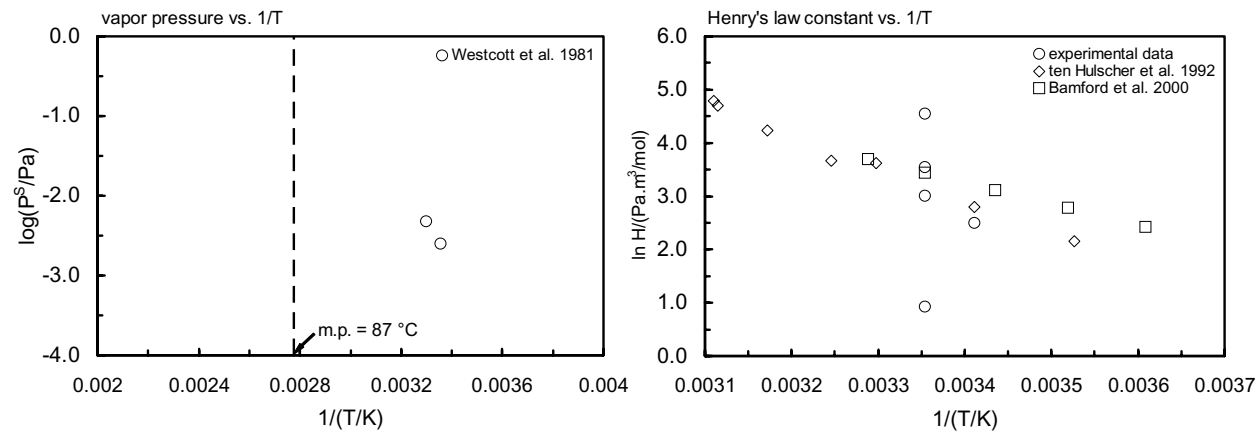
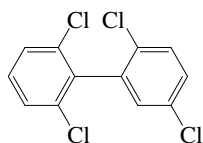


FIGURE 7.1.1.52.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for 2,2',5,5'-tetrachlorobiphenyl (PCB-52).

7.1.1.53 2,2',5,6'-Tetrachlorobiphenyl (PCB-53)



Common Name: 2,2',5,6'-Tetrachlorobiphenyl

Synonym: PCB-53, 2,2',5,6'-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',5,6'-tetrachlorobiphenyl

CAS Registry No: 41464-41-9

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

103–104.5 (Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.168 (mp at $104^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0923 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.109 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0945, 0.0786, 0.0717, 0.0335 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0476 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.288 (supercooled liquid S_L , calculated-mp, Dunnivant & Elzerman 1988)

0.292 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.044 (calculated-MCI χ , Patil 1991)

0.0520 (calculated-QSPR, Dunnivant et al. 1992)

0.0306 (calculated-group contribution, Kühne et al. 1995)

0.0114, 0.0306 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.114 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00493 (Neely 1983; quoted, Erickson 1986)

0.0273 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

0.0356 (supercooled liquid P_L , GC-RT correlation, Burkhard 1984)

0.0372 (GC-RI correlation, Burkhard et al. 1985a)

0.0356 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0268, 0.0331 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.011 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00671; 0.0405 (calculated- $S \times HLC$, solid P_S ; supercooled liquid P_L , Dunnivant & Elzerman 1988)

$\log(P/mmHg) = 10.40 - 4310/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0214, 0.0347 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/a) = -4114/(T/K) + 12.24$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.0162 ($20^{\circ}C$, supercooled liquid P_L , from Falconer & Bidleman 1994. Harner & Bidleman 1996)

0.00161–0.0204; 0.0107–0.0385 (literature P_S range; literature P_L range, Delle Site 1997)

0.00955 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], reported as 2,2',5,6- Saçan & Balcioglu 1998)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C as indicated):

- 30.40 (calculated-P/C, Murphy et al. 1983)
 - 112.5 (calculated-P/C, Burkhard et al. 1985b)
 - 28.67 (20°C , calculated-P/C, Murphy et al. 1987)
 - 41.14 (batch stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
 - 47.26 (calculated-molecular connectivity indices, Sabljic & Güsten 1989)
 - 43.62 (calculated-QSPR, Dunnivant et al. 1992)
 - 17.21 (calculated-QSPR, Achman et al. 1993)
 - 44.8 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
- $\ln K_{\text{AW}} = -\Delta H_{\text{H}}/RT + \Delta S_{\text{H}}/R$; R is the ideal gas constant, $\Delta H_{\text{H}} = 25 \pm 2 \text{ kJ/mol}$, $\Delta S_{\text{H}} = 0.05 \pm 0.01 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 5.96 (calculated-TSA, Burkhard 1984)
- 5.90 (calculated-regression analysis with chlorine substituents, Oliver 1987c)
- 5.39, 5.57, 5.43, 5.80 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 5.46 (generator column-GC, Hawker & Connell 1988a)
- 5.62 (calculated-TSA, Hawker & Connell 1988a)
- 5.87 (calculated-MCI χ , Patil 1991)
- 5.55 (recommended, Sangster 1993)
- 7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
- 5.98 (quoted, Hansch et al. 1995)
- 6.12, 5.55–5.90 (calculated-Characteristic Root Index CRI, min.-max. range, Saçan & Inel 1995)
- 5.4429 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
- 6.13 (calculated-CLOGP ver. 4, Ran et al. 2002)
- 5.67 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated and reported temperature dependence equations.

- 9.28, 8.70, 8.24, 7.64 (0, 10, 20, 30°C , generator column-GC, Harner & Mackay 1995)
- $\log K_{\text{OA}} = -5.26 + 3965/(T/K)$; temp range 0 – 30°C (generator column-GC, Harner & Bidleman 1996)
- 9.18, 8.18; 8.25 (0, 20°C , multi-column GC- k' correlation; calculated at 20°C , Zhang et al. 1999)
- 8.02 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 5.76 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{aq.}) = 5.7 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C , half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{\text{OH}}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation: 91% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0019 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 88 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

Groundwater:

Sediment:

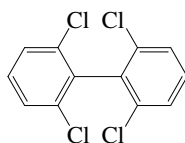
Soil:

Biota: $t_{1/2} = 365 \text{ d}$ in rainbow trout, d and $t_{1/2} = 107 \text{ d}$ in its muscle 107 d (Niimi & Oliver 1983);

$t_{1/2} = 30 \text{ d}$ in worms at 8°C, 30 d (Oliver 1987c).

depuration $t_{1/2} = 91 \text{ d}$ for high-dose treatment, $t_{1/2} = 88 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.54 2,2',6,6'-Tetrachlorobiphenyl (PCB-54)



Common Name: 2,2',6,6'-Tetrachlorobiphenyl

Synonym: PCB-54, 2,2',6,6'-tetrachloro-1,1'-biphenyl

Chemical Name: 2,2',6,6'-tetrachlorobiphenyl

CAS Registry No: 15968-05-5

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

198 (Van Roosmalen 1934; Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0201 (mp at $198^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.412, 0.221, 0.143, 0.0882 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0027 ($22^{\circ}C$, generator column-GC/ECD, Opperhuizen et al. 1988)

0.0119 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0659 (supercooled liquid P_L , Burkhard 1984)

0.00132 (GC-RI correlation, Burkhard et al. 1985a)

0.0659 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0392, 0.0517 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0566 (supercooled liquid P_L , Dunnivant & Elzerman 1988)

0.00227; 0.118 (calculated- $S \times HLC$, P_S ; supercooled liquid P_L , Dunnivant & Elzerman 1988)

$\log(P_L/Pa) = -3751/(T/K) + 11.17$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

0.000396–0.0219; 0.00388–0.104 (literature P_S range; literature P_L range, Delle Site 1997)

0.0114 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioglu 1998)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

188.5 (calculated-P/C, Burkhard et al. 1985b)

15.0 (calculated, Coates & Elzerman 1986)

55.73 (batch stripping-GC/ECD, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)

50.0 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

20.27 (wetted-wall column-GC/ECD, Brunner et al. 1990)

50.04 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.63 (calculated after Rekker 1977, Könemann 1981)

4.16, 713, 7.01 (HPLC- k' correlation; calculated- π const.; calculated-fragment const., McDuffie 1981)

- 5.94 (RP-TLC-retention, Bruggeman et al. 1982)
 4.95, 5.27, 5.22, 5.52 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.48 (generator column-GC, Hawker & Connell 1988a)
 5.936 \pm 0.031 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 5.24 (recommended, Sangster 1993)
 5.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 7.30 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 3.85; 5.38 (zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.106, 4.91, 4.89, 4.72 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
 5.72 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.63 (river sediment, Coates & Elzerman 1986)
 4.79 (correlated literature values in soils, Sklarew & Girvin 1987)
 5.01 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 5.11; 5.01 (soil, quoted lit.; calculated-Characteristic Root Index [CRI], Saçan & Balcioglu 1996)
 4.91, 4.84 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 2740 \text{ d}^{-1}$; $k_2 = 0.387 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 190 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 100 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{1/2} = 72.5 \text{ min}$ when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5 kW high pressure Xenon lamp (De Felip et al. 1996).

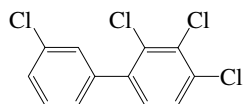
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 190 \text{ d}$ for high-dose treatment, $t_{1/2} = 100 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.55 2,3,3',4-Tetrachlorobiphenyl (PCB-55)



Common Name: 2,3,3',4-Tetrachlorobiphenyl

Synonym: PCB-55, 2,3,3',4-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4-tetrachlorobiphenyl

CAS Registry No: 74338-24-2

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

89 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.122 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.81×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00517 (GC-RI correlation, Burkhard et al. 1985b)

0.00579, 0.00349 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4382/(T/K) + 12.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

11.55 (calculated-P/C, Burkhard 1984)

23.51 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

18.48 (calculated-QSPR, Dunnivant et al. 1992)

35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 2$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.86 (calculated-TSA, Burkhard 1984)

6.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.0161 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.66 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Life, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2): $k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 91 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004) $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 157 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

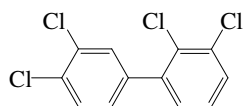
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 91 \text{ d}$ for high-dose treatment, $t_{1/2} = 157 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.56 2,3,3',4'-Tetrachlorobiphenyl (PCB-56)



Common Name: 2,3,3',4'-Tetrachlorobiphenyl

Synonym: PCB-56, 2,3,3',4'-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4'-tetrachlorobiphenyl

CAS Registry No: 41464-41-9

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

95 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.122 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0389 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0989 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0146 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0115 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.96×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00517 (GC-RI correlation, Burkhard et al. 1985b)

0.00434, 0.00327 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.17×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00331, 0.00468 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4382/(T/K) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa- m^3/mol at $25^{\circ}C$ or as indicated):

9.45 (calculated-P/C, Burkhard 1984)

16.41 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

13.27 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

15.34 (calculated-QSAR, Dunnivant et al. 1992)

8.24 (calculated-QSAR, Achman et al. 1993)

13.9 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

27.6 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 32 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.86 (calculated-TSA, Burkhard 1984)

5.85 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.11 (calculated, Miertus & Jakus 1990)

5.85 (recommended, Sangster 1993)

- 5.90 (calculated-TSA, Murray & Andren 1992)
 5.9815 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.66 (suspended particulate matter, Burkhard 1984)
 6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 5.4 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from ~4–11 d in freshwater systems, 0.1–10 d in cloud water, > 1000 d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

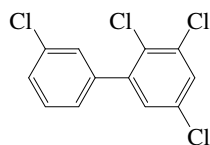
Ground water:

Sediment:

Soil:

Biota:

7.1.1.57 2,3,3',5-Tetrachlorobiphenyl (PCB-57)



Common Name: 2,3,3',5-Tetrachlorobiphenyl

Synonym: PCB-57

Chemical Name: 2,3,3',5-tetrachlorobiphenyl

CAS Registry No: 70424-87-8

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

68 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0718 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00767 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

19.76 (calculated-P/C, Burkhard 1984)

37.59 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

27.40 (calculated-QSPR, Dunnivant et al. 1992)

35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.91 (calculated, Burkhard 1984)

6.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.1376 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.69 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

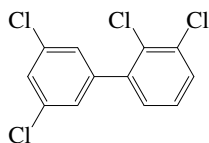
Ground water:

Sediment:

Soil:

Biota:

7.1.1.58 2,3,3',5'-Tetrachlorobiphenyl (PCB-58)



Common Name: 2,3,3',5'-Tetrachlorobiphenyl

Synonym: PCB-58

Chemical Name: 2,3,3',5'-tetrachlorobiphenyl

CAS Registry No: 41464-43-1

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

68 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00558 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$):

9.62×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.000167 (GC-RI correlation, Burkhard et al. 1985b)

$\log(P/mmHg) = 10.80 - 5600/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

16.11 (calculated-P/C, Burkhard 1984)

45.46 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

25.33 (calculated-QSPR, Dunnivant et al. 1992)

35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.91 (calculated-TSA, Burkhard 1984)

6.17 (calculated-TSA, Hawker & Connell 1988a)

6.17 (recommended, Hansch et al. 1995)

6.0904 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.73 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

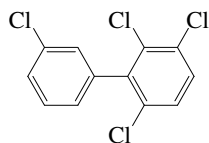
Ground water:

Sediment:

Soil:

Biota:

7.1.1.59 2,3,3',6-Tetrachlorobiphenyl (PCB-59)



Common Name: 2,3,3',6-Tetrachlorobiphenyl

Synonym: PCB-59

Chemical Name: 2,3,3',6-tetrachlorobiphenyl

CAS Registry No: 74472-33-6

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

42 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):Density (g/cm^3):Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):0.131 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00733 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):0.0155 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0164 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

34.65 (calculated-P/C, Burkhard 1984)

36.58 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

30.81 (calculated-QSPR, Dunnivant et al. 1992)

35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004
Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.84 (calculated, Burkhard 1984)

5.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.8476 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:Sorption Partition Coefficient, $\log K_{OC}$:

5.64 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 132 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 135 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

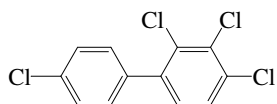
Surface water:

Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 132 \text{ d}$ for high-dose treatment, $t_{1/2} = 135 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.60 2,3,4,4'-Tetrachlorobiphenyl (PCB-60)

Common Name: 2,3,4,4'-Tetrachlorobiphenyl

Synonym: PCB-60, 2,3,4,4'-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3,4,4'-tetrachlorobiphenyl

CAS Registry No: 33025-41-1

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

128 (Weast 1972–73; Ruelle & Kesselring 1997)

142 (Saeki et al. 1971; Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2024

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.0695 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.058 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.0168 (calculated-TSA, Mackay et al. 1980)

0.121 (calculated-TSA, supercooled liquid S_L , Burkhard et al. 1985b)

0.0389 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0902, 0.0485, 0.0254, 0.0243 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0359, 0.0273 (Nirmalakhandan & Speece 1989)

0.0146 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.045 (calculated-MCI χ , Patil 1991)

0.00274 (calculated-QSPR, Dunnivant et al. 1992)

0.0067, 0.0176 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.000319 (GC-RI correlation, Burkhard et al. 1985a)

0.00427 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00527, 0.00414 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00217 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 10.90 - 4660/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00331, 0.00458 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4282/(T/K) + 12.42$ (supercooled liquid P_L , GC-RT correlation, Falconer Bidleman 1994)

0.0157 (supercooled liquid P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

84.20 (batch stripping, Atlas et al. 1982)

10.34 (calculated-P/C, Burkhard et al. 1985b)

16.41 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

- 15.40 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
 15.48 (calculated-QSPR, Dunnivant et al. 1992)
 35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.87 (calculated-TSA, Burkhard 1984)
 5.84 (HPLC-RT correlation calculated- π , Rapaport & Eisenreich 1984)
 5.90 (selected, Shiu & Mackay 1986)
 5.89, 6.15, 6.57, 6.37 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 6.11 (calculated-TSA, Hawker & Connell 1988a)
 5.88 (calculated-MCI χ , Patil 1991)
 7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
 6.01 (recommended, Sangster 1993)
 5.84 (quoted, Hansch et al. 1995)
 5.95, 5.33–6.24 (calculated-Characteristic Root Index CRI, minimum-maximum range, Saçan & Inel 1995)
 6.0108 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.82 (10°C, estimated, Thomas et al. 1998)
 9.21 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 6.20, 5.0 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.67 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 6.10 (organic carbon, obs., Murray & Andren 1992)
 5.03 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioglu 1996)
 5.30 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 5.4 \times 10^9$ dm³ mol⁻¹ s⁻¹, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40$ d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 10$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.10$ d⁻¹ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

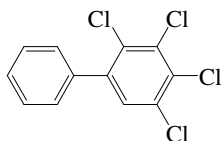
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 7$ d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.61 2,3,4,5-Tetrachlorobiphenyl (PCB-61)



Common Name: 2,3,4,5-Tetrachlorobiphenyl

Synonym: PCB-61, 2,3,4,5-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3,4,5-tetrachlorobiphenyl

CAS Registry No: 33284-53-6

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

92.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2024

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.2 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

69.45 (Miller et al. 1984)

69.25, 64.3 (exptl., calculated, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.217 (Mackay et al. 1980)

0.218 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0192 (generator column-GC/ECD, Weil et al. 1974)

0.0209 (shake flask-GC/ECD, Haque & Schmedding 1975)

0.0099 (generator column-HPLC/UV, Billington 1982; Billington et al. 1988)

0.0209 (generator column-GC/ECD, Miller et al. 1984, 1985)

0.0207, 0.030, 0.0180, 0.0243 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.014 (generator column-GC, Dunnivant & Elzerman 1988)

0.0137 (generator column-GC/ECD, Li et al. 1992; Li & Doucette 1993)

0.0136 (shake flask-GC/ECD, Li & Andren 1994)

$0.0156^* \pm 0.0004$ (generator column-GC/ECD, measured range $5-45^{\circ}C$, Shiu et al. 1997)

$\ln x = -3.967 - 4970.5/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.0624 (calculated-mp and K_{ow} , Ran et al. 2002)

0.106, 0.101 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

$\log [S_L/(mol\ m^{-3})] = -839/(T/K) - 0.626$ (supercooled liquid, linear regression of literature data, Li et al. 2003)

$\log [S_L/(mol\ m^{-3})] = -1043/(T/K) + 0.037$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0013 (GC-RT correlation, Burkhard et al. 1985a)

0.00558 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

$\log (P_L/Pa) = -4382/(T/K) + 12.78$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

1.854×10^{-4} ($20^{\circ}C$, gas saturation-GC/ECD, measured range -20 to $20^{\circ}C$, Wania et al. 1994)

$\log (P_S/Pa) = 12.10 - 4632/(T/K)$; temp range -20 to $+20^{\circ}C$ (gas saturation-GC, Wania et al. 1994)

0.0144 (supercooled liq. P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)
 0.00724, 0.00692 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log (P_L/Pa) = -4330/(T/K) + 12.38$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
 $\log (P_L/Pa) = -4193/(T/K) + 11.91$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

11.45 (calculated-P/C, Burkhard et al. 1985b)
 17.53 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)
 24.14 (calculated-QSPR, Dunnivant et al. 1992)
 35.1 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004
 20.42, 19.95 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
 $\log [H/(Pa \text{ m}^3/\text{mol})] = -3150/(T/K) + 11.87$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.78 (HPLC-RT correlation, Sugiura et al. 1979)
 5.90 (shake flask-GC, Platford 1982)
 6.39 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 6.74 (calculated-fragment const., Yalkowsky et al. 1983)
 5.81 (calculated-TSA, Burkhard 1984)
 5.72 (generator column-GC/ECD, Miller et al. 1984,1985)
 5.90 (selected, Shiu & Mackay 1986)
 6.38, 6.31, 6.57, 6.37 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 6.18; 6.04 (generator column-GC/ECD; calculated-TSA, Hawker & Connell 1988a)
 5.92, 6.74 (calculated-solvatochromic parameters and V_f , calculated- fragment additivity., Kamlet et al. 1988)
 6.88, 6.74, 5.89, 6.04, 6.02 (calculated- π const., f const., MW, MCI χ , TSA, Doucette & Andren 1988)
 6.39 (calculated- π const., De Bruijn et al. 1989)
 6.406 \pm 0.069 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 5.89 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 6.34 (generator column-GC, Li & Doucette 1993)
 7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
 6.44 (recommended, Sangster 1993)
 6.41 (recommended, Hansch et al. 1995)
 5.97, 5.72–6.74 (calculated-Characteristic Root Index CRI; minimum-maximum range, Saçan & Inel 1995)
 6.1472 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
 6.00 (calculated-QSPR, Yeh & Hong 2002)
 6.51 (calculated-CLOGP ver. 4, Ran et al. 2002)
 6.17, 6.11 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.901* (20°C, generator column-GC, measured range –10 to 20°C, Harner & Mackay 1995)
 $\log K_{OA} = -2.90 + 3464/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Mackay 1995)
 8.90 (20°C, generator column-GC, Harner & Bidleman 1996)
 $\log K_{OA} = -2.89 + 3464.1/(T/K)$; temp range –10 to + 20°C (generator column-GC, Harner & Bidleman 1996)
 9.38–9.65 (10°C, estimated, Thomas et al. 1998)
 10.19, 8.93; 8.90 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 8.76 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
 8.80; 8.75 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
 8.64, 8.55 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log K_{OA} = 4660/(T/K) - 7.08$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$:

4.29, 3.57, 3.94, 3.90 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)

Sorption Partition Coefficient, log K_{OC} :

- 5.61 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.93 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.038 \text{ d}^{-1}$ (golden orfe, Sugiura et al. 1979)

$k_2 = 0.0022 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 312 \text{ d}$ in rainbow trout, and $t_{1/2} = 93 \text{ d}$ in its muscle 93 d (Niimi & Oliver 1983)

TABLE 7.1.1.61.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,3,4,5-tetrachlorobiphenyl (PCB-61) at various temperatures

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1997		Wania et al. 1994		Harner & Mackay 1995	
generator column-GC/ECD		gas saturation-GC/ECD		generator column-GC	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	log K_{OA}
5	0.0056	–20	5.298×10^{-7}	–10	10.268
15	0.0102	–10	3.817×10^{-6}	0	9.80
25	0.0156	0	1.439×10^{-5}	10	9.40
35	0.0285	10	6.163×10^{-5}	20	8.901
45	0.0560	20	1.854×10^{-4}	25	8.74
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 41.3$		log (P/Pa) = $A - B/(T/K)$		$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 66.3$	
for 5–45°C		A 12.10		log $K_{OA} = A + B/T$	
		B 4632		A –2.9	
		temp range –20 to 20°C		B 3464.1	
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 88.7$			

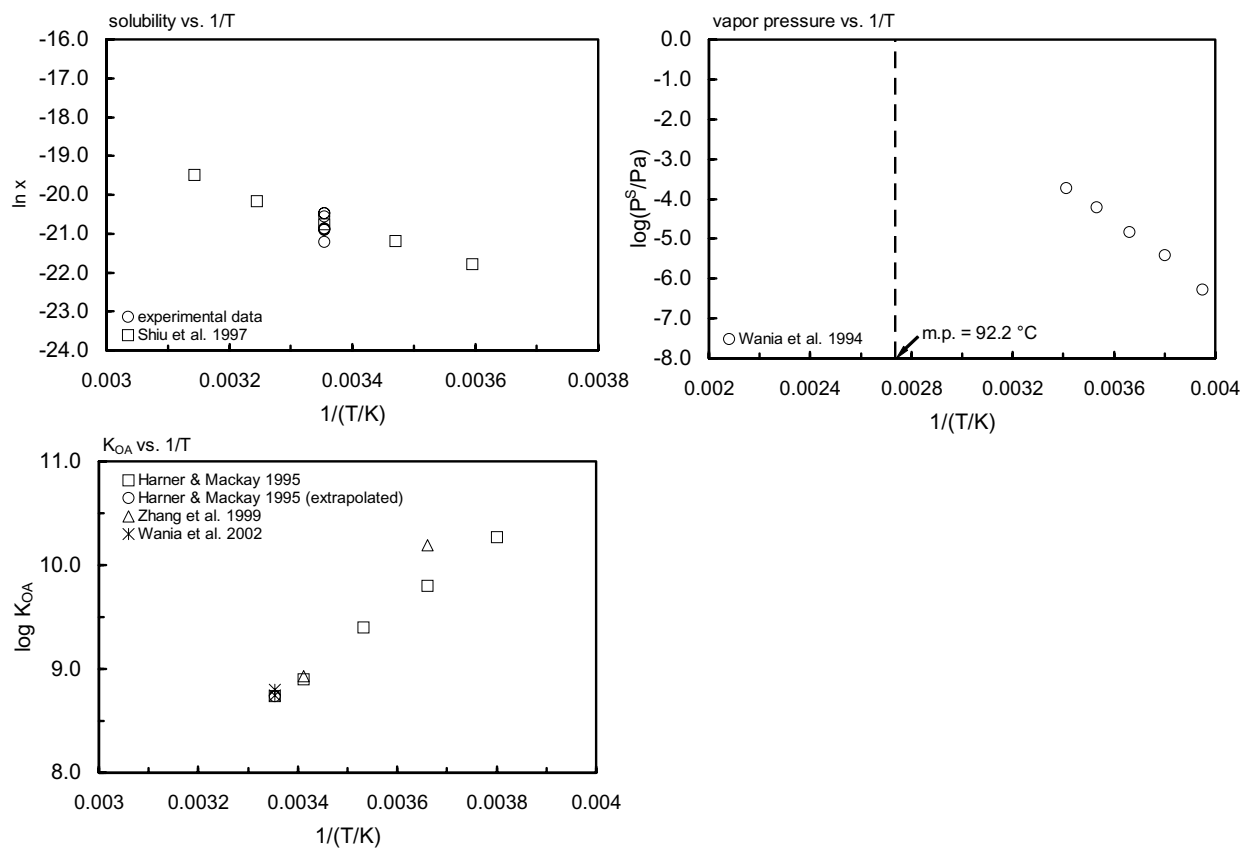
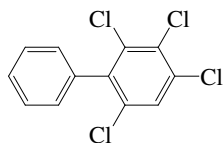


FIGURE 7.1.1.61.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,3,4,5-tetrachlorobiphenyl (PCB-61).

7.1.1.62 2,3,4,6-Tetrachlorobiphenyl (PCB-62)



Common Name: 2,3,4,6-Tetrachlorobiphenyl

Synonym: PCB-62

Chemical Name: 2,3,4,6-tetrachlorobiphenyl

CAS Registry No: 54230-23-7

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

77 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.151 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0463 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0158 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0167 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

30.70 (calculated-P/C, Burkhard 1984)

37.08 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

21.28 (wetted-wall column-GC, Brunner et al. 1990)

37.47 (calculated-QSPR, Dunnivant et al. 1992)

35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2 kJ/mol$, $\Delta S_H = 0.05 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.79 (calculated, Burkhard 1984)

5.89 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.0323 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.59 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

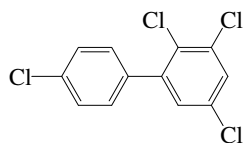
Ground water:

Sediment:

Soil:

Biota:

7.1.1.63 2,3,4',5-Tetrachlorobiphenyl (PCB-63)



Common Name: 2,3,4',5-Tetrachlorobiphenyl

Synonym: PCB-63, 2,3,4',5-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3,4',5-tetrachlorobiphenyl

CAS Registry No: 74472-34-7

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

83 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.105 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0263 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0496 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00727 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.36×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00681 (GC-RI correlation, Burkhard et al. 1985b)

2.64×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00724 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4382/(T/K) + 12.53$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant (Pa- m^3/mol at $25^{\circ}C$ or as indicated):

17.73 (calculated-P/C, Burkhard 1984)

29.28 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

29.60 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

8.24 (calculated-QSAR, Achman et al. 1993)

25.59 (calculated-QSPR, Dunnivant et al. 1992)

24.5 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

42.1 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.91 (calculated-TSA, Burkhard 1984)

6.10 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.17 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.10 (recommended, Sangster 1993)

6.1262 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

10.15, 9.06 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)

8.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 219 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 172 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

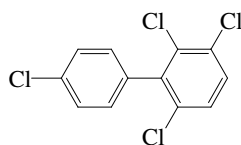
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 219 \text{ d}$ for high-dose treatment, $t_{1/2} = 172 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.64 2,3,4',6-Tetrachlorobiphenyl (PCB-64)



Common Name: 2,3,4',6-Tetrachlorobiphenyl

Synonym: PCB-64, 2,3,4',6-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3,4',6-tetrachlorobiphenyl

CAS Registry No: 52663-58-8

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

57 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.130 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0937 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.028 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0138 (P_L supercooled liquid, GC-RT correlation Burkhard et al. 1985a)

0.0146 (GC-RI correlation, Burkhard et al. 1985b)

5.51×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 10.70 - 4510/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00776, 0.0141 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.30$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

31.01 (calculated-P/C, Burkhard 1984)

17.25 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

28.37 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

14.2 (wetted-wall column-GC, Brunner et al. 1990)

27.59 (calculated-QSPR, Dunnivant et al. 1992)

24.7 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

42.4 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 2 kJ/mol$, $\Delta S_H = 0.05 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.84 (calculated-TSA, Burkhard 1984)

5.76 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.0 (calculated-TSA, Murray & Andren 1992)

5.76 (recommended, Sangster 1993)

5.8251 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

- 8.41; 7.91 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -6.43 + 4420/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 8.80 (quoted, Kömp & McLachlan 1997b)
- 9.62, 8.63; 8.74 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- 8.54 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.64 (suspended particular matter, Burkhard 1984)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25 - 60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5 - 40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 140 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 160 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

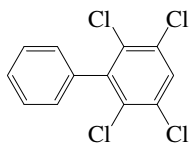
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 140 \text{ d}$ for high-dose treatment, $t_{1/2} = 160 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.65 2,3,5,6-Tetrachlorobiphenyl (PCB-65)



Common Name: 2,3,5,6-Tetrachlorobiphenyl

Synonym: PCB-65, 2,3,5,6-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3,5,6-tetrachlorobiphenyl

CAS Registry No: 33284-54-7

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

77–77.5 (Bolgar 1973)

79.0 (Burkhard 1984; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.295 (mp at $79^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.162 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0099, 0.0216, 0.0119, 0.0279 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0431 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0151 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00467 (GC-RI correlation, Burkhard et al. 1985b)

0.0151 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.33$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

0.0238 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index [CRI], Saçan & Balcioglu 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

27.26 (calculated-P/C, Burkhard 1984)

31.01 (calculated-QSAR- MCI χ , Sabljic & Güsten 1989)

34.10 (calculated-QSPR, Dunnivant et al. 1992)

35.0 (predicted from homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.77 (calculated-TSA, Burkhard 1984)

6.07, 5.95, 5.98, 5.85 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.94; 5.86 (generator column-GC; calculated-TSA, Hawker & Connell 1988a)

5.96 (recommended, Sangster 1993)

7.8733 (calculated-UNIFAC group contribution method, Chen et al. 1993)

- 5.86 (recommended, Hansch et al. 1995)
 5.81; 5.46–5.96 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
 6.0133 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
 5.83 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 8.40 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 2.46 (*Poecillia reticulata*, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.57 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

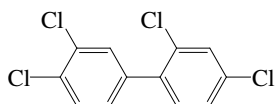
Ground water:

Sediment:

Soil:

Biota:

7.1.1.66 2,3',4,4'-Tetrachlorobiphenyl (PCB-66)



Common Name: 2,3',4,4'-Tetrachlorobiphenyl

Synonym: PCB-66, 2,3',4,4'-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3',4,4'-tetrachlorobiphenyl

CAS Registry No: 32598-10-0

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

124 (Saeki et al. 1971; Hutzinger et al. 1974)

127–127.5 (Webb & McCall 1972)

127–128 (Wallnöfer et al. 1973, Bolgar 1973)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.105 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.058 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.0168 (calculated-TSA, Mackay et al. 1980)

0.098 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.00474 (calculated-fragment solubility constants, Wakita et al. 1986)

0.0368 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.068 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0273 (calculated-MCI χ , Nirmalakhandan & Speece 1989)

0.0116 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.045 (calculated-MCI χ , Patil 1991)

0.00446 (calculated-QSPR, Dunnivant et al. 1992)

0.0216 (calculated-group contribution method, Kühne et al. 1995)

0.0266 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00616 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

0.000494 (GC-RI correlation, Burkhard et al. 1985a)

0.00459 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00569, 0.00507 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00252 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 10.90 - 4650/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00427, 0.0059 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4349/(T/K) + 12.38$ (GC-RT correlation, Falconer & Bidleman 1994)

0.00347 (supercooled liquid P_L , from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

84.20 (calculated-P/C, Murphy et al. 1983)

13.68 (calculated-P/C, Burkhard et al. 1985b)

- 14.18 (quoted, Eisenreich 1987)
 20.37 (20°C, calculated-P/C, Murphy et al. 1987)
 25.84 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
 12.16 (wetted-wall column-GC, Brunner et al. 1990)
 20.55 (calculated-QSPR, Dunnivant et al. 1992)
 36.97* \pm 0.48 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
 $\ln K_{AW} = 7.4573 - 3488.7/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(29.0/kJ \cdot mol^{-1})/RT] + (0.062/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314 J \cdot K^{-1} \cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
 35.4 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.90 (HPLC-RT correlation, Shaw & Connell 1982)
 5.80, 6.31 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
 5.98 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
 6.31 (generator column-GC/ECD, Hawker & Connell 1988a)
 6.09 (generator column-GC, Larsen et al. 1992)
 6.12 (recommended, Sangster 1993)
 6.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 9.22* (20°C, generator column-GC, measured range 0–30°C, Harner & Bidleman 1996)
 $\log K_{OA} = -3.82 + 3827/(T/K)$; temp range 0–30°C (generator column-GC, Harner & Bidleman 1996)
 9.73 (10°C, estimated, Thomas et al. 1998)
 10.33, 9.29; 9.22 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 9.36 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 4.45 (worms, Oliver 1987c)
 3.18–4.62 (various marine species, mean dry wt. BCF, Hope et al. 1998)
 4.55–5.76 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.80, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.74 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.72 (soil, calculated-S, Chou & Griffin 1986)
 5.23 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
 4.90 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
 6.10 (organic carbon, obs., Murray & Andren 1992)
 4.90 (soil, calculated-QSPR Characteristic Root Index [CRI], Saçan & Balçioğlu 1996)
 5.20 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Hydrolysis:

Photolysis: photodegradation $k = (0.11 \pm 0.02) h^{-1}$ with $t_{1/2} = 7.1$ h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60$ d, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{aq.}) = 5.1 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{\text{OH}}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40$ d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.001 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; selected, Clark et al. 1990)

$k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 82$ d and $k_2 = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 55$ d for food concn of 21 ng/g and 158 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 164$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 225$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991);

photodegradation $t_{1/2} = (7.1 \pm 1.5) \text{ h}$ in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Groundwater:

Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.067 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.75 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 1.18 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.32 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00081 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.0024 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00443 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.000295 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{1/2} = 670$ d in rainbow trout, and $t_{1/2} = 108$ d its muscle (Niimi & Oliver 1983)

$t_{1/2} = 33$ d in worms at 8°C (Oliver 1987c)

depuration $t_{1/2} = 55\text{--}82$ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 164$ d for high-dose treatment, $t_{1/2} = 225$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.66.1

Reported Henry's law constants and octanol-air partition coefficients of 2,3',4,4'-tetrachlorobiphenyl (PCB-66) at various temperatures and temperature dependence equations

Henry's law constant		log K _{OA}			
Bamford et al. 2000		Harner & Bidleman 1996		Zhang et al. 1999	
gas stripping-GC/MS		generator column-GC		multicolumn-GC-k' correlation	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}	t/°C	log K _{OA}
4	14.17	0	10.21	0	10.33
11	19.80	10	9.65	20	9.29
18	27.25	20	9.22		
25	36.97	30	8.82		
31	47.51				

$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 73.28$

$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\log K_{OA} = A + B/T$	
	K _{AW}	A	-3.82
A	7.4573	B	3827
B	3488.09		

enthalpy, entropy change:
 $\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 29.0 \pm 2.6$
 $\Delta S/(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) = 62 \pm 8$

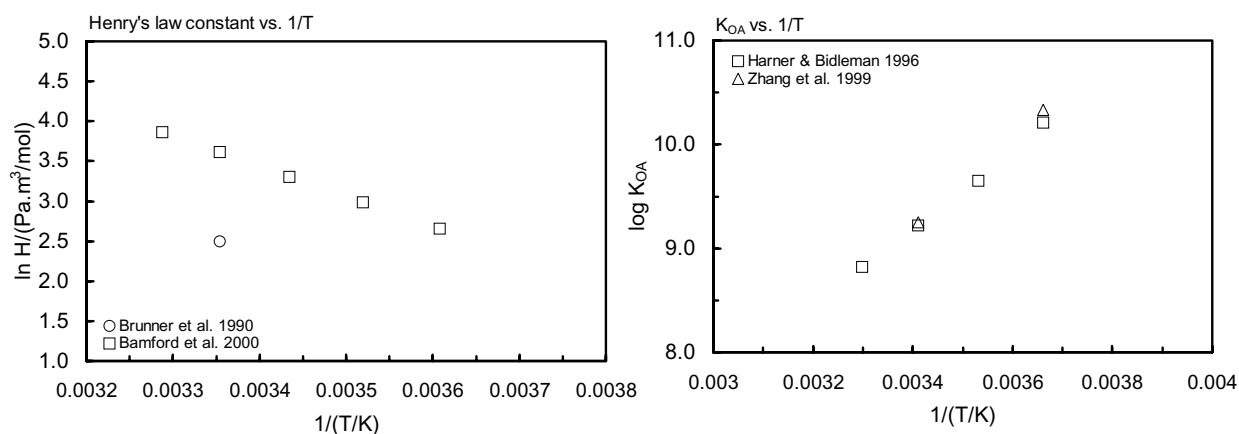
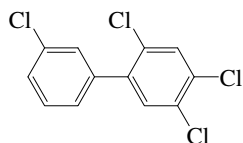


FIGURE 7.1.1.66.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,3',4,4'-tetrachlorobiphenyl (PCB-66).

7.1.1.67 2,3',4,5-Tetrachlorobiphenyl (PCB-67)



Common Name: 2,3',4,5-Tetrachlorobiphenyl

Synonym: PCB-67, 2,3',4,5-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3',4,5-tetrachlorobiphenyl

CAS Registry No: 73575-53-8

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

83 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0987 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0351, 0.0298, 0.00804, 0.0266 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00654 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0070 (GC-RI correlation, Burkhard et al. 1985b)

$\log(P/mmHg) = 10.70 - 4530/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00708 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4382/(T/K) + 12.52$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

19.35 (calculated-P/C, Burkhard 1984)

29.18 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)

23.70 (calculated-QSPR, Dunnivant et al. 1992)

35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3\ kJ/mol$, $\Delta S_H = 0.06 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.93 (calculated-TSA, Burkhard 1984)

6.22, 6.32, 6.40, 6.33 (RP-HPLC- k' correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.32 (recommended, Sangster 1993)

6.2276 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.06 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.73 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

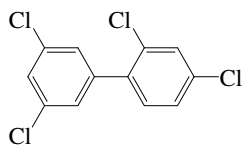
Ground water:

Sediment:

Soil:

Biota:

7.1.1.68 2,3',4,5'-Tetrachlorobiphenyl (PCB-68)



Common Name: 2,3',4,5'-Tetrachlorobiphenyl

Synonym: PCB-68

Chemical Name: 2,3',4,5'-tetrachlorobiphenyl

CAS Registry No: 73575-52-7

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

71 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.085 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0184 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00679 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00726 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

23.30 (calculated-P/C, Burkhard 1984)

55.02 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

38.17 (calculated-QSPR, Dunnivant et al. 1992)

35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.99 (calculated-TSA, Burkhard 1984)

6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.2624 (calculated molecular properties MNDO-AM method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.66 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.79 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 11 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2 = 0.08 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

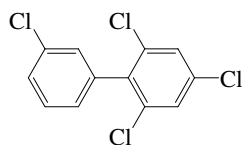
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 8 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.69 2,3',4,6-Tetrachlorobiphenyl (PCB-69)



Common Name: 2,3',4,6-Tetrachlorobiphenyl

Synonym: PCB-69

Chemical Name: 2,3',4,6-tetrachlorobiphenyl

CAS Registry No: 60233-24-1

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

45 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.105 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0097, 0.0146, 0.0184, 0.0243 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0169 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0179, (GC-RI correlation, Burkhard et al. 1985b)

$\log(P/mmHg) = 10.60 - 4440/T$ (GC-RT correlation, Tateya et al. 1988)

0.01911 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.43$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

47.12 (calculated-P/C, Burkhard 1984)

63.53 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

21.28 (wetted-wall column-GC/ECD, Brunner et al. 1990)

51.22 (calculated-QSAR, Dunnivant et al. 1992)

35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.91 (calculated-TSA, Burkhard 1984)

6.09, 6.06, 6.09, 5.89 (RP-HPLC- k' correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.0068 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.47 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

5.71 (suspended particulate matter, Burkhard et al. 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

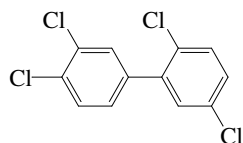
Ground water:

Sediment:

Soil:

Biota:

7.1.1.70 2,3',4',5-Tetrachlorobiphenyl (PCB-70)



Common Name: 2,3',4',5-Tetrachlorobiphenyl

Synonym: PCB-70, 2,3',4',5-tetrachloro-1,1'-biphenyl

Chemical Name: 2,3',4',5-tetrachlorobiphenyl

CAS Registry No: 32598-11-1

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

104 (Bellavita 1935; Hutzinger et al. 1974)

104–107 (Wallnöfer et al. 1973, Bolgar 1973)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2024

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.168 (mp at $104^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.041 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.029 (calculated-TSA, Mackay et al. 1980)

0.022 (generator column-GC, Bruggeman et al. 1981)

0.099 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.0091 (generator column-GC/ECD, Opperhuizen et al. 1985)

0.0104 (calculated-fragment solubility constants, Wakita et al. 1986)

0.0362 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0254, 0.0368, 0.0432, 0.030 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0273 (calculated-MCI χ , Nirmalakhandan & Speece 1989)

0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.045 (calculated-MCI χ , Patil 1991)

0.0111 (calculated-QSPR, Dunnivant et al. 1992)

0.0114, 0.0306 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.0463 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00544, 0.00642 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Bidleman 1984)

0.00769 (calculated $S \times HLC$, Burkhard et al. 1985a)

0.000919 (GC-RI correlation, Burkhard et al. 1985a)

0.00519 (supercooled liquid P_L , calculated-GC-RI, Burkhard et al. 1985b)

0.00526, 0.00551 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.0060 (selected P_L , supercooled liquid, Shiu & Mackay 1986)

0.00236 (20°C, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
 $\log (P/\text{mmHg}) = 10.90 - 4640/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
 0.00447, 0.0063 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/P_a) = -4431/(T/K) + 12.60$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

20.26 (calculated-P/C, Murphy et al. 1983)
 15.30 (calculated-P/C, Burkhard et al. 1985b)
 19.05 (20°C, calculated-P/C, Murphy et al. 1987)
 19.15 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
 10.13 (wetted-wall column-GC, Brunner et al. 1990)
 20.50 (calculated-QSPR, Dunnivant et al. 1992)
 17.2 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
 32.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 3 \text{ kJ/mol}$, $\Delta S_H = 0.06 \pm 0.01 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.95 (shake flask-GC, Tulp & Hutzinger 1978)
 5.95 (HPLC- k' correlation, McDuffie 1981)
 6.39 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 6.30 (HPLC-RT correlation, Shaw & Connell 1982)
 5.72, 6.23 (HPLC-RT correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
 6.18 (HPLC-RT correlation, Opperhuizen et al. 1985)
 6.01, 6.24, 6.36, 6.29 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 5.99 (generator column-GC, Larsen et al. 1992)
 5.99 (HPLC- k' correlation, Neogrohati & Hammers 1992)
 5.7833 (calculated-UNIFAC group contribution, Chen et al. 1993)
 6.23 (recommended, Sangster 1993)
 6.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

10.29, 9.22; 9.29 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 8.92 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

6.15 (goldfish, 3% lipid, static equilibration system-GC/ECD, 23-d exposure, Bruggeman et al. 1981)
 6.20 (goldfish, 3% lipid, calculated- K_{OW} , Bruggeman et al. 1981)
 4.62, 5.11 (goldfish, exptl., correlated, Mackay & Hughes 1984)
 4.32, 5.50 (guppy, lipid phase, Opperhuizen et al. 1985)
 4.92 (guppy, Gobas et al. 1987)
 4.62, 4.32 (fish, calculated- C_B/C_W or k_1/k_2 , Connell & Hawker 1988; Hawker 1990)
 5.08; 6.61 (22°C, zebrafish: $\log BCF_W$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)
 4.32, 5.62; 4.742, 4.257 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW} , Lu et al. 1999)
 5.08, 6.61 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

5.70, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.02, 4.86, 4.85, 4.69 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
- 5.73 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 5.6–6.8, 6.3 (suspended sediment, average, Oliver 1987a)
- 7.20 (algae > 50 μm , Oliver 1987a)
- 4.81 (soil, calculated-S, Chou & Griffin 1986)
- 4.76 (correlated literature values in soils, Sklarew & Girvin 1987)
- 6.04 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 5.52 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.84 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 5.02; 5.07 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 5.30 (soil, calculated- K_{OW} , Girvin & Scott 1997)
- 4.86, 4.80 (sediments: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 5.5 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C , half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 420 \text{ d}^{-1}$; $k_2 = 0.01 \text{ d}^{-1}$ (23°C , goldfish, 3% lipid content, Bruggeman et al. 1981; quoted, Waid 1986, Clark et al. 1990)

$k_2 = 0.01, 0.0104 \text{ d}^{-1}$ (goldfish, exptl., correlated, Mackay & Hughes 1984)

$k_1 = 380 \text{ d}^{-1}$; $k_2 = 0.018 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1985)

$k_1 = 17.5 \text{ h}^{-1}$; $1/k_2 = 2400 \text{ h}$ (goldfish, quoted, Hawker & Connell 1985)

$\log k_1 = 2.58, 2.62 \text{ d}^{-1}$; $\log 1/k_2 = 1.74, 2.0 \text{ d}$ (fish, quoted, Connell & Hawker 1988)

$\log k_2 = -2.0 \text{ d}^{-1}$ (fish, quoted, Thomann 1989)

$k_1 = 3340 \text{ d}^{-1}$; $k_2 = 0.0280 \text{ d}^{-1}$ (22°C , zebrafish, 30-d exposure, Fox et al. 1994)

$k_1 = 0.00043 \text{ h}^{-1}$; $k_2 = 0.170 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_1 = 10$ (food lipid $\text{mg}/(\text{g worm lipid-d})$; $k_2 = 0.09 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 167 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 217 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of $25\text{--}60 \text{ d}$ due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of $8.5\text{--}40 \text{ d}$ based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991); photodegradation $t_{1/2} = 4.87$ min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

Groundwater:

Sediment:

Soil:

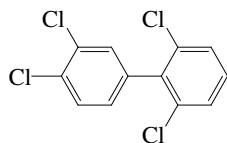
Biota: clearance $t_{1/2} = 60$ d in goldfish (static equilibration system, 23-d exposure, Bruggeman et al. 1981)

$t_{1/2} = 38.6$ d in guppy (Opperhuizen et al. 1985);

elimination $t_{1/2} = 8$ d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2} = 167$ d for high-dose treatment, $t_{1/2} = 217$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.71 2,3',4',6-Tetrachlorobiphenyl (PCB-71)



Common Name: 2,3',4',6-Tetrachlorobiphenyl

Synonym: PCB-71

Chemical Name: 2,3',4',6-tetrachlorobiphenyl

CAS Registry No: 41464-46-4

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

57 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.123 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0278 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0583 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

9.59×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)

0.0102 (GC-RI correlation, Burkhard et al. 1985b)

0.00912, 0.00877 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00776, 0.0115 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4229/(T/K) + 12.14$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

22.80 (calculated-P/C, Burkhard 1984)

32.53 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

14.31 (calculated-QSPR, Achman et al. 1993)

31.82 (calculated-QSPR, Dunnivant et al. 1992)

35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2 kJ/mol$, $\Delta S_H = 0.05 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.86 (calculated-TSA, Burkhard 1984)

5.76 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.98 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.7206 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

9.78, 8.84; 8.98 (0, $20^{\circ}C$, multi-column GC- k' correlation; calculated at $20^{\circ}C$, Zhang et al. 1999)

8.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

5.66 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 5.7 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

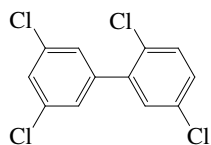
Ground water:

Sediment:

Soil:

Biota:

7.1.1.72 2,3',5,5'-Tetrachlorobiphenyl (PCB-72)



Common Name: 2,3',5,5'-Tetrachlorobiphenyl

Synonym: PCB-72

Chemical Name: 2,3',5,5'-tetrachlorobiphenyl

CAS Registry No: 41464-42-0

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

56 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0861 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0232 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0107 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.66×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0204, 0.00818, 0.00957 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.010, 0.00988 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4382/(T/K) + 12.70$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

25.34 (calculated-P/C, Burkhard 1984)

48.33 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

36.70 (calculated-QSAR, Dunnivant et al. 1992)

35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3 kJ/mol$, $\Delta S_H = 0.06 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.98 (calculated, Burkhard 1984)

6.26 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)

6.2101 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.78 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

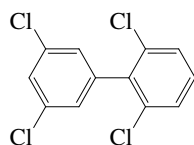
Ground water:

Sediment:

Soil:

Biota:

7.1.1.73 2,3',5',6-Tetrachlorobiphenyl (PCB-73)



Common Name: 2,3',5',6-Tetrachlorobiphenyl

Synonym: PCB-73

Chemical Name: 2,3',5',6-tetrachlorobiphenyl

CAS Registry No: 74338-23-1

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

66 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0368 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0142 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0204, 0.0150, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

38.91 (calculated-P/C, Burkhard 1984)

61.81 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

52.69 (calculated-QSPR, Dunnivant et al. 1992)

35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.91 (calculated-TSA, Burkhard 1984)

6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.8026 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.97 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.71 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–0 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–0 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

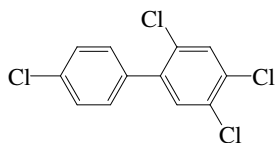
Ground water:

Sediment:

Soil:

Biota:

7.1.1.74 2,4,4',5-Tetrachlorobiphenyl (PCB-74)



Common Name: 2,4,4',5-Tetrachlorobiphenyl

Synonym: PCB-74, 2,4,4',5-tetrachloro-1,1'-biphenyl

Chemical Name: 2,4,4',5-tetrachlorobiphenyl

CAS Registry No: 32690-93-0

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

125 (Burkhard et al. 1985a; Shiu & Mackay 1986; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F:

0.102 (calcd-assuming $\Delta S_{fus} = 56$ J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0978 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0306 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0496 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0116 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00453 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0058 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00209, 0.000636, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00731, 0.00692 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.12×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 10.80 - 4600/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00479, 0.00631 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4382/(T/K) + 12.56$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

0.0116 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balçioğlu 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

17.33 (calculated-P/C, Burkhard 1984)

21.18 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

21.18 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

10.13 (wetted-wall column-GC/ECD, Brunner et al. 1990)

21.76 (calculated-QSPR, Dunnivant et al. 1992)

23.1 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

40.2 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 25 \pm 2$ kJ/mol, $\Delta S_H = 0.05 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW} :

- 6.16, 6.67 (HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
- 6.10 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
- 6.10 (recommended, Sangster 1993)
- 6.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

- 10.25, 9.14; 8.96 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 9.38–9.65 (10°C, estimated, Thomas et al. 1998)
- 9.11 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Biota Sediment Accumulation Factor, BSAF:

- 51 (trout in Lake Ontario, Niimi 1996)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_p or log K_d

- 5.80, 4.90 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC} :

- 5.74 (suspended particulate matter, Burkhard 1984)
- 6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.0 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 5.50 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25-60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 5.4 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4-11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1-10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5-40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 172 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 220 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11$ d in freshwater systems, $t_{1/2} = 0.1\text{--}10$ d in cloud water, $t_{1/2} > 1000$ d in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

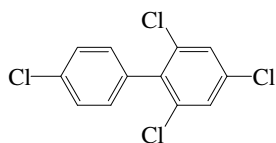
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 172$ d for high-dose treatment, $t_{1/2} = 220$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.75 2,4,4',6-Tetrachlorobiphenyl (PCB-75)



Common Name: 2,4,4',6-Tetrachlorobiphenyl

Synonym: PCB-75, 2,4,4',6-tetrachloro-1,1'-biphenyl

Chemical Name: 2,4,4',6-tetrachlorobiphenyl

CAS Registry No: 32598-12-2

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

93.0 (calculated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.104 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.00967, 0.0127, 0.0122, 0.0180 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.091 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.045 (calculated-MCI χ , Patil 1991)

0.0804 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0204, 0.0158, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.0150 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0179, 0.0202 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4229/(T/K) + 12.44$ (GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

42.25 (calculated-P/C, Burkhard et al. 1985b)

42.25 (batch stripping, Dunnivant & Elzerman 1988)

55.32 (calculated- QSPR-MCI χ , Sabljic & Güsten 1989)

47.07 (calculated-QSPR, Dunnivant et al. 1992)

35.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 2\ kJ/mol$, $\Delta S_H = 0.05 \pm 0.01\ kJ/mol\ K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.08, 6.10, 5.97, 5.97 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.03 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.19 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.72 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

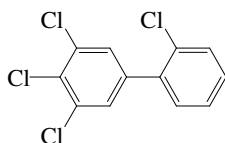
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.76 2,3',4',5'-Tetrachlorobiphenyl (PCB-76)



Common Name: 2,3',4',5'-Tetrachlorobiphenyl

Synonym: PCB-76, 2,3',4',5'-tetrachlorobiphenyl

Chemical Name: 2,3',4',5'-tetrachlorobiphenyl

CAS Registry No: 70362-48-0

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

89 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.114 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0551 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0569 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0184 (calculated-TSA, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0150 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0204, 0.00512, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00602, 0.00426 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.44×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00447, 0.00646 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4382/(T/K) + 12.48$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

12.16 (calculated-P/C, Burkhard 1984)

12.97 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

22.60 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

10.13 (calculated-QSPR, Achman et al. 1993)

24.19 (calculated-QSPR, Dunnivant et al. 1992)

35.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 28 \pm 3\ kJ/mol$, $\Delta S_H = 0.06 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.88 (calculated-TSA, Burkhard 1984)

5.98 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.05 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.23 (Hawker & Connell 1988b)

5.90 (calculated-QSPR, Murray & Andren 1992)

- 5.98 (recommended, Sangster 1993)
 6.0763 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 8.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.68 (suspended particulate matter, Burkhard 1984)
 6.0 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 5.5 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C , half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 153 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 164 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of $25\text{--}60 \text{ d}$ due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of $8.5\text{--}40 \text{ d}$ based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

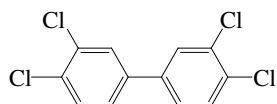
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 153 \text{ d}$ for high-dose treatment, $t_{1/2} = 164 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.77 3,3',4,4'-Tetrachlorobiphenyl (PCB-77)



Common Name: 3,3',4,4'-Tetrachlorobiphenyl

Synonym: PCB-77, 3,3',4,4'-tetrachloro-1,1'-biphenyl

Chemical Name: 3,3',4,4'-tetrachlorobiphenyl

CAS Registry No: 32598-13-3

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

180 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2024

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.10 (Ruelle et al. 1993)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.6 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.029 (calculated, assuming $\Delta S_{fus} = 56 J/mol K$, Shiu & Mackay 1986)

0.0202 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.175 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

7.50×10^{-4} (generator column-GC/ECD, Weil et al. 1974)

5.69×10^{-4} * (generator column-GC/ECD, measured $4-32^{\circ}C$, Dickhut et al. 1986)

5.84×10^{-4} * (generator column-GC/ECD, measured range $4-32^{\circ}C$, Dickhut et al. 1986)

$\ln x = -6098/(T/K) - 3.586$, temp range $4-32^{\circ}C$, $\Delta H_{ss} = 50.7 kJ/mol$ (generator column-GC/ECD, Dickhut et al. 1986)

$\log x = -2636/(T/K) - 1.558$, $\Delta H_{ss} = 50.5 kJ/mol$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or

$S/(mol/L) = 3.59 \times 10^{-10} \exp(0.072 \cdot t/^{\circ}C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)

8.23×10^{-4} , 1.01×10^{-3} , 1.16×10^{-3} (RP-HPLC- k' correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0018 ($22^{\circ}C$, generator column-GC/ECD, Opperhuizen et al. 1988)

5.50×10^{-4} ; 0.0161 (generator column-GC; supercooled liquid S_L , Dunnivant & Elzerman 1988)

6.10×10^{-4} (generator column-GC/ECD, room temp., Hong & Qiao 1995)

2.02×10^{-3} , 5.44×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

$\log S_L (mol/L) = -0.246 + 1339/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -3.58245 - 6074.34/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.00270* (generator column-GC/ECD, measured range $5-35^{\circ}C$. Huang & Hong 2002).—See Comment by van Noort 2004

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00219, 0.00196 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

0.0014 (supercooled liquid P_L , GT-RT correlation, Burkhard 1984)

5.97×10^{-4} ; 4.46×10^{-5} , 8.04×10^{-4} (calculated-MW, GC-RT correlation, calculated-MCI χ , Burkhard et al. 1985a)
 0.0014 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)
 0.00213, 0.00144 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 5.88×10^{-5} ; 0.0020 (selected P_S , supercooled liquid P_L , Shiu & Mackay 1986)
 0.00212 (supercooled liquid P_L , Dunnivant & Elzerman 1988)
 1.82×10^{-5} ; 5.26×10^{-4} (calculated-S \times HLC, solid P_S ; supercooled liquid P_L , Dunnivant & Elzerman 1988)
 0.00141, 0.00191 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log(P_L/P_a) = -4552/(T/K) + 12.61$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)
 1.202×10^{-3} (supercooled liquid P_L , 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
 6.46×10^{-5} ; 2.21×10^{-3} (solid, supercooled liquid, Passivirta et al. 1999)
 $\log(P_S/P_a) = 15.56 - 5889/(T/K)$ (solid, Passivirta et al. 1999)
 $\log(P_L/P_a) = 12.61 - 4552/(T/K)$ (liquid, Passivirta et al. 1999)
 $(1.82 - 80.4) \times 10^{-5}$; $(4.71 - 22.0) \times 10^{-4}$ (quoted lit. P_S range; lit. P_L range, Delle Site 1997)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4.37 (calculated-P/C, Burkhard et al. 1985b)
 1.72 (calculated-P/C, Shiu & Mackay 1986)
 9.52 (gas stripping-GC/ECD, Dunnivant et al. 1988; Dunnivant & Elzerman 1988)
 40.88 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
 10.39 (calculated-QSPR, Dunnivant et al. 1992)
 $\log H$ (Pa m³/mol) = $12.86 - 3214/(T/K)$ (Passivirta et al. 1999)
 $16.20^* \pm 0.41$ (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
 $\ln K_{AW} = 11.0657 - 4787.1/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(39.8/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.092/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)
 16.7 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 40 \pm 6 \text{ kJ/mol}$, $\Delta S_H = 0.09 \pm 0.02 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.04 (HPLC-RT correlation, Sugiura et al. 1979)
 6.52 (RP-TLC-retention, Bruggeman et al. 1982)
 5.62 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
 6.77 (HPLC- k' correlation, De Kock & Lord 1987)
 6.11, 6.40, 6.37 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 6.21 (generator column-GC, Hawker & Connell 1988a)
 6.630 ± 0.018 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 6.13 (generator column-GC, Larsen et al. 1992)
 5.98 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 7.8733 (calculated-UNIFAC group contribution, Chen et al. 1993)
 6.11 (recommended, Sangster 1993)
 6.63 (recommended, Hansch et al. 1995)
 6.48 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

9.08 (calculated, Paterson et al. 1991)
 9.96* (20°C, generator column-GC, measured range 0 to 30°C, Harner & Bidleman 1996)
 $\log K_{OA} = -3.14 + 3828/(T/K)$; (temp range 0 to 30°C, Harner & Bidleman 1996)
 10.92, 9.92; 10.03 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)

9.70 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
 9.29; 9.19 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.46 (killifish, Goto et al. 1978)
 3.90, 3.24, 3.63, 4.15 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
 2.77, 2.63 (human fat in lipid, wet wt. basis, calculated- K_{OW} , Geyer et al. 1987)
 5.36; 6.89 (22°C, zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
 4.59, 5.87; 4.745, 4.943 (quoted-whole fish, fish lipid; calculated-molecular connectivity indices, K_{OW} , Lu et al. 1999)
 2.56–4.26 (various marine species, mean dry wt. BCF, Hope et al. 1998)
 4.19–5.23 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
 5.36 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
 5.36, 6.90 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.41, 6.37 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
 2.62, 2.77 (human: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} :

5.75 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.41 (soil, calculated, Chou & Griffin 1986)
 5.02 (soil, calculated-QSPR Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.029, 0.0047 \text{ d}^{-1}$ (golden orfe, guppy, Sugiura et al. 1979)
 $k_2 = 0.0157 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
 $k_1 = 5160 \text{ d}^{-1}$; $k_2 = 0.0224 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 $k_1 = 17 \text{ L d}^{-1} \text{ g}^{-1} \text{ dry wt.}$; $k_2 = 0.073 \text{ d}^{-1}$ (Baltic Sea blue mussel, flow-through expt., Gustafsson et al. 1999)
 $k_2 = 0.0251 \text{ d}^{-1}$ with $t_{1/2} = 28 \text{ d}$ (newly contaminated oysters, Gardinali et al. 2004)
 $k_2 = 0.0166 \text{ d}^{-1}$ with $t_{1/2} = 42 \text{ d}$ (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995);
 $t_{1/2} = 1500 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).
 Surface water: $t_{1/2} = 805 \text{ d}$ in Lake Michigan (Neely 1983);
 photodegradation $t_{1/2} = 528 \text{ min}$ when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996);
 $t_{1/2} = 30000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{1/2} = 87600$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2} = 87600$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} = 44$ d in rainbow trout, and its muscle, 29 d (Niimi & Oliver 1983);

theoretical half-life to reach 90% steady-state tissue concn 9.5 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)

Depuration $t_{1/2} = 28$ d for newly contaminated oysters, and $t_{1/2} = 42$ d for chronically contaminated oysters (Gardinali et al. 2004)

TABLE 7.1.1.77.1

Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 3,3',4,4'-tetrachlorobiphenyl (PCB 77) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility				Henry's law constant		log K_{OA}	
Dickhut et al. 1986		Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OA}
4	1.46×10^{-4}	5	1.25×10^{-3}	4	4.46	0	10.88
20	4.38×10^{-4}	15	1.77×10^{-3}	11	6.99	10	10.36
25	5.84×10^{-4}	25	2.70×10^{-3}	18	10.75	20	9.96
32	1.17×10^{-3}	35	4.35×10^{-3}	25	16.20	30	9.47
				31	22.69		
$\ln x = A - B/(T/K)$		mp/°C 180–181				$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 73.30$	
A -3.586				enthalpy, entropy change:		$\log K_{OA} = A + B/T$	
B 6098.15		$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 29.6$		$\Delta H/(\text{kJ} \cdot \text{mol}^{-1}) = 39.8 \pm 6.0$		A -3.14	
				$\Delta S/(\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}) = 92 \pm 20$		B 3828	
enthalpy of solution:				$\ln K_{AW} = -\Delta H/RT + \Delta S/R$			
$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 50.7 \pm 4.8$				A 11.6567			
for 4–32°C				B 4787.11			

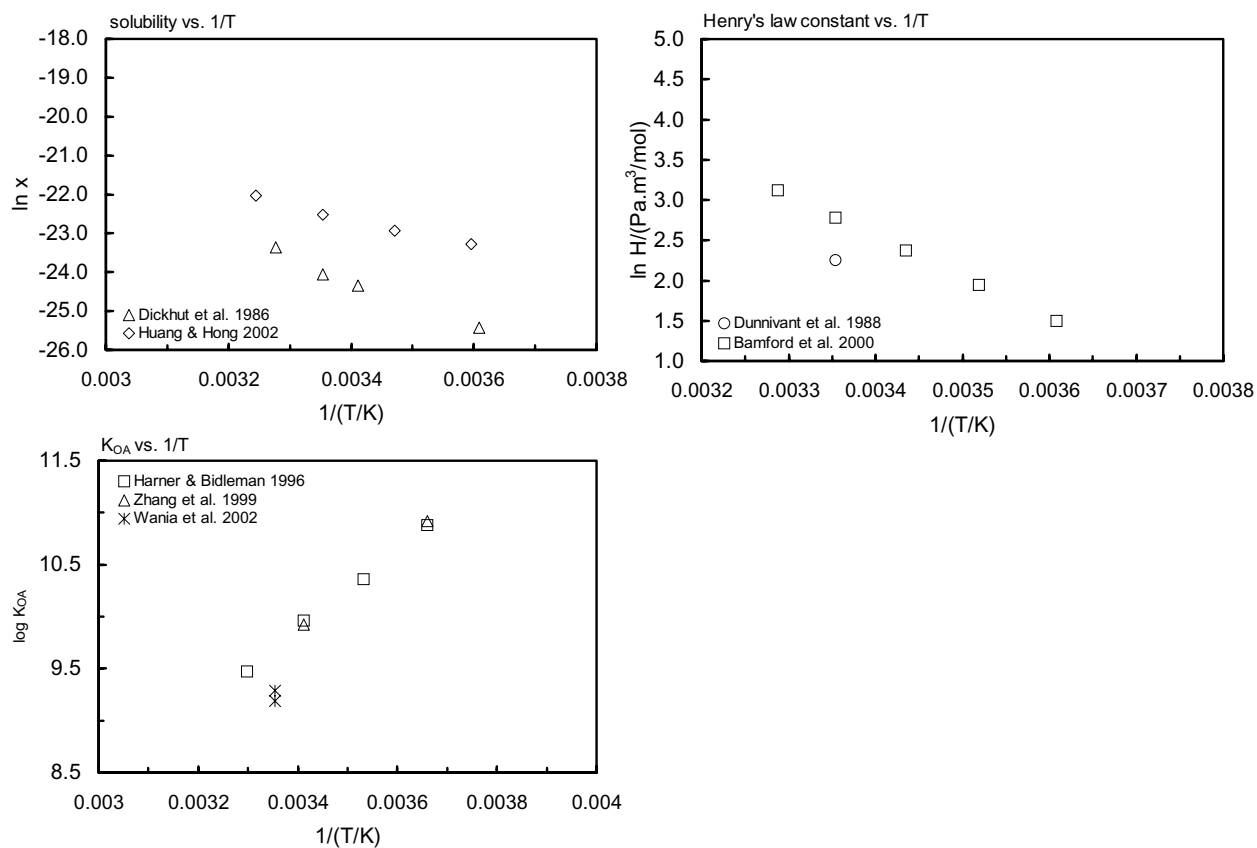
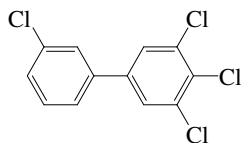


FIGURE 7.1.1.77.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 3,3',4,4'-tetrachlorobiphenyl (PCB-77).

7.1.1.78 3,3',4,5-Tetrachlorobiphenyl (PCB-78)



Common Name: 3,3',4,5-Tetrachlorobiphenyl

Synonym: PCB-78

Chemical Name: 3,3',4,5-tetrachlorobiphenyl

CAS Registry No: 70362-49-1

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

94 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0943 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00186 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00116, 0.000167, 0.000223 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00319, 0.00206 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4598/T + 12.92$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

5.76 (calculated-P/C, Burkhard 1984)

22.90 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

21.77 (calculated-QSPR, Dunnivant et al. 1992)

20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5$ kJ/mol, $\Delta S_H = 0.08 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.95 (calculated, Burkhard 1984)

6.35 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.2278 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.75 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2): k_1 : 8 (food lipid mg)/(g worm lipid-d); k_2 : 0.09 d⁻¹ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

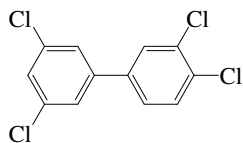
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 7 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.79 3,3',4,5'-Tetrachlorobiphenyl (PCB-79)



Common Name: 3,3',4,5'-Tetrachlorobiphenyl

Synonym: PCB-79

Chemical Name: 3,3',4,5'-tetrachlorobiphenyl

CAS Registry No: 41464-48-6

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

83 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0815 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00923 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0036 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.07×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0204, 0.00224, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00341, 0.00206 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4598/(T/K) + 12.95$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

7.39 (calculated-P/C, Burkhard 1984)

11.75 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

3.94 (calculated-QSPR, Achman et al. 1993)

12.73 (calculated-QSAR, Dunnivant et al. 1992)

20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5\ kJ/mol$, $\Delta S_H = 0.08 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.00 (calculated-TSA, Burkhard 1984)

6.42 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.3035 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.67 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.80 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

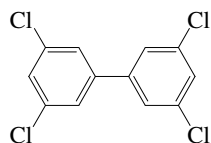
Ground water:

Sediment:

Soil:

Biota:

7.1.1.80 3,3',5,5'-Tetrachlorobiphenyl (PCB-80)



Common Name: 3,3',5,5'-Tetrachlorobiphenyl

Synonym: PCB-80, 3,3',5,5'-tetrachloro-1,1'-biphenyl

Chemical Name: 3,3',5,5'-tetrachlorobiphenyl

CAS Registry No: 33284-52-5

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

164 (Van Roosmalen 1934; Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.2 (calculated-Le Bas method at normal boiling point)

211.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.0421 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0712 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.000306, 0.000496, 0.000786, 0.000902 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00124 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.0295 (supercooled liquid S_L , calculated-mp, Dunnivant & Elzerman 1988)

0.00292 (calculated-TSA, Abramowitz & Yalkowsky 1990)

2.92×10^{-3} , 7.68×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

4.96×10^{-3} (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.000859, 0.000139, 0.0219 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.00305 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00547, 0.00511 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4598/(T/K) + 13.16$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

12.46 (calculated-P/C, Burkhard et al. 1985b)

63.02 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

38.0 (calculated-QSPR, Dunnivant et al. 1992)

20.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 36 \pm 5\ kJ/mol$, $\Delta S_H = 0.08 \pm 0.01\ kJ/mol\ K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.85 (HPLC-RT correlation, Sugiura et al. 1978; quoted, Hansch et al. 1995)

6.58 (RP-TLC-retention, Bruggeman et al. 1982)

6.77, 6.77, 6.45, 6.41 (RP-HPLC- k' correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.60 (recommended, Sangster 1993)

6.48, 6.85 (quoted lit. values, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.26 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

5.85 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

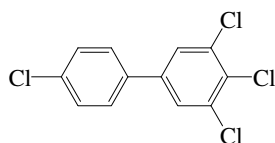
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.81 3,4,4',5-Tetrachlorobiphenyl (PCB-81)



Common Name: 3,4,4',5-Tetrachlorobiphenyl

Synonym: PCB-81

Chemical Name: 3,4,4',5-Tetrachlorobiphenyl

CAS Registry No: 70362-50-4

Molecular Formula: $C_{12}H_6Cl_4$

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

137 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0929 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985)

0.00292 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0010 (room temp., generator column-GC/ECD, Hong & Qiao 1995)—see comment by van Noort 2004

0.00313 (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)

0.00140, 0.00213, 0.00313, 0.00505 ($5, 15, 25, 35^{\circ}C$, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00165 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.0204, 0.0018, 0.00804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00290, 0.00182. (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4598/(T/K) + 12.88$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.20 (calculated-P/C, Burkhard et al. 1985a)

15.0 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

10.06 (calculated-QSPR, Dunnivant et al. 1992)

5.97 (calculated-QSPR, Achman et al. 1993)

12.7 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

25.8 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 33 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.96 (calculated-TSA, Burkhard 1984)

6.36 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.1949 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

6.53; 6.16 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)

6.64, 6.24 (calculated-MCI χ , calculated-molecular properties MNDO-MI method, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.88 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

5.10, 6.40 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

5.76 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 25\text{--}60 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36\text{--}1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for tetrachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 8.5\text{--}40 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.0185 \text{ d}^{-1}$ with $t_{1/2} = 37 \text{ d}$ (newly contaminated oysters, Gardinali et al. 2004)

$k_2 = 0.0186 \text{ d}^{-1}$ with $t_{1/2} = 37 \text{ d}$ (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radical for tetrachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radical for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

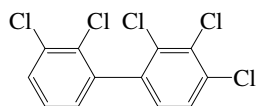
Soil:

Biota: clearance $t_{1/2} = 21 \text{ d}$ in guppy for tetrachlorobiphenyl (Bruggeman et al. 1984);

reported biological half-lives for tetrachlorobiphenyls: $t_{1/2} = 2\text{--}290 \text{ d}$ in trout, $t_{1/2} = 29\text{--}127 \text{ d}$ in trout muscle; $t_{1/2} = 51\text{--}81 \text{ d}$ in goldfish, $t_{1/2} = 7\text{--}200 \text{ d}$ in carp and $t_{1/2} = 4\text{--}53 \text{ d}$ in guppy (Niimi 1987)

Depuration $t_{1/2} = 37 \text{ d}$ for newly contaminated oysters, and $t_{1/2} = 37 \text{ d}$ for chronically contaminated oysters (Gardinali et al. 2004)

7.1.1.82 2,2',3,3',4-Pentachlorobiphenyl (PCB-82)



Common Name: 2,2',3,3',4-Pentachlorobiphenyl

Synonym: PCB-82

Chemical Name: 2,2',3,3',4-pentachlorobiphenyl

CAS Registry No: 52663-62-4

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

85 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0467 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0291 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0028 (calculated-QSPR, Dunnivant et al. 1992)

0.00622 (calculated-group contribution method, Kühne et al. 1995)

0.0221 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0020 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00218, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

1.06×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 11.0 - 4780/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

12.46 (calculated-P/C, Burkhard 1984)

11.86 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

12.36 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

14.82 (calculated-QSPR, Dunnivant et al. 1992)

5.97 (calculated-QSPR, Achman et al. 1993)

16.3 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

40.3 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 42 \pm 8$ kJ/mol, $\Delta S_H = 0.11 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.20 (calculated-TSA, Burkhard 1984)

6.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.30 (estimated, Girvin & Scott 1997)

6.0458 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

6.73 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.16 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.00 (suspended particulate matter, Burkhard 1984)

4.770 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

5.80 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2-0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60-120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3-0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16-48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 174 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 196 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

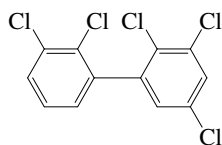
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 174 \text{ d}$ for high-dose treatment, $t_{1/2} = 196 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.83 2,2',3,3',5-Pentachlorobiphenyl (PCB-83)



Common Name: 2,2',3,3',5-Pentachlorobiphenyl

Synonym: PCB-83

Chemical Name: 2,2',3,3',5-pentachlorobiphenyl

CAS Registry No: 60145-20-2

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

65 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

224.5 (Ruelle et al. 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.405 (mp at $65^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0045 (generator column-GC/ECD, Weil et al. 1974)

0.023 (shake flask-GC/ECD, Wallnöfer et al. 1973)

0.046 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.0282 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0260 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.0103, 0.0278 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00735, 0.00324, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.00299 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00274, 0.00303 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00154 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 11.0 - 4760/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00204 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.60$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated):

21.28 (calculated-P/C, Burkhard et al. 1985b)

16.62 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

26.65 (calculated- QSPR-MCI χ , Sabljic & Güsten 1989)

21.46 (calculated-QSPR, Dunnivant et al. 1992)

23.6 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

45.4 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 6$ kJ/mol, $\Delta S_H = 0.07 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.24	(calculated-TSA, Burkhard 1984)
6.26	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.51	(calculated, Miertus & Jakus 1990; quoted, Sangster 1993)
6.0458	(calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

10.44, 9.39	(0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
9.01	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.04	(suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
4.748	(marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2-0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60-120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3-0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16-48 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 172 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 217 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1996).

Surface water:

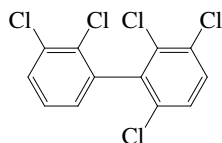
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 172 \text{ d}$ for high-dose treatment, $t_{1/2} = 217 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.84 2,2',3,3',6-Pentachlorobiphenyl (PCB-84)



Common Name: 2,2',3,3',6-Pentachlorobiphenyl

Synonym: PCB-84, 2,2',3,3',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',6-pentachlorobiphenyl

CAS Registry No: 52663-60-2

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

91 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.047 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0542 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.48×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00693, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00372, 0.00441 supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.64×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 11.0 - 4740/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00302, 0.0055 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4399/(T/K) + 12.32$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

51.68 (calculated-P/C, Burkhard 1984)

17.63 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

24.82 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

5.97 (calculated-QSPR, Achman et al. 1993)

25.45 (calculated-QSPR, Dunnivant et al. 1992)

51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.04 (RP-HPLC- k' correlation, Rapaport & Eisenreich 1984)

5.60 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.24 (generator column-GC, Larsen et al. 1992)

5.96 (recommended, Sangster 1993)

6.04 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

- 8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -5.84 + 4360/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 8.80 (quoted, Kömp & McLachlan 1997b)
- 10.28, 9.28 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
- 8.94 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Biota Sediment Accumulation Factor, BSAF:

- 80 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.09 (suspended particulate matter, Bukhard 1984)
- 4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 4.7 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 135 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 141 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991)

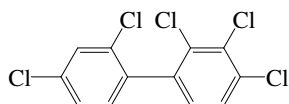
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 135 \text{ d}$ for high-dose treatment, $t_{1/2} = 141 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.85 2,2',3,4,4'-Pentachlorobiphenyl (PCB-85)



Common Name: 2,2',3,4,4'-Pentachlorobiphenyl

Synonym: PCB-85, 2,2',3,4,4'-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4'-pentachlorobiphenyl

CAS Registry No: 65510-45-4

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

87 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0428 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0219 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00782 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00233 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00253, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00472, 0.00218 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.12×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P_L/Pa) = -4522/(T/K) + 12.54$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

0.00248 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

17.83 (calculated-P/C, Burkhard 1984)

16.72 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

24.82 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

6.69 (wetted-wall column-GC/ECD, Brunner et al. 1990)

19.49 (calculated-QSPR, Dunnivant et al. 1992)

26.4 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

47.2 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 26 \pm 7$ kJ/mol, $\Delta S_H = 0.05 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.61 (RP-HPLC- k' correlation, Rapaport & Eisenreich 1984)

6.18 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)

6.18 (recommended, Sangster 1993)

6.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.29 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.07 (suspended particulate matter, Burkhard 1984)
 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)
 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 5.70 (soil-organic carbon, Girvin & Scott 1997)
 5.51 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioğlu 1996)
 5.70 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

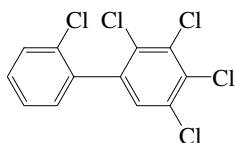
Ground water:

Sediment:

Soil:

Biota:

7.1.1.86 2,2',3,4,5-Pentachlorobiphenyl (PCB-86)



Common Name: 2,2',3,4,5-Pentachlorobiphenyl

Synonym: PCB-86, 2,2',3,4,5-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,5-pentachlorobiphenyl

CAS Registry No: 55312-69-1

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

100 (Mackay et al. 1980; Burkhard et al. 1985a; Opperhuizen et al. 1988; Brodsky & Ballschmiter 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.181 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0098 (generator column-GC/ECD, Weil et al. 1974)

0.0349 (generator column-HPLC/UV, Huang 1983)

0.034 (generator column-HPLC, Billington et al. 1988)

0.00334, 0.00554, 0.00297, 0.00651 (RP-HPLC- k' correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00933 (quoted, Neely 1981)

0.051 (P_L calculated from P_S using fugacity ratio F, Neely 1981)

0.00643 (supercooled liquid P_L , Neely 1981)

0.000077 (calculated, Neely 1983; quoted, Erickson 1986)

0.00133, 0.00245, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.0128 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00288 (supercooled liquid P_L , GC-RI correlations, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.61$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

84.1 (calculated-P/C, Burkhard et al. 1985b)

17.23 (calculated-MCI χ , Sabljic & Güsten 1989)

24.14 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8\ kJ/mol$, $\Delta S_H = 0.06 \pm 0.01\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.38 (Neely 1983; quoted, Erickson 1986)

7.49 (calculated-fragment const., Yalkowsky et al. 1983)

6.22 (calculated-TSA, Burkhard 1984)

- 6.38 (calculated- π const., Woodburn et al. 1984)
- 6.20 (selected, Shiu & Mackay 1986)
- 6.44, 6.38, 6.43, 6.29 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.23 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.26 (calculated-MCI χ , Patil 1991)
- 6.39 (recommended, Sangster 1993)
- 6.325 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
- 6.97 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/air Partition Coefficient, $\log K_{OA}$:

- 9.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 4.43 (oyster, Vreeland 1974; quoted, Hawker & Connell 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.02 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 4.770 (marine humic substances, calculated-MCI χ , reported as $\log K_h$ at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2 - 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation: microbial degradation with pseudo first-order rate constant $k = 0.005 \text{ yr}^{-1}$ in the water column and $k = 0.05 \text{ yr}^{-1}$ in the sediment (Furukawa et al. 1978; quoted, Neely 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

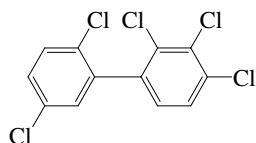
Surface water: $t_{1/2} = 108 \text{ d}$ in Lake Michigan (Neely 1983).

Groundwater:

Sediment:

Soil:

Biota:

7.1.1.87 2,2',3,4,5'-Pentachlorobiphenyl (PCB-87)

Common Name: 2,2',3,4,5'-Pentachlorobiphenyl

Synonym: PCB-87, 2,2',3,4,5'-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,5'-pentachlorobiphenyl

CAS Registry No: 38380-02-8

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

111.5–113 (Hutzinger et al. 1974; Erickson 1986)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2803

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.132 (Mackay et al. 1980)

0.138 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.022 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.0045 (generator column-GC/ECD, Weil et al. 1974)

0.0294 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0082, 0.00783, 0.00543, 0.0070 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00226 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

0.000392 (GC-RI correlation, Burkhard et al. 1985a)

0.00141, 0.00262 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00261, 0.00248 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00116 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 11.10 - 4800/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0017, 0.00275 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4562/(T/K) + 12.66$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

33.44 (calculated, Murphy et al. 1983)

19.86 (calculated-P/C, Burkhard et al. 1985b)

24.81 (calculated-P/C, Shiu & Mackay 1986)

12.87 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

18.24 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

7.50 (wetted-wall column-GC, Brunner et al. 1990)

18.61 (calculated-QSPR, Dunnivant et al. 1992)

5.966 (calculated-QSPR, Achman et al. 1993)

37.71 ± 0.69 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)

12.97, 18.83, 26.86, 37.71, 49.80 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 8.9006 - 3909.07/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(32.5/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.074/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)

36.5 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 33 \pm 4 \text{ kJ/mol}$, $\Delta S_H = 0.07 \pm 0.01 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.85 (RP-TLC- k' correlation, Bruggeman et al. 1982)

6.30 (HPLC-RT correlation, Shaw & Connell 1982)

5.45, 6.37 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)

6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)

6.14, 6.23, 6.24, 6.27 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.36 (HPLC- k' correlation, Noegrohati & Hammers 1992)

6.23 (recommended, Sangster 1993)

6.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

9.96 (10°C, estimated, Thomas et al. 1998)

9.25 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

4.43 (oyster, Vreeland 1974)

5.38; 6.91 (22°C, zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

5.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

4.54 (Koch 1983)

6.07 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

4.88 (calculated, Bahnick & Doucette 1988)

4.761, 4.748 (marine humic substances of 5 mg/L DOC, selected, calculated-MCI χ , reported as $\log K_h$, Sabljic et al. 1989)

4.76, 4.87, 4.85, 3.75 (marine humic substance in concentrations. of 5,10, 20, 40 mg/L DOC, reported as $\log K_h$, Lara & Ernst 1989)

6.18 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)

5.08 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)

5.73 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted and selected, Baker et al. 2000)

5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

4.62 (soil, calculated-MCI, Sabljic et al. 1995)

5.02 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioglu 1996)

6.00 (soil, calculated- K_{OW} , Girvin & Scott 1997)

5.80; 4.50 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Sorption Partition Coefficient, $\log K_{OM}$:

4.50, 4.85 (selected, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2 - 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0045 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 0.049 \text{ h}^{-1}$; $k_2 = 0.013 \text{ h}^{-1}$ (mayfly-sediment model II, Gobas et al. 1989)

$k_1 = 3360 \text{ d}^{-1}$; $k_2 = 0.0140 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 154 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 195 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

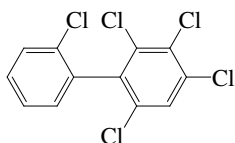
Sediment:

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.027 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.57 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, and $k = 0.27 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are: $k = 0.00152 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00223 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, and $k = 0.0039 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997).

Biota: $t_{1/2} = 155 \text{ d}$ in rainbow trout and $t_{1/2} = 62 \text{ d}$ its muscle (Niimi & Oliver 1983).

depuration $t_{1/2} = 154 \text{ d}$ for high-dose treatment, $t_{1/2} = 195 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.88 2,2',3,4,6-Pentachlorobiphenyl (PCB-88)



Common Name: 2,2',3,4,6-Pentachlorobiphenyl

Synonym: PCB-88

Chemical Name: 2,2',3,4,6-pentachlorobiphenyl

CAS Registry No: 55215-17-3

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

100 (Mackay et al. 1980; Burkhard et al. 1985a; Opperhuizen et al. 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2803

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.182 (Mackay et al. 1980)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.012 (generator column-GC/ECD, Weil et al. 1974)

0.0129 (calculated-TSA, Mackay et al. 1980)

0.0385 (supercooled liquid S_L , calculated- TSA, Burkhard et al. 1985b)

0.00242 (calculated-fragment solubility constants, Wakita et al. 1986)

0.009 (calculated-MCI χ , Nirmalakhandan & Speece 1989)

0.0206 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.011 (calculated-MCI χ , Patil 1991)

0.00801 (calculated-group contribution, Kühne et al. 1995)

0.0124, 0.00472 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.0265 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00309 (GC-RI correlation, Burkhard et al. 1985a)

0.0161 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00646 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4399/(T/K) + 12.53$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

136.8 (calculated-P/C, Burkhard et al. 1985b)

34.65 (calculated-molecular connectivity indices χ , Sabljic & Güsten 1989)

38.97 (calculated-QSPR, Dunnivant et al. 1992)

51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.51 (calculated-fragment const., Yalkowsky et al. 1983)

- 6.31 (calculated-TSA, Burkhard 1984)
- 6.07 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.26 (calculated-MCI χ , Patil 1991)
- 6.1452 (calculated-molecular properties, MNDO-AM1 method, Makino 1998)
- 6.84 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.39 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.11 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 4.611 (marine humic substances, calculated-MCI χ , reported as association coefficient $\log K_h$ at 5 mg/L of DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(calc) = (0.2-0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 60-120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(calc) = (0.3-0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(calc) = 16-48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

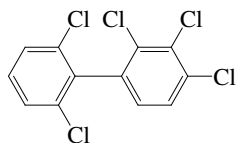
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.89 2,2',3,4,6'-Pentachlorobiphenyl (PCB-89)



Common Name: 2,2',3,4,6'-Pentachlorobiphenyl

Synonym: PCB-89, 2,2',3,4,6'-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,6'-pentachlorobiphenyl

CAS Registry No: 73575-57-2

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

99 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0382 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0542 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0206 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

4.82×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00522 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa- m^3/mol at $25^{\circ}C$ or as indicated):

41.64 (calculated-P/C, Burkhard 1984)

29.49 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

30.18 (calculated-QSPR, Dunnivant et al. 1992)

5.97 (calculated-QSPR, Achman et al. 1993)

30.6 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

49.4 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 21 \pm 6$ kJ/mol, $\Delta S_H = 0.04 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.31 (calculated-TSA, Burkhard 1984)

6.07 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.60 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.40 (calculated-TSA, Murray & Andren 1992)

5.60 (recommended, Sangster 1993)

5.8981 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.11 (suspended particulate matter, Burkhard 1984)
- 4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

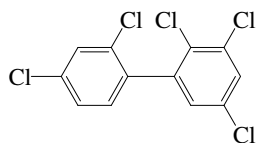
Ground water:

Sediment:

Soil:

Biota:

7.1.1.90 2,2',3,4',5-Pentachlorobiphenyl (PCB-90)



Common Name: 2,2',3,4',5-Pentachlorobiphenyl

Synonym: PCB-90, 2,2',3,4',5-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',5-pentachlorobiphenyl

CAS Registry No: 68194-07-0

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

67 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0375 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.01344 ($20^{\circ}C$, supercooled liquid S_L , Murphy et al. 1987)

0.00494 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00714 (calculated-group contribution method, Kühne et al. 1995)

0.00107, 0.00198 (generator column-GC/ECD, estimated, Hong & Qiao 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00375 (GC-RI correlation, Burkhard et al. 1985b)

$\log(P/mmHg) = 11.0 - 4740/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00347 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.69$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

30.19 (calculated-P/C, Burkhard 1984)

39.11 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

29.83 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.32 (calculated-TSA, Burkhard 1984)

6.32 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988a)

6.36 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)

6.32 (recommended, Sangster 1993)

6.339 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.92 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

6.12 (suspended particulate matter, Burkhard 1984)

4.66, 4.68, 4.75, 3.75 (marine humic substance in concentrations of 5, 10, 20, 40 mg/L DOC, reported as log K_h , Lara & Ernst 1989)

4.659, 4.726 (marine humic substance, observed, calculated-MCI, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

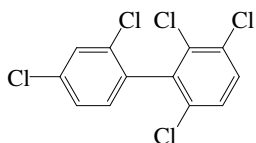
Ground water:

Sediment:

Soil:

Biota:

7.1.1.91 2,2',3,4',6-Pentachlorobiphenyl (PCB-91)



Common Name: 2,2',3,4',6-Pentachlorobiphenyl

Synonym: PCB-91, 2,2',3,4',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',6-pentachlorobiphenyl

CAS Registry No: 58194-05-8

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

93 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0336 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0395 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0221 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00803 (GC-RI correlation, Burkhard et al. 1985b)

0.00487, 0.00667 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.32×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 10.90 - 4650/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0038, 0.00589 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4399/(T/K) + 12.44$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

73.16 (calculated-P/C, Burkhard 1984)

27.46 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

35.78 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

12.16 (wetted-wall column-GC/ECD, Brunner et al. 1990)

35.05 (calculated-QSPR, Dunnivant et al. 1992)

9.03 (calculated-QSPR, Achman et al. 1993)

42.2 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

54.9 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 10 \pm 5$ kJ/mol, $\Delta S_H = 0.00 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.31 (RP-HPLC- k' correlation, Rapaport & Eisenreich 1984)

6.31 (calculated-TSA, Burkhard 1984)

- 5.87 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
 6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
 5.87 (recommended, Sangster 1993)
 5.9623 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.07 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.11 (suspended particulate matter, Burkhard 1984)
 4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_1 = 10 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2 = 0.08 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)
 $k_2 = 0.08 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 166 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 217 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

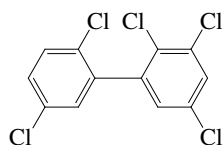
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 8 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)
 depuration $t_{1/2} = 166 \text{ d}$ for high-dose treatment, $t_{1/2} = 217 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.92 2,2',3,5,5'-Pentachlorobiphenyl (PCB-92)



Common Name: 2,2',3,5,5'-Pentachlorobiphenyl

Synonym: PCB-92, 2,2',3,5,5'-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,5,5'-pentachlorobiphenyl

CAS Registry No: 52663-61-3

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

53 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0379 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00494 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.92×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00422, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00394, 0.00458 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P/mmHg) = 11.0 - 4740/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00302, 0.00447 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.76$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

33.64 (calculated-P/C, Burkhard 1984)

32.63 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

26.35 (calculated-QSPR, Dunnivant et al. 1992)

5.97 (calculated-QSPR, Achman et al. 1993)

28.4 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

48.2 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 24 \pm 6$ kJ/mol, $\Delta S_H = 0.05 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.05, 6.97 (RP-HPLC- k' correlation:uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

6.32 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.11 (generator column-GC, Larsen et al. 1992)

6.32 (recommended, Sangster 1993)

6.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.11 (suspended particulate matter, Burkhard 1984)

4.726 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 135 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 141 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

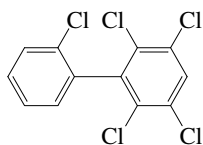
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 135 \text{ d}$ for high-dose treatment, $t_{1/2} = 141 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.93 2,2',3,5,6-Pentachlorobiphenyl (PCB-93)



Common Name: 2,2',3,5,6-Pentachlorobiphenyl

Synonym: PCB-93, 2,2',3,5,6-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,5,6-pentachlorobiphenyl

CAS Registry No: 73575-56-1

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

91 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0411 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0149, 0.0164, 0.00986, 0.0119 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0151 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.0160, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00708 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4399/(T/K) + 12.57$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

120.6 (calculated-P/C, Burkhard 1984)

28.78 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

34.49 (calculated-QSPR, Dunnivant et al. 1992)

51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.29 (calculated-TSA, Burkhard 1984)

5.99, 6.06, 6.07, 6.12 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.04 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.06 (recommended, Sangster 1993)

6.1176 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.09 (suspended particulate matter, Burkhard 1984)
4.611 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h , calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

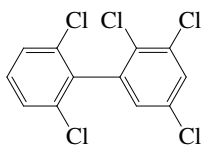
Ground water:

Sediment:

Soil:

Biota:

7.1.1.94 2,2',3,5,6'-Pentachlorobiphenyl (PCB-94)



Common Name: 2,2',3,5,6'-Pentachlorobiphenyl

Synonym: PCB-94

Chemical Name: 2,2',3,5,6'-pentachlorobiphenyl

CAS Registry No: 73575-55-0

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

79 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0336 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

7.24×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00774, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

70.62 (calculated-P/C, Burkhard 1984)

43.98 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

39.69 (calculated-QSPR, Dunnivant et al. 1992)

51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6\ kJ/mol$, $\Delta S_H = 0.03 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.36 (calculated-TSA, Burkhard 1984)

6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.0371 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.64 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.16 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

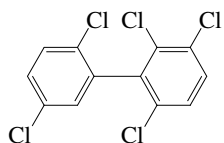
Ground water:

Sediment:

Soil:

Biota:

7.1.1.95 2,2',3,5',6-Pentachlorobiphenyl (PCB-95)



Common Name: 2,2',3,5',6-Pentachlorobiphenyl

Synonym: PCB-95, 2,2',3,5',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',3,5',6-pentachlorobiphenyl

CAS Registry No: 38379-99-6

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

98.5–100 (Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.184 (mp at $100^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0336 (supercooled liquid S_L , calculated-TSA, Burkhard 1985b)

0.0541 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0291, 0.0216, 0.0192, 0.0156; 0.021 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0259 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.011 (calculated-MCI χ , Patil 1991)

0.00190 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00735, 0.00905, 0.00278 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.00849 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00537, 0.00744 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00335 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 10.90 - 4650/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00427, 0.00741 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4399/(T/K) + 12.48$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

0.00295 ($20^{\circ}C$, supercooled liquid P_L , from Falconer & Bidleman 1994; Harner & Bidleman 1996)

0.00211 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

82.78 (calculated-P/C, Burkhard 1985b)

20.06 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

29.38 (calculated-molecular connectivity indices χ , Sabljic & Güsten 1989)

30.39 (calculated-QSPR, Dunnivant et al. 1992)

30.8 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

49.5 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 21 \pm 5\ kJ/mol$, $\Delta S_H = 0.04 \pm 0.02\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 5.18 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 6.63 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
- 5.67, 5.98, 5.86, 6.05 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.08 (generator column-GC, Larsen et al. 1992)
- 5.92 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

- 9.06 (20°C, generator column-GC, measured range -10 to 30°C, Harner & Bidleman 1996)
- 10.51, 9.06, 9.51, 9.06, 8.55 (-10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
- $\log K_{OA} = -4.30 + 3904/(T/K)$; temp range -10 to 30°C (generator column-GC, Harner & Bidleman 1996)
- 8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -5.84 + 4360/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 8.80 (quoted, Kömp & McLachlan 1997b, Kaupp & McLachlan 1999)
- 10.07, 9.06; 9.07 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 9.04 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:Sorption Partition Coefficient, $\log K_{OC}$:

- 6.16 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 5.3–6.8, 6.1; 7.40 (suspended sediment, average; algae > 50 μm , Oliver 1987a)
- 6.30 (Lake Michigan water column, Swackhamer & Armstrong 1987)
- 4.60, 4.66, 4.61, 3.70 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
- 4.603, 4.589 (marine humic substances, observed; calculated-MCI χ , reported as association coefficient $\log K_h$ at 5 mg/L DOC, Sabljic et al. 1989)
- 5.68, 5.70, 5.64 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
- 5.55 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
- 6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_1 = 0.00030 \text{ h}^{-1}$; $k_2 = 0.184 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 164 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 225 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{1/2} = 8.29$ min when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

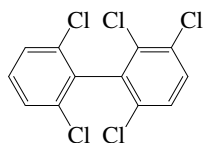
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 164$ d for high-dose treatment, $t_{1/2} = 225$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.96 2,2',3,6,6'-Pentachlorobiphenyl (PCB-96)



Common Name: 2,2',3,6,6'-Pentachlorobiphenyl

Synonym: PCB-96

Chemical Name: 2,2',3,6,6'-pentachlorobiphenyl

CAS Registry No: 73575-54-9

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

53 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0368 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0157 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00166, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

139.8 (calculated-P/C, Burkhard 1984)

38.60 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

41.56 (calculated-QSPR, Dunnivant et al. 1992)

62.0 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 15 \pm 3\ kJ/mol$, $\Delta S_H = 0.02 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.33 (calculated-TSA, Burkhard 1984)

5.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

5.5365 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ as or as indicated and reported temperature dependence equations:

8.77 ($20^{\circ}C$, generator column-GC/ECD, measured range -10 to $30^{\circ}C$, Harner & Bidleman 1996)

10.28, 9.72, 9.22, 8.77, 8.30 (-10 , 0 , 10 , 20 , $30^{\circ}C$, generator column-GC, Harner & Mackay 1995)

$\log K_{OA} = -4.60 + 3913/(T/K)$, temp range -10 to $30^{\circ}C$ (Harner & Bidleman 1996)

9.87, 8.79; 8.76 (0 , $20^{\circ}C$, multi-column GC- k' correlation; calculated at $20^{\circ}C$, Zhang et al. 1999)

8.82 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.13 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

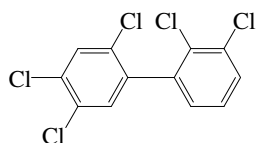
Ground water:

Sediment:

Soil:

Biota:

7.1.1.97 2,2',3,4',5'-Pentachlorobiphenyl (PCB-97)



Common Name: 2,2',3,4',5'-Pentachloro

Synonym: PCB-97

Chemical Name: 2,2',3',4,5-pentachlorobiphenyl

CAS Registry No: 41464-51-1

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

82 (Burkhard et al. 1984b; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

53.77 (quoted, Shiu & Mackay 1986)

Fugacity Ratio at $25^{\circ}C$, F:

0.279 (assuming $\Delta S_{fus} = 56$ J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0431 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0284 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00622, 0.00651, 0.00383, 0.00682 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0099 (literature average, Paya-Perez et al. 1991)

0.00847 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

2.01×10^{-3} , 8.05×10^{-4} , 8.04×10^{-4} (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00251, 0.00265 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.31×10^{-3} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 11.10 - 4790/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

1.85×10^{-3} , 2.88×10^{-3} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.56$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

0.0026 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

20.67 (calculated-P/C, Burkhard 1984)

15.1 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

18.14 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

7.50 (wetted-wall column-GC/ECD, Brunner et al. 1990)

18.23 (calculated-QSPR, Dunnivant et al. 1992)

- 23.5 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
 45.3 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 6$ kJ/mol, $\Delta S_H = 0.07 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.75, 6.67 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
 6.25, 6.33, 6.35, 6.28 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 6.31 (recommended, Sangster 1993)
 6.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 10.49, 9.44 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 9.21 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.43; 6.96 (zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.40, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.40, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.07 (suspended particulate matter, Burkhard 1984)
 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)
 5.83, 5.89, 5.78 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
 5.69 (soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
 5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
 6.10 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.2-0.4) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60-120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{calc}) = (0.3-0.9) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16-48$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_1 = 3400$ d⁻¹; $k_2 = 0.0126$ d⁻¹ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 $k_2 = 0.004$ d⁻¹ with $t_{1/2} = 163$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004$ d⁻¹ with $t_{1/2} = 188$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

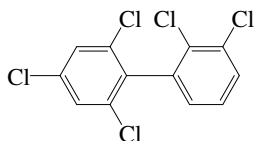
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 163$ d for high-dose treatment, $t_{1/2} = 188$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.98 2,2',3,4',6'-Pentachlorobiphenyl (PCB-98)



Common Name: 2,2',3,4',6'-Pentachlorobiphenyl

Synonym: PCB-98

Chemical Name: 2,2',3,4',6'-pentachlorobiphenyl

CAS Registry No: 60233-25-2

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

93 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

268.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0333 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0153, 0.0116, 0.0124 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.05×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00753, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00615, 0.00751 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00692 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4399/(T/K) + 12.54$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

68.90 (calculated-P/C, Burkhard 1984)

50.26 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

39.69 (calculated-QSPR, Dunnivant et al. 1992)

51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6 kJ/mol$, $\Delta S_H = 0.03 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.36 (calculated-TSA, Burkhard 1984)

5.98, 6.16, 5.99 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.13 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.071 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.16 (suspended particulate matter, Burkhard 1984)
 4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h , calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 153 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 164 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

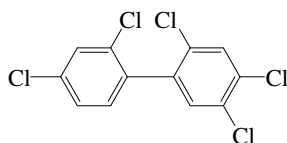
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 153 \text{ d}$ for high-dose treatment, $t_{1/2} = 164 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.99 2,2',4,4',5-Pentachlorobiphenyl (PCB-99)



Common Name: 2,2',4,4',5-Pentachlorobiphenyl

Synonym: PCB-99, 2,2',4,4',5-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',4,4',5-pentachlorobiphenyl

CAS Registry No: 38380-01-7

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

81.0 (calculated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0353 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.0222 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00366 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0103 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.011 (calculated-MCI χ , Patil 1991)

0.00597 (estimated-EPIWIN v3.04, Hardy 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0029 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

0.00735, 0.00342, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.00316 (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)

0.00328, 0.00375 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00147 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 11.0 - 4740/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.0024, 0.00347 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4533/(T/K) + 12.68$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

0.00229 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

0.000293 (estimated-EPIWIN v3.04, Hardy 2002)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

29.28 (calculated-P/C, Burkhard et al. 1985b)

21.68 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

30.50 (calculated-QSAR MCI χ , Sabljic & Güsten 1989)

7.90 (wetted-wall column-GC/ECD, Brunner et al. 1990)

57.0 (calculated-QSPR, Dunnivant et al. 1992)

9.39 (estimated-bond method EPIWIN v3.04, Hardy 2002)

35.4 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

51.8 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 16 \pm 6$ kJ/mol, $\Delta S_H = 0.02 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.29, 7.21 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 6.41 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
- 6.39 (calculated-TSA, Hawker & Connell 1988a)
- 6.26 (calculated-MCI χ , Patil 1991)
- 6.41 (recommended; Sangster 1993)
- 7.21 (recommended, Hansch et al. 1995)
- 6.60, 6.26–7.21 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
- 6.4014 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
- 6.9795 (estimated-EPIWIN v3.04, Hardy 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.38 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 4.09 (fish, microcosm, Garten & Trabalka 1983)
- 5.14 (estimated-EPIWIN v3.04, Hardy 2002)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.70, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.14 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 4.73 (marine humic substance, calculated-MCI χ , reported as $\log K_h$ at 5 mg /L DOC, Sabljic et al. 1989)
- 7.00 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 5.68 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.54 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 6.10 (soil, calculated- K_{OW} , Girvin & Scott 1997)
- 4.87 (estimated-EPIWIN v3.04, Hardy 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 0.6419$ d from river, $t_{1/2} = 13.31$ d from lake (estimated-EPIWIN v3.04, Hardy 2002).

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120$ d, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48$ d at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_1 = 8$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.07 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)
- $k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 2252$ d (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 172$ d (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: volatilization $t_{1/2} = 0.6419$ d from river, $t_{1/2} = 13.31$ d from lake (estimated-EPIWIN v.3.04, Hardy 2002).

Groundwater:

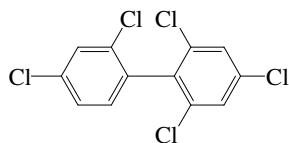
Sediment:

Soil:

Biota: elimination $t_{1/2} = 9$ d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2} = 252$ d for high-dose treatment, $t_{1/2} = 172$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.100 2,2',4,4',6-Pentachlorobiphenyl (PCB-100)



Common Name: 2,2',4,4',6-Pentachlorobiphenyl

Synonym: PCB-100, 2,2',4,4',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',4,4',6-pentachlorobiphenyl

CAS Registry No: 39485-83-1

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

95 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0275 (supercooled liq. S_L , calculated-TSA, Burkhard et al. 1985b)

0.031 (unpublished data of Weil 1978; quoted, Kilzer et al. 1979; Geyer et al. 1980)

0.00666, 0.00580, 0.00941 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.011 (calculated-MCI χ , Patil 1991)

0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00735, 0.00872, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.00818 (supercooled liquid, GC-RT correlation, Burkhard et al. 1985b; quoted, Eisenreich 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

97.27 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)

62.62 (calculated-MCI χ , Sabljic & Güsten 1989)

56.98 (calculated-QSPR, Dunnivant et al. 1992)

51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.23, 6.37, 6.08 (RP-HPLC-RI correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.23 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.66 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

1.11, 1.06 (adipose tissue of male, female Albino rats, Geyer et al. 1980)

0.32 (rodent, Garten & Trabalka 1983)

4.06, 3.91 (algae, calculated, Geyer et al. 1984)

4.06, 3.37, 4.44 (algae, fish, activated sludge, Freitag et al. 1984, 1985; quoted, Halfon & Reggiani 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.24 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.567 (marine humic substance, calculated-MCI χ , reported as association coefficient $\log K_h$ at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.010 \text{ d}^{-1}$ (10°C, sandworm, Goerke & Ernst 1977; quoted, Waid 1986)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

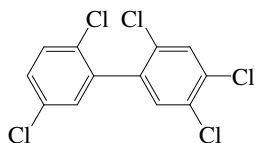
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.101 2,2',4,5,5'-Pentachlorobiphenyl (PCB-101)



Common Name: 2,2',4,5,5'-Pentachlorobiphenyl

Synonym: PCB-101, 2,2',4,5,5'-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',4,5,5'-pentachlorobiphenyl

CAS Registry No: 37680-72-3

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

78.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.2803

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.8 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

53.56 (Miller et al. 1984)

53.7, 65.6 (exptl., calculated, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.318 (assuming $\Delta S_{fus} = 56$ J/mol K, Shiu & Mackay 1986)

0.0321 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.031 (shake flask-GC/ECD, Wallnöfer et al. 1973; Hutzinger et al. 1974)

0.0103 (shake flask-GC/ECD, Haque & Schmedding 1975; Chiou et al. 1977)

0.0042 (generator column-GC/ECD, Weil et al. 1974)

0.019 (shake flask-LSC, Metcalf et al. 1975)

0.010 ($24^{\circ}C$, shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977)

0.00424 ($16.5^{\circ}C$, shake flask-GC/ECD, Wiese & Griffin 1978)

0.0005; 0.004 (generator column-HPLC/UV; RP-HPLC-RT correlation, Swann et al. 1983)

0.0194 (generator column-GC/ECD, Miller et al. 1984, 1985)

0.0356 (supercooled liquid P_L , calculated-TSA, Burkhard et al. 1985b)

0.0154* (generator column-GC/ECD, measured range $4-32^{\circ}C$, Dickhut et al. 1986)

$\ln x = -3837/(T/K) - 8.0159$, temp range $4-32^{\circ}C$, $\Delta H_{ss} = 31.9$ kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)

$\log x = -1664/(T/K) - 3.478$, $\Delta H_{ss} = 31.8$ kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or

$S/(mol/L) = 1.54 \times 10^{-10} \exp(0.046 \cdot t/^{\circ}C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)

0.011 (shake flask-GC/ECD, Chiou et al. 1986, 1991)

0.0263 ($20^{\circ}C$, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00402, 0.00517, 0.0070, 0.0070 (RP-HPLC- k' correlations, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00674; 0.0222(generator column-GC/ECD, supercooled liquid S_L , Dunnivant & Elzerman 1988)

$\log [S_L/(mol/L)] = 0.875 - 982.6/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -8.026 - 3836.44/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.0334 (calculated-mp and K_{ow} , Ran et al. 2002)
 0.0312, 0.0333 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)
 $\log S_L/(\text{mol m}^{-3}) = -1113/(T/K) - 0.27$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.0016 (P_s from GC-RT correlation, Westcott & Bidleman 1981)
 0.00096, 0.00173 (solid P_s : 25, 30°C, gas saturation-GC/ECD, Westcott et al. 1981)
 $\log (P/\text{mmHg}) = 11.1 - 4840/(T/K)$; temp range 30–40°C (gas saturation-GC, Westcott et al. 1981)
 0.0031 (P_L calculated from P_s using fugacity ratio F , Westcott & Bidleman 1981)
 0.0053, 0.00316 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
 0.00315 (supercooled liquid P_L , converted from literature P_s with ΔS_{fus} Bidleman 1984)
 0.00336, 0.00402 (supercooled liquid P_L , calculated from P_{GC} , GC-RT correlation, different stationary phases, Bidleman 1984)
 0.00358 (supercooled liquid P_L , GC-RT correlation, Burkhard 1984, Burkhard et al. 1985b)
 0.00225, 0.00118, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)
 0.00361, 0.00403 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 0.00109; 0.0035 (selected solid P_s ; supercooled liquid P_L , Shiu & Mackay 1986)
 0.00142 (20°C, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
 0.00359 (supercooled liquid P_L , Dunnivant & Elzerman 1988)
 0.000527; 0.00173 (calculated-S \times HLC, solid P_s ; supercooled liquid P_L , Dunnivant & Elzerman 1988)
 $\log (P/\text{mmHg}) = 11.0 - 4750/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
 0.00152 (calculated-UNIFAC group contribution, Banerjee et al. 1990)
 0.00315, 0.00296 (supercooled P_L , converted from literature P_s with different ΔS_{fus} values, Hinckley et al. 1990)
 0.00504, 0.0034 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log (P_L/\text{Pa}) = 12.13 - 4369/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
 0.00257, 0.00398 (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/\text{Pa}) = -4514/(T/K) + 12.67$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
 1.86×10^{-3} (supercooled liquid P_L , 20°C, from Falconer & Bidleman 1994, Harner & Bidleman 1996)
 1.33×10^{-4} , 4.16×10^{-4} (solid, supercooled liquid, Passivirta et al. 1999)
 $\log (P_s/\text{Pa}) = 15.47 - 5495/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 12.67 - 4514/(T/K)$ (liquid, Passivirta et al. 1999)
 $(4.04-22.5) \times 10^{-4}$; $(1.46-40.4) \times 10^{-3}$ (literature solid P_s range; literature liquid P_L range, Delle Site 1997)
 0.0020 (supercooled P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)
 0.0024, 0.00245 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log P_L/\text{Pa} = -4632/(T/K) + 12.92$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
 $\log P_L/\text{Pa} = -4346/(T/K) + 11.94$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

11.46–35.46 (calculated-P/C, Westcott et al. 1981)
 32.73 (calculated-P/C, Burkhard et al. 1985b)
 7.09 (20°C, gas stripping-GC, Oliver 1985)
 35.48 (calculated-P/C, Shiu & Mackay 1986)
 18.14 (20°C, calculated-P/C, Murphy et al. 1987)
 25.43 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
 47.19 (calculated-QSAR- χ , Sabljic & Güsten 1989)
 9.12 (wetted-wall column-GC/ECD, Brunner et al. 1990)
 24.87 (calculated-QSPR, Dunnivant et al. 1992)
 1.424, 4.166 (0, 15°C, from modified two-film model, Hornbuckle et al. 1994)
 $\log H (\text{Pa m}^3/\text{mol}) = 13.55 - 3531/(T/K)$ (Passivirta et al. 1999)
 $42.07^* \pm 0.70$ (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
 $\ln K_{AW} = 7.9384 - 3572.29/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(29.7/\text{kJ}\cdot\text{mol}^{-1})/RT + (0.066/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R]$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C (gas stripping-GC, Bamford et al. 2000)

43.2 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 30 \pm 3$ kJ/mol, $\Delta S_H = 0.07 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

31.62, 24.0 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

$\log [H/(\text{Pa m}^3/\text{mol})] = -3233/(T/K) + 12.21$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.12 (radiolabeled- ^{14}C , Metcalf et al. 1975)

6.11 (shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977; Chiou et al. 1982)

7.64 (Hansch & Leo 1979)

6.44 (HPLC-RT correlation, Veith et al. 1979)

6.85 (RP-TLC- k' correlation, Bruggeman et al. 1982)

6.42 (HPLC-RT correlation, Swann et al. 1983)

5.92 (generator column-GC/ECD, Miller et al. 1984)

6.15, 7.07 (RP-HPLC- k' correlation, Rapaport & Eisenreich 1984)

7.64 (HPLC-RT correlation, Woodburn et al. 1984)

6.50 (generator column-HPLC, Woodburn et al. 1984)

6.88, 7.0 (HPLC- k' correlation, calculated, De Kock & Lord 1987)

6.50 (generator column-GC/ECD, Doucette & Andren 1987, 1988)

6.36, 6.39, 6.18, 6.27 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.88 (HPLC-RT correlation, Doucette & Andren 1988)

6.23, 6.18 (RP-HPLC- k' correlation, different stationary phases, Sherblom & Eganhouse 1988)

6.41 (HPLC- k' correlation, Noegrohati & Hammers 1992)

6.16 (recommended, Sangster 1993)

6.50 (recommended, Hansch et al. 1995)

6.15, 6.33 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and the reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section.

8.30 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)

9.31* (20°C, generator column-GC, measured range -10 to 30°C, Harner & Bidleman 1996)

$\log K_{OA} = -3.82 + 3841/(T/K)$; temp range -10 to 30°C (generator Column-GC, Harner & Bidleman 1996)

8.80; 8.20 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)

$\log K_{OA} = -5.84 + 4360/(T/K)$ (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)

9.79 (10°C, estimated, Thomas et al. 1998)

10.49, 9.44; 9.29 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)

9.37 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

9.14; 9.05 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

8.90, 8.73 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log K_{OA} = 4291/(T/K) - 5.50$ (LDV linear regression of literature data, Li et al. 2003)

$\log K_{OA} = 3785/(T/K) - 5.35$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log \text{BCF}$:

3.18 (green sunfish, 15 d in static water, Sanborn et al. 1975)

3.74, 4.78, 4.08, 4.24 (algae, snail, fish, mosquito, Metcalf et al. 1975)

4.66 (fish, flowing water, Kenaga & Goring; Kenaga 1980)

3.92, 3.60 (calculated-S, calculated- K_{OC} , Kenaga 1980)

4.09 (fish, microcosm, Garten & Trabalka 1983)

3.30–4.15 highest value, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7- to 96-d laboratory study, Oliver & Niimi 1985)

> 5.40, 4.15; 6.92 (rainbow trout, laboratory data: kinetic BCF; steady state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)

2.73, 2.60 (human fat of lipid, wet wt. basis, calculated- K_{OW} , Geyer et al. 1987)

4.15 (fish, quoted, Isnard & Lambert 1988)

- 6.55 (rainbow trout, lipid basis, Noegrohati & Hammers 1992)
- 5.47; 7.00 (22°C, zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
- 3.32–5.15 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 4.84–6.26 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
- 4.06, 6.06 (*Daphnia*, 21-d renewal: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 5.47, 7.0 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 5.10, 7.02 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 4.03; 3.98 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_p or log K_d

- 5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, log K_{OC}:

- 4.63 (Kenaga & Goring 1980)
- 4.74, 4.80 (estimated-S, K_{OW}, Lyman 1982)
- 5.13, 4.67 (estimated-BCF, Lyman 1982)
- 4.70; 5.45 (soil, slurry method; HPLC-RT correlation, Swann et al. 1983)
- 6.14 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
- 5.60; 5.50; 6.60 (field data of sediment trap material; Niagara River-organic matter; calculated-K_{OW}, Oliver & Charlton 1984)
- 5.65 (suspended solids-Lake Superior, field measurement-GC/ECD, Baker et al. 1986)
- 6.68, 5.58 (suspended solids-Lake Superior: calculated-K_{OW}, Baker et al. 1986)
- 4.87, 4.07 (Sanhedron soil, Suwannee River, humic acid, shake flask-GC/ECD, Chiou et al. 1986,1987)
- 4.12, 4.10 (Sanhedron soil, Suwannee River, fulvic acid, shake flask-GC/ECD, Chiou et al. 1986,1987)
- 5.1–6.7, 6.2 (suspended sediment, average, Oliver 1987a)
- 5.41, 5.41, 4.81, 4.09, 4.01 (Aldrich humic acid Na salt, Fluka-Tridon humic acid, Calcasieu River humic extract, Suwannee River water sample, Sopchoppy River water sample, Chiou et al. 1987)
- 6.25 (Lake Michigan water column, Swackhamer & Armstrong 1987)
- 4.77, 4.86, 4.80, 3.86 (humic substances, in concentrations. of 5, 10, 20, 40 mg C/L, reported as log K_h, Lara & Ernst 1989)
- 4.772, 4.726 (marine humic substances of 5 mg/L DOC, reported as association coefficient log K_h, quoted exptl; calculated-MCI χ , Sabljic et al. 1989)
- 5.86 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 5.58 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 5.81, 5.83, 5.78 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
- 5.67 (soil, shake flask-GC, Paya-Perez et al. 1991)
- 5.90 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 4.63 (soil, Sabljic et al. 1995)
- 5.80; 5.58 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 5.90; 4.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
- 5.73 (sediment: organic carbon OC \geq 0.5%, average, Delle Site 2001)
- 4.78–7.03; 4.60–6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.59; 6.19, 5.53, 6.04 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Sorption Partition Coefficient, log K_{OM}:

- 4.63, 4.84 (quoted, calculated-molecular connectivity indices χ , Sabljic 1984)

Sorption Partition Coefficient, log K_p:

- 4.87–5.35 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodegradation rate constants $k = (0.20 \pm 0.01) \text{ h}^{-1}$, $(0.20 \pm 0.04) \text{ h}^{-1}$, with $t_{1/2} = 3.4 \text{ h}$, 3.7 h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{\text{OH}}(\text{aq.}) = 4.6 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C , half-lives range from $\sim 4\text{--}11 \text{ d}$ in freshwater systems, $0.1\text{--}10 \text{ d}$ in cloud water, $> 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{\text{OH}}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: degradation rate, $k = 1.5 \times 10^{-8} \text{ nmol cell}^{-1} \text{ h}^{-1}$ by species of *Alcaligenes* and *Acinetobacter* (Furukawa et al. 1978, selected, NAS 1979);

85% degradation at 24 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986);

aerobic biodegradation $t_{1/2} = 1.32 \text{ d}$ with the addition of polymer chitin, $t_{1/2} = 0.80 \text{ d}$ with chitin plus adapted microbes in flow microcosm with water and sedimentary materials from the field (Abramowicz 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 180 \text{ d}^{-1}$; $k_2 = 0.0007 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1 = 0.049 \text{ h}^{-1}$; $k_2 = 0.014 \text{ h}^{-1}$ (mayfly-sediment model II, Gobas et al. 1989)

$\log 1/k_2 > 3.1$, 3.6 h (fish, quoted, calculated- K_{OW} , Hawker & Connell 1988b).

$k_1 = 3850 \text{ d}^{-1}$; $k_2 = 0.0130 \text{ d}^{-1}$ (22°C , zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.054 \text{ d}^{-1}$ with an elimination $t_{1/2} = 12.9 \text{ d}$ (earthworm, Belfroid et al. 1995)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 131 \text{ d}$ and $k_2 = 0.012 \text{ d}^{-1}$ with $t_{1/2} = 56 \text{ d}$ for food concn of 20 ng/g and 148 ng/g , respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_1 = 0.00082 \text{ h}^{-1}$; $k_2 = 0.160 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_1(\text{calc}) = 6$ (food lipid $\text{mg}/(\text{g worm lipid-d})$; $k_2(\text{calc}) = 0.06 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 172 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 246 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of $60\text{--}120 \text{ d}$ due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of $16\text{--}48 \text{ d}$ based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995);

suggested $t_{1/2} = 3000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: aerobic biodegradation $t_{1/2} = 1.32 \text{ d}$ with the addition of polymer chitin, $t_{1/2} = 0.80 \text{ d}$ with chitin plus adapted microbes in flow microcosm with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990);

half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH-oxidation (Sedlak & Andren 1991);

photodegradation $t_{1/2} = (3.4 \pm 0.15) \text{ h}$, $(3.7 \pm 0.8) \text{ h}$ in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995);

$t_{1/2} = 60000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{1/2} = 87600 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: Sorption-Desorption Rate Constants: release rate constants k_d for labile PCBs sorbed to utility substation soils are: $k = 0.039 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.65 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.54 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.24 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from first day gas-purge experiments; release rate constants k_d for nonlabile PCBs sorbed to utility substation soils are $k = 0.00064 \text{ d}^{-1}$ from Conkelley surface soil consist of sand and silt with 0.05% OC-organic carbon, $k = 0.00188 \text{ d}^{-1}$ from Conkelley subsurface soil, 0.4-m deep, consist of sand and silt with 0.13% OC, $k = 0.00073 \text{ d}^{-1}$ from Tarehee surface soil consist of sand and silt with 0.02% OC and $k = 0.00247 \text{ d}^{-1}$ from Conkelley surface soil consist of silt with 0.01% OC, rates derived from 120–195 d experiments (Girvin et al. 1997)

$t_{1/2} = 87600 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} = 1000 \text{ d}$ in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{1/2} = 85 \text{ d}$ in its muscle, (Niimi & Oliver 1983);

elimination $t_{1/2} = 12.9$ from earthworm (Belfroid et al. 1995)

depuration $t_{1/2} = 56\text{--}131 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$t_{1/2} = 4.3 \text{ h}$ in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination $t_{1/2} = 12 \text{ d}$ in earthworm given contaminated food (predicted, Wågman et al. 2001).

depuration $t_{1/2} = 172 \text{ d}$ for high-dose treatment, $t_{1/2} = 24446 \text{ d}$ for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.101.1

Reported aqueous solubilities, vapor pressures, Henry's law constants and octanol-air partition coefficients of 2,2',4,5,5'-pentachlorobiphenyl (PCB-101) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure		Henry's law constant		log K_{OA}	
Dickhut et al. 1986		Westcott et al. 1981		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas saturation-GC		gas stripping-GC/MS		generator column-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	$H/(\text{Pa}\cdot\text{m}^3/\text{mol})$	$t/^\circ\text{C}$	log K_{OA}
4	0.0061	25	0.00096	4	15.75	-10	10.70
20	0.0121	30	0.00173	11	22.20	0	10.31
25	0.0154			18	30.78	10	9.78
32	0.0223			25	42.07	20	9.31
		log $P/\text{mmHg} = A - B/(T/K)$		31	54.40	30	8.78
	$\ln x = A - B/(T/K)$	A	11.1				
	A	-8.0159	B	$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(\text{kJ}\cdot\text{mol}^{-1}) = 73.54$	
	B	3836.90	temp range $30\text{--}40^\circ\text{C}$	A	7.9384		
				B	3572.3	log $K_{OA} = A + B/T$	
$\Delta H_{sol}/(\text{kJ}\cdot\text{mol}^{-1}) = 31.9 \pm 1.9$						A	-3.82
for $4\text{--}32^\circ\text{C}$						B	3841
				enthalpy, entropy change:			
				$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 29.7 \pm 3.2$			
				$\Delta S/(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) = 66 \pm 10$			

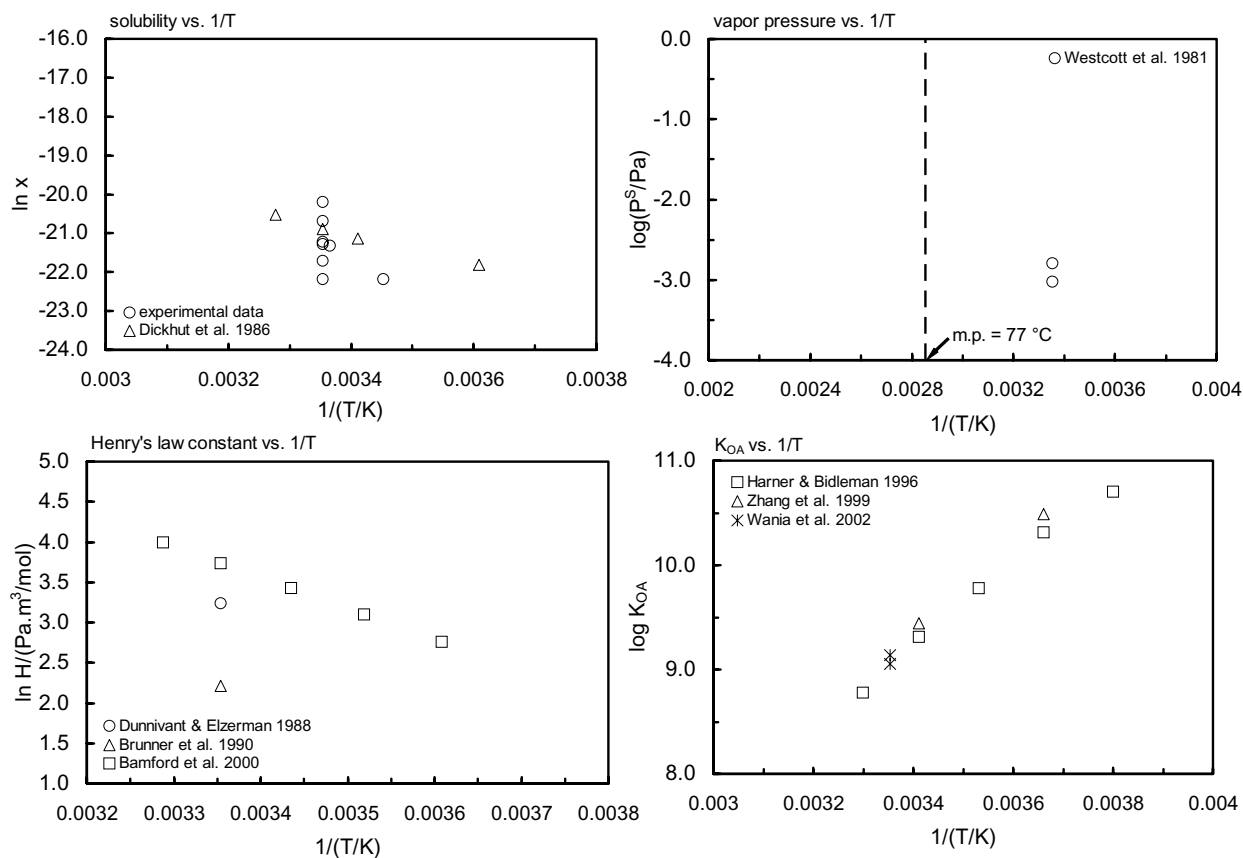
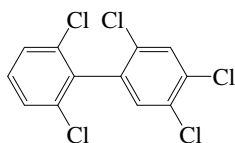


FIGURE 7.1.1.101.1 Logarithm of mole fraction solubility, vapor pressure, Henry's law constant and K_{OA} versus reciprocal temperature for 2,2',4,5,5'-pentachlorobiphenyl (PCB-101).

7.1.1.102 2,2',4,5,6'-Pentachlorobiphenyl (PCB-102)



Common Name: 2,2',4,5,6'-Pentachlorobiphenyl

Synonym: PCB-102, 2,2',4,5,6'-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',4,5,6'-pentachlorobiphenyl

CAS Registry No: 68194-06-9

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

93 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0314 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0065 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

6.61×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00706, 0.00184 (calculated-MW, GC-RI correlation, calculated- χ , Burkhard et al. 1985b)

0.00527, 0.00667 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P/mmHg) = 10.80 - 4630/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

$\log(P_L/Pa) = -4399/(T/K) + 12.48$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

68.60 (calculated-P/C, Burkhard 1984)

35.26 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

9.12 (wetted-wall column-GC/ECD, Brunner et al. 1990)

37.6 (calculated-QSPR, Dunnivant et al. 1992)

51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6\ kJ/mol$, $\Delta S_H = 0.03 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.39 (calculated-TSA, Burkhard 1984)

6.16 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)

6.0959 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.13 (calculated-QSPR/quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.19 (suspended particulate matter, Burkhard 1984)
4.589 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

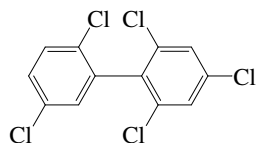
Ground water:

Sediment:

Soil:

Biota:

7.1.1.103 2,2',4,5',6-Pentachlorobiphenyl (PCB-103)



Common Name: 2,2',4,5',6-Pentachlorobiphenyl

Synonym: PCB-103, 2,2',4,5',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',4,5',6-pentachlorobiphenyl

CAS Registry No: 60145-21-3

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

81 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0275 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00986, 0.00859, 0.0164, 0.0113 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0164 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

9.23×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00983, 0.00804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00887, 0.0112 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00617 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4399/(T/K) + 12.70$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

109.43 (calculated-P/C, Burkhard 1984)

56.24 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

51.02 (calculated-QSPR, Dunnivant et al. 1992)

51.2 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 18 \pm 6$ kJ/mol, $\Delta S_H = 0.03 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.44 (calculated-TSA, Burkhard 1984)

6.11, 6.25, 5.92, 6.14 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.22 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)

6.11 (recommended, Sangster 1993)

8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)

6.1499 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.00 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.24 (suspended particulate matter, Burkhard 1984)

4.567 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

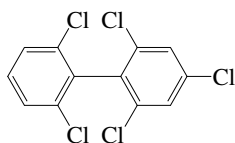
Ground water:

Sediment:

Soil:

Biota:

7.1.1.104 2,2',4,6,6'-Pentachlorobiphenyl (PCB-104)



Common Name: 2,2',4,6,6'-Pentachlorobiphenyl

Synonym: PCB-104, 2,2',4,6,6'-pentachloro-1,1'-biphenyl

Chemical Name: 2,2',4,6,6'-pentachlorobiphenyl

CAS Registry No: 56558-16-8

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

85.0 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)

224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.258 (mp at $85^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.030 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.0156 (generator column-GC, Dunnivant & Elzerman 1988)

0.0411 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.00986 (calculated-group contribution method, Kühne et al. 1995)

0.00651, 0.0175 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.0666 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$):

0.017 (supercooled liquid P_L , Burkhard 1984)

0.00735, 0.018, 0.00419 (supercooled liquid P_L , calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.0170 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00434 (supercooled liquid P_L , GC-RT correlation, Foreman & Bidleman 1985)

0.00434 (calculated-S \times HLC, solid P_S , Dunnivant & Elzerman 1988)

0.00225 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balçioğlu 1998)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

185.4 (calculated-P/C, Burkhard et al. 1985b)

90.9 (gas stripping, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)

55.4 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

75.11 (calculated-QSPR, Dunnivant et al. 1992)

39.40, 47.17, 56.0, 66.0* \pm 1.4, 75.50 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 2.1650 - 1774.05/(T/K)$; temp range $4-31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(14.5/kJ \cdot mol^{-1})/RT] + (0.018/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314$ J $\cdot K^{-1} \cdot mol^{-1}$ and temp range: $4-31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

62.0 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 15 \pm 3$ kJ/mol, $\Delta S_H = 0.02 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.40	(calculated-TSA, Burkhard 1984)
5.37	(generator column-GC, Hawker & Connell 1988a; quoted, Sangster 1993)
5.81	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
8.7057	(calculated-UNIFAC group contribution, Chen et al. 1993)
6.61	(calculated-Characteristic Root Index CRI, Saçan & Inel 1995)
5.7636	(calculated-molecular properties MNDO-AM1, Makino 1998)
5.96	(calculated-QSPR, Yeh & Hong 2002)
6.59	(calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.46	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
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Bioconcentration Factor, $\log BCF$:Sorption Partition Coefficient, $\log K_{OC}$:

6.20	(suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
4.431	(marine humic substances, reported as association coefficient $\log K_h$ at 5 mg L ⁻¹ DOC, calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 6 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2 = 0.10 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

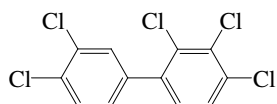
Sediment:

Soil:

Biota: $t_{1/2} > 1000 \text{ d}$ in rainbow trout, and $t_{1/2} = 101 \text{ d}$ in its muscle (Niimi & Oliver 1983);

elimination $t_{1/2} = 7 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.105 2,3,3',4,4'-Pentachlorobiphenyl (PCB-105)



Common Name: 2,3,3',4,4'-Pentachlorobiphenyl

Synonym: PCB-105, 2,3,3',4,4'-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,4'-pentachlorobiphenyl

CAS Registry No: 32598-14-4

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

103 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, assuming $\Delta S_{fus} = 56$ J/mol K, F: 0.164 (at mp $103^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0405 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00236, 0.0119, 0.00636, 0.00517 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00206 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00190 (calculated-QSPR, Dunnivant et al. 1992)

0.000982, 0.00190(generator column-GC/ECD, estimated, Hong & Qiao 1995)

0.00166* (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see comment by Van Noort 2004.

0.0362, 0.08243(supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

$\log [S_L/(mol\ m^{-3})] = -1285/(T/K) + 0.18$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

8.7×10^{-4} , 9.35×10^{-4} (supercooled liquid P_L by GC-RT correlation, different stationary phases, Bidleman 1984)

7.07×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00124, 0.000132, 0.000233 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

8.85×10^{-4} , 6.77×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

5.62×10^{-4} , 7.76×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = -4758/(T/K) + 12.90$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

6.76×10^{-4} (supercooled liquid P_L , $20^{\circ}C$, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

2.54×10^{-3} (P_L , calculated-MCI χ and Characteristic Root Index [CRI], Saçan & Balçioğlu 1998)

8.71×10^{-4} , 1.23×10^{-3} (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log P_L/Pa = -4554/(T/K) + 12.29$ (supercooled liquid P_L , FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

5.68 (calculated-P/C, Burkhard 1985a)

6.08 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

10.06 (calculated-QSPR, Dunnivant et al. 1992)

2.43 (calculated-QSPR, Achman et al. 1993)

33.6* \pm 1.3 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)

$\ln K_{AW} = 26.221 - 9093.1/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(75.6/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.218/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)

33.9 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 76 \pm 8 \text{ kJ/mol}$, $\Delta S_H = 0.22 \pm 0.03 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

33.88, 13.80 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

$\log H/(\text{Pa m}^3/\text{mol}) = -3269/(T/K) + 12.1$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.41, 6.68, 7.14, 6.93 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.82 (generator column-GC; Hawker & Connell 1988a)

6.79 (recommended, Sangster 1993)

6.65 (recommended, Hansch et al. 1995)

4.97–5.10 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)

6.61 (generator column-GC/ECD, Yeh & Hong 2002)

6.61, 6.82 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

10.27* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)

$\log K_{OA} = -5.68 + 4678/(T/K)$; (temp range –10 to 30°C, Harner & Bidleman 1996)

11.41, 10.20; 10.02 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)

10.17 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

7.40, 7.34 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log K_{OA} = 4630/(T/K) - 6.0$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.82–4.26 (various marine species, mean dry weight, Hope et al. 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

6.09 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

4.906 (as $\log K_h$, association coefficient with marine humic substance, calculated-MCI χ , Sabljic et al. 1989)

5.81 (soil, shake flask-GC, Paya-Perez et al. 1991)

6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.014 \text{ d}^{-1}$ with $t_{1/2} = 48 \text{ d}$ and $k_2 = 0.014 \text{ d}^{-1}$ with $t_{1/2} = 50 \text{ d}$ for food concn of 17 ng/g and 133 ng/g, respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 181 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 204 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment: $t_{1/2} = 7 \text{ yr}$ (Geyer et al. 2000)

Soil:

Biota: reported biological $t_{1/2} = 155$ to $> 1000 \text{ d}$ for trout, $t_{1/2} = 62$ –101 d for trout muscle; $t_{1/2} = 73$ to $> 200 \text{ d}$ for carp for pentachlorobiphenyls (Niimi 1987)

Depuration $t_{1/2} = 49$ –50 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 181 \text{ d}$ for high-dose treatment, $t_{1/2} = 204 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.105.1

Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,3,3',4,4'-pentachlorobiphenyl (PCB 105) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{H}/(\text{Pa m}^3/\text{mol})$	$t/^{\circ}\text{C}$	log K_{OA}
5	5.58×10^{-4}	4	3.09	-10	12.12
15	8.89×10^{-4}	11	7.10	0	11.43
25	1.66×10^{-3}	18	15.73	10	10.84
35	2.98×10^{-3}	25	33.6	20	10.27
		31	62.5	30	9.77
$\ln x = A - B/(T/K)$		$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 89.57$	
mole fraction x					
A		A	26.2208	$\log K_{OA} = A + B/T$	
B	$\Delta H_{sol}/R$	B	9093.1	A	-5.68
mp/ $^{\circ}\text{C}$	116.5–117.5	enthalpy, entropy change:		B	4678
$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 40.1$		$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 75.6 \pm 8.4$			
		$\Delta S/(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) = 218 \pm 28$			

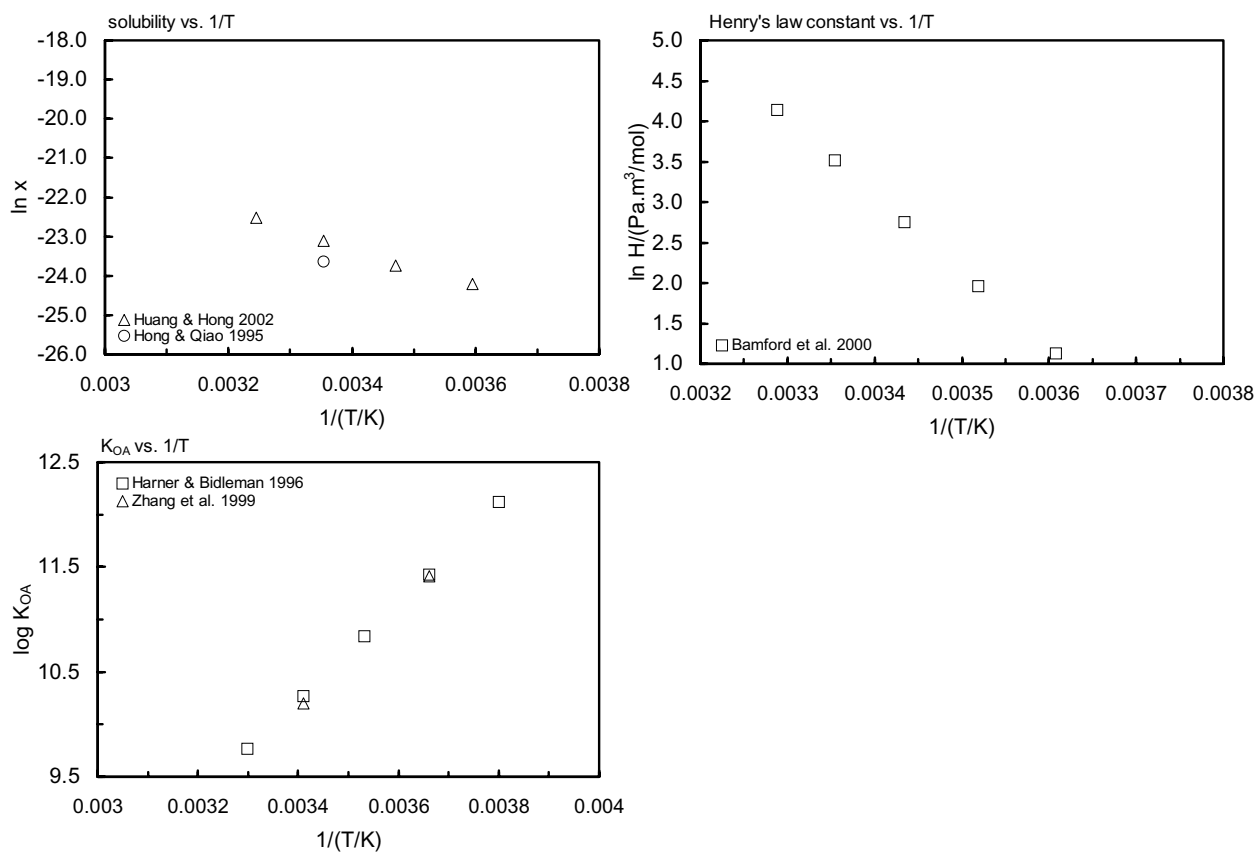
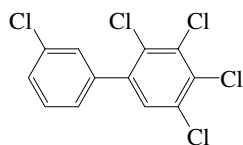


FIGURE 7.1.1.105.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,3,3',4,4'-pentachlorobiphenyl (PCB-105).

7.1.1.106 2,3,3',4,5-Pentachlorobiphenyl (PCB-106)

Common Name: 2,3,3',4,5-Pentachlorobiphenyl

Synonym: PCB-106, 2,3,3',4,5-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,5-pentachlorobiphenyl

CAS Registry No: 70424-69-0

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

105 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0411 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0082, 0.0088, 0.00517, 0.0058 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00326 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0050 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.0180, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00138, 0.00127 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4688/(T/K) + 12.86$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

39.82 (calculated-P/C, Burkhard 1984)

19.66 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

16.7 (calculated-QSPR, Dunnivant et al. 1992)

36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.29 (calculated-TSA, Burkhard 1984)

6.79, 6.79, 7.22, 6.89 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.64 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)

6.92 (recommended, Sangster 1993)

6.6213 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.09 (suspended particulate matter, Burkhard 1984)
4.906 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h , calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

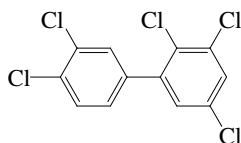
Ground water:

Sediment:

Soil:

Biota:

7.1.1.107 2,3,3',4',5-Pentachlorobiphenyl (PCB-107)



Common Name: 2,3,3',4',5-Pentachlorobiphenyl

Synonym: PCB-107, 2,3,3',4',5-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4',5-pentachlorobiphenyl

CAS Registry No: 70424-68-9

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

105 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0359 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0148 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0026 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00105 (P_L supercooled liquid, Burkhard et al. 1985a)

0.00735, 0.00116, 0.000532 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

2.61×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00105, 0.00132 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4688/(T/K) + 12.82$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

9.63 (calculated-P/C, Burkhard 1984)

8.61 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

20.27 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

16.13 (calculated-QSPR, Dunnivant et al. 1992)

3.94 (calculated-QSPR, Achman et al. 1993)

16.1 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

40.1 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 43 \pm 7$ kJ/mol, $\Delta S_H = 0.11 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.34 (calculated-TSA, Burkhard 1984)

6.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.5952 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.58 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.14 (suspended particulate matter, Burkhard 1984)
 4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 194 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.002 \text{ d}^{-1}$ with $t_{1/2} = 283 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

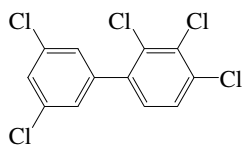
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 194 \text{ d}$ for high-dose treatment, $t_{1/2} = 283 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.108 2,3,3',4,5'-Pentachlorobiphenyl (PCB-108)



Common Name: 2,3,3',4,5'-Pentachlorobiphenyl

Synonym: PCB-108, 2,3,3',4,5'-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,5'-pentachlorobiphenyl

CAS Registry No: 70362-41-3

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

73 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0356 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0153 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00517 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00103 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00115, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00142, 0.00118 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00105 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4688/(T/K) + 12.87$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

9.57 (calculated-P/C, Burkhard 1984)

35.26 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

17.81 (calculated-QSPR, Dunnivant et al. 1992)

36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 7$ kJ/mol, $\Delta S_H = 0.15 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.34 (calculated-TSA, Burkhard 1984)

6.57 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.6672 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.86 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.14 (suspended particulate matter, Burkhard 1984)
4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

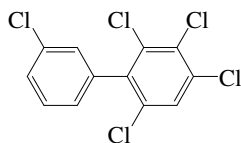
Ground water:

Sediment:

Soil:

Biota:

7.1.1.109 2,3,3',4,6-Pentachlorobiphenyl (PCB-109)



Common Name: 2,3,3',4,6-Pentachlorobiphenyl

Synonym: PCB-109, 2,3,3',4,6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,6-pentachlorobiphenyl

CAS Registry No: 74472-35-8

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

73 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0434 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0063 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00675, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

47.52 (calculated-P/C, Burkhard 1984)

28.56 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

39.42 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8 kJ/mol$, $\Delta S_H = 0.06 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.27 (calculated-TSA, Burkhard 1984)

6.48 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.5063 (quoted exptl., calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.59 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.07 (suspended particulate matter, Burkhard 1984)

4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

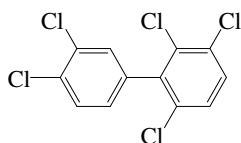
Ground water:

Sediment:

Soil:

Biota:

7.1.1.110 2,3,3',4',6-Pentachlorobiphenyl (PCB-110)



Common Name: 2,3,3',4',6-Pentachlorobiphenyl

Synonym: PCB-110, 2,3,3',4',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4',6-pentachlorobiphenyl

CAS Registry No: 38380-03-9

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

79 (calculated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0434 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.0288 ($20^{\circ}C$, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00731 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0082 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.011 (calculated-MCI χ , Patil 1991)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00735, 0.00248, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.00228 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00182, 0.00199 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

9.48×10^{-4} ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 11.0 - 4780/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00141, 0.00224 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.43$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

0.00258 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

37.48 (calculated-P/C, Murphy et al. 1983)

17.12 (calculated-P/C, Burkhard et al. 1985b)

10.74 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

19.15 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

19.89 (calculated-QSPR, Dunnivant et al. 1992)

5.966 (calculated-QSPR, Achman et al. 1993)

18.5 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

42.0 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 38 \pm 7$ kJ/mol, $\Delta S_H = 0.09 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.20 (RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
- 6.48 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.22 (generator column-GC, Larsen et al. 1992)
- 6.20 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ or as indicated and reported temperature dependence equations:

- 9.06; 8.58 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -6.16 + 4540/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 10.14 (10°C, estimated, Thomas et al. 1998)
- 9.06 (quoted, Kömp & McLachlan 1997b, Kaupp & McLachlan 1999)
- 10.61, 9.58; 9.80 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- 9.19 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 5.18, 6.48 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.60, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
- 5.50 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.06 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 5.6–6.8, 6.4; 7.70 (suspended sediment, average; algae > 50µm, Oliver 1987a)
- 4.72, 4.80, 4.77, 3.79 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
- 4.72, 4.75 (marine humic substances of 5 mg/L DOC, quoted, calculated-MCI χ , Sabljic et al. 1989)
- 6.32 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
- 5.20 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
- 5.71 (soil, shake flask-GC, Paya-Perez et al. 1991)
- 6.20 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 5.50 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
- 5.80 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodegradation rate constant $k = (0.07 \pm 0.01) \text{ h}^{-1}$ with $t_{1/2} = 9.9 \text{ h}$ in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{aq.}) = 4.3 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, PCB in Aroclor 1242 mixture, oxidized by hydroxyl radicals generated with Fenton's reagent in aqueous solutions at 25°C, half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines (relative rate method, Sedlak & Andren 1991)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.00064 \text{ h}^{-1}$; $k_2 = 0.094 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 171 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 204 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: half-lives range from $t_{1/2} \sim 4\text{--}11 \text{ d}$ in freshwater systems, $t_{1/2} = 0.1\text{--}10 \text{ d}$ in cloud water, $t_{1/2} > 1000 \text{ d}$ in oceans for PCBs with as many as 8 chlorines for OH- oxidation (Sedlak & Andren 1991); photodegradation $t_{1/2} = (9.9 \pm 1.6) \text{ h}$ in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

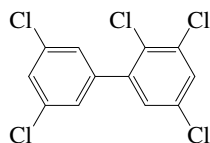
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 171 \text{ d}$ for high-dose treatment, $t_{1/2} = 204 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.111 2,3,3',5,5'-Pentachlorobiphenyl (PCB-111)



Common Name: 2,3,3',5,5'-Pentachlorobiphenyl

Synonym: PCB-111, 2,3,3',5,5'-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',5,5'-pentachlorobiphenyl

CAS Registry No: 39635-32-0

Molecular Formula: $C_{12}H_4Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

79 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0315 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00411 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00156 (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00633, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

16.21 (calculated-P/C, Burkhard 1984)

49.45 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

19.89 (calculated-QSPR, Dunnivant et al. 1992)

36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17 kJ/mol$, $\Delta S_H = 0.15 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.39 (calculated-TSA, Burkhard 1984)

6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.7224 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.08 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.19 (suspended particulate matter, Burkhard 1984)

4.862 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

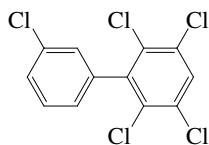
Ground water:

Sediment:

Soil:

Biota:

7.1.1.112 2,3,3',5,6-Pentachlorobiphenyl (PCB-112)



Common Name: 2,3,3',5,6-Pentachlorobiphenyl

Synonym: PCB-112, 2,3,3',5,6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',5,6-pentachlorobiphenyl

CAS Registry No: 74472-36-9

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

65 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0463 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00382, 0.00783, 0.00430, 0.00765 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0130 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.91×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00633, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00316 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.65$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

41.75 (calculated-P/C, Burkhard 1984)

33.34 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

27.02 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8 kJ/mol$, $\Delta S_H = 0.06 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.24 (calculated-TSA, Burkhard 1984)

6.40, 6.28, 6.70, 6.25 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.45 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.41 (recommended, Sangster 1993)

6.4916 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.16 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.04 (suspended particulate matter, Burkhard 1984)
- 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h , calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 12 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2 = 0.06 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

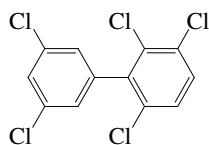
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 11 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.113 2,3,3',5',6-Pentachlorobiphenyl (PCB-113)



Common Name: 2,3,3',5',6-Pentachlorobiphenyl

Synonym: PCB-113, 2,3,3',5',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,3',5',6-pentachlorobiphenyl

CAS Registry No: 68194-10-5

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

65 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0382 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0036 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.372×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00365, 0.00184 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00306, 0.00368 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00240 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.63$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

28.88 (calculated-P/C, Burkhard 1984)

48.43 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

33.02 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8 kJ/mol$, $\Delta S_H = 0.06 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.31 (calculated-TSA, Burkhard 1984)

6.45 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.54 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.45 (recommended, Sangster 1993)

6.3808 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

6.11 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: measured rate constant $k < 0.05 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.3 and $23 \pm 2^\circ\text{C}$, with $t_{1/2} > 8 \text{ d}$ at pH 7 (Yao & Haag 1991).

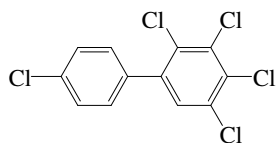
Ground water:

Sediment:

Soil:

Biota:

7.1.1.114 2,3,4,4',5-Pentachlorobiphenyl (PCB-114)



Common Name: 2,3,4,4',5-Pentachlorobiphenyl

Synonym: PCB-114, 2,3,4,4',5-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,4,4',5-pentachlorobiphenyl

CAS Registry No: 74472-37-0

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

99 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)

109 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.188 (at mp $99^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0121, 0.00879(RP-HPLC- k' correlation, different mobile phases, Brodsky & Ballschmiter 1988)

0.00146; 0.00246(generator column-GC/ECD; estimated, Hong & Qiao 1995)

0.00263 (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see comment by Van Noort 2004.

0.000732, 0.00157, 0.00263, 0.00505 ($5, 15, 25, 35^{\circ}C$, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.58×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00136, 0.000881, 0.000352 (calculated-MW, GC-RI correlation, calculated- χ , Burkhard et al. 1985b)

3.45×10^{-4} ($20^{\circ}C$, supercooled liquid P_L , Murphy et al. 1987)

0.00124, 0.000115(supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

6.92×10^{-4} (supercooled liquid P_L ; GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4688/(T/K) + 12.82$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

42.56 (calculated-P/C, Burkhard et al. 1985a)

6.99 ($20^{\circ}C$, calcd-P/C, Murphy et al. 1987)

11.55 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

14.48 (calculated-QSPR, Dunnivant et al. 1992)

4.96 (calculated-QSPR, Achman et al. 1993)

36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.29 (calculated-TSA, Burkhard 1984)

- 6.45, 6.78 (RP-HPLC- k' correlation, different mobile phases, Brodsky & Ballschmiter 1988)
 6.65 (calculated, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
 6.72 (recommended, Sangster 1993)
 6.5879 (calculated-molecular properties MNDO-AM1, Makino 1998)
 6.47 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.62 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.34, 6.65 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.09 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.906 (as $\log K_h$, association coefficient with marine humic substance, calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 164 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 187 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

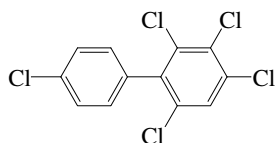
Sediment:

Soil:

Biota: reported biological $t_{1/2} = 155$ to $> 1000 \text{ d}$ for trout, $t_{1/2} = 62\text{--}101 \text{ d}$ for trout muscle; $t_{1/2} = 73$ to $> 200 \text{ d}$ for carp for pentachlorobiphenyls (Niimi 1987)

depuration $t_{1/2} = 164 \text{ d}$ for high-dose treatment, $t_{1/2} = 187 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.115 2,3,4,4',6-Pentachlorobiphenyl (PCB-115)



Common Name: 2,3,4,4',6-Pentachlorobiphenyl

Synonym: PCB-115, 2,3,4,4',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,4,4',6-pentachlorobiphenyl

CAS Registry No: 74472-38-1

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

87 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0428 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00342, 0.00517, 0.00142, 0.00494 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0082 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.41×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00599, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00224 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.50$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

42.56 (calculated-P/C, Burkhard 1984)

31.11 (calculated-QSAR- MCI χ , Sabljic & Güsten 1989)

24.87 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8\ kJ/mol$, $\Delta S_H = 0.06 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.27 (calculated-TSA, Burkhard 1984)

6.43, 6.40, 6.55, 6.38 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.49 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.44 (recommended, Sangster 1993)

6.4654 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.07 (suspended particulate matter, Burkhard 1984)
 4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 9 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2 = 0.07 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

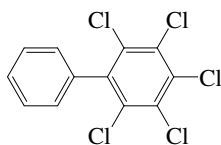
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 11 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.116 2,3,4,5,6-Pentachlorobiphenyl (PCB-116)



Common Name: 2,3,4,5,6-Pentachlorobiphenyl

Synonym: PCB-116, 2,3,4,5,6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,4,5,6-pentachlorobiphenyl

CAS Registry No: 18259-05-7

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

123.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

381 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)

Density (g/cm^3 at $20^{\circ}C$): 1.2803

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.80 (differential scanning calorimetry, Miller et al. 1984; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

54.81 (Miller et al. 1984)

54.83, 65.6 (exptl., calculated, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.108 (mp at $123.5^{\circ}C$)

0.105 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0068 (generator column-GC/ECD, Weil et al. 1974)

0.0207 (shake flask-GC/ECD, Dexter & Pavlou 1978)

0.00548 (generator column-GC/ECD, Miller et al. 1984,1985)

0.00139, 0.00517, 0.00158, 0.00608 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00401 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.0136 ($22^{\circ}C$, generator column-GC/ECD, Oppenhuizen et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.000788, 0.000394, 0.00419 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)

0.00341 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.0024 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.53$ (GC-RT correlation, Falconer & Bidleman 1994)

0.00326 (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

18.34 (calculated-P/C, Burkhard et al. 1985b)

23.41 (calculated-QSPR-MCI χ , Sabljic et al. 1989)

29.97 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 6.85 (RP-TLC-retention time correlation, Bruggeman et al. 1982)
- 7.49 (calculated-f const., Yalkowsky et al. 1983)
- 6.30 (generator column-GC/ECD, Miller et al. 1984, 1985)
- 6.30; 6.70, 6.40, 6.65, 6.32 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.754 ± 0.015 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
- 6.25 (HPLC- k' correlation, Noegrohati & Hammers 1992)
- 6.52 (recommended, Sangster 1993)
- 6.74 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$

- 9.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Bioaccumulation Factor, $\log BAF$:

- 5.46 (fish, lipid based-L/kg(Ip), Thomann 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.94 (suspended particulate matter, calculated- K_{ow} , Burkhard 1984)
- 4.791 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)
 $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2: > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

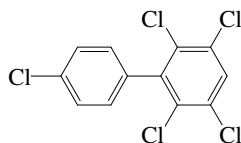
Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} > 1000 \text{ d}$ in rainbow trout, and $t_{1/2} = 100 \text{ d}$ in its muscle, 100 d (Niimi & Oliver 1983).

7.1.1.117 2,3,4',5,6-Pentachlorobiphenyl (PCB-117)



Common Name: 2,3,4',5,6-Pentachlorobiphenyl

Synonym: PCB-117, 2,3,4',5,6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3,4',5,6-pentachlorobiphenyl

CAS Registry No: 68194-11-6

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

115 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0457 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0042, 0.00651, 0.0248, 0.00494 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00411 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.23×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00561, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

$\log(P/mmHg) = 11.10 - 4800/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

0.00257 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.56$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

37.29 (calculated-P/C, Burkhard 1984)

25.13 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

33.02 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.25 (calculated-TSA, Burkhard 1984)

6.37, 6.33, 6.49, 6.28 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.46 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.39 (recommended, Sangster 1993)

6.4587 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.20 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

6.05 (suspended particulate matter, Burkhard 1984)

4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h , calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

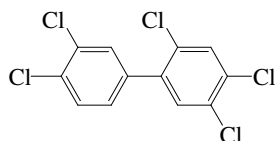
Ground water:

Sediment:

Soil:

Biota:

7.1.1.118 2,3',4,4',5-Pentachlorobiphenyl (PCB-118)



Common Name: 2,3',4,4',5-Pentachlorobiphenyl

Synonym: PCB-118, 2,3',4,4',5-pentachloro-1,1'-biphenyl

Chemical Name: 2,3',4,4',5-pentachlorobiphenyl

CAS Registry No: 31508-00-6

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

106 (Burkhard et al. 1985; Brodsky & Ballschmiter 1988)

109 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

224.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K, F: 0.158 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.01344 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.0153 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00107; 0.00198 (generator column-GC/ECD; estimated, Hong & Qiao 1995)

0.00207* (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see comment by Van Noort 2004.

0.0290, 0.0223 (supercooled liquid S_L : derivation of literature-derived value, final-adjusted value, Li et al. 2003)
 $\log [S_L/(mol\ m^{-3})] = -1339/(T/K) + 0.32$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00120 (P_L supercooled liquid, GC-RT correlation, Bidleman 1984)

9.62×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.000167 (GC-RI correlation, Burkhard et al. 1985b)

0.00123, 0.00104 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.54×10^{-4} ($20^{\circ}C$, supercooled liquid P_L , Murphy et al. 1987)

8.32×10^{-4} , 1.12×10^{-3} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = -4664/(T/K) + 12.72$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

8.91×10^{-4} , 1.0×10^{-4} (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log P_L/Pa = -4853/(T/K) + 13.23$ (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)

$\log P_L/Pa = -4627/(T/K) + 12.52$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

40.8 (concn ratio-GC, Murphy et al. 1983)

8.61 ($20^{\circ}C$, gas stripping-GC, Murphy et al. 1987)

- 11.75 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)
 12.73 (calculated-QSPR, Dunnivant et al. 1992)
 3.94 (calculated-QSPR, Achman et al. 1993)
 36.12* \pm 1.0 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
 $\ln K_{AW} = 15.877 - 5989.9/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(49.8/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.132/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
 36.3 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 50 \pm 6 \text{ kJ/mol}$, $\Delta S_H = 0.13 \pm 0.02 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004
 32.36, 14.45 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
 $\log H/(\text{Pa m}^3/\text{mol}) = -2699/(T/K) + 10.56$ (LDV linear regression of literature data, Li et al. 2003)
 $\log H/(\text{Pa m}^3/\text{mol}) = -3289/(T/K) + 12.19$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.42 (HPLC-RT correlation, Shaw & Connell 1982)
 6.66, 7.12 (HPLC- k' correlation, Rapaport & Eisenreich 1984)
 6.57 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
 6.74 (calculated-TSA, Hawker & Connell 1988a)
 6.24 (generator column-GC, Larsen et al. 1992)
 6.57 (recommended, Sangster 1993)
 6.49 (generator column-GC/ECD, Yeh & Hong 2002)
 6.49, 6.69 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ as or as indicated and reported temperature dependence. Additional data at other temperatures designated * are compiled at the end of this section:

- 10.08* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
 $\log K_{OA} = -5.92 + 4693/(T/K)$; temp range –10 to 30°C (generator column-GC, Harner & Bidleman 1996)
 11.13, 10.04; 10.02 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 9.86 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
 9.80, 9.36 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log K_{OA} = 4646/(T/K) - 6.22$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 3.60–5.19 (various marine species, mean dry weight, Hope et al. 1998)
 5.43 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.16 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.88 (as $\log K_h$, association coefficient with marine humic substance, calculated- χ , Sabljic et al. 1989)
 5.81 (soil from Ispra near Lake Maggiore, Italy, batch equilibrium-GC/ECD, Paya-Perez et al. 1991)
 5.20 (colloids and micro-particulates, GC/ECD, Murray & Andren 1992)
 5.80 (calculated- K_{OW} , Girvin & Scott 1997)
 5.52 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
 4.79–7.42 (range, calculated from sequential desorption of 11 urban soils; Krauss & Wilcke 2001)
 5.46; 6.03, 6.67, 6.26 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of exptl 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
 6.16–7.20 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Sorption Partition Coefficient, $\log K_p$ of $\log K_d$:

- 5.55–5.82 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)
 5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2): $k_2 = 0.034 \text{ d}^{-1}$ with an elimination $t_{1/2} = 20.3 \text{ d}$ (earthworm, Belfroid et al. 1995) $k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 103 \text{ d}$ and $k_2 = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53 \text{ d}$ for food concn of 20 ng/g and 133 ng/g respectively in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998) $k_1 = 14 \text{ L d}^{-1} \text{ g}^{-1}$ dry wt.; $k_2 = 0.052 \text{ d}^{-1}$ (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999) $k_2 = 0.052 \text{ d}^{-1}$ (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999) $k_1 = 6$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.06 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001) $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 180 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004) $k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 225 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota: reported biological half-lives: $t_{1/2} = 155$ to $> 1000 \text{ d}$ for trout, $t_{1/2} = 62\text{--}101 \text{ d}$ for trout muscle; $t_{1/2} = 73$ to $> 200 \text{ d}$ for carp for pentachlorobiphenyls (Niimi 1987);elimination $t_{1/2} = 20.3 \text{ d}$ from earthworm (Belfroid et al. 1995)elimination $t_{1/2} = 95 \text{ d}$ in rainbow trout, based on 228 d of elimination (Coristine et al. 1996)depuration $t_{1/2} = 53\text{--}103 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

theoretical half-life to reach 90% steady-state tissue concn 13.3 d (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);

elimination $t_{1/2} = 12 \text{ d}$ in earthworm given contaminated food (predicted, Wågman et al. 2001).depuration $t_{1/2} = 180 \text{ d}$ for high-dose treatment, $t_{1/2} = 225 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.118.1
Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,3',4,4',5-pentachlorobiphenyl (PCB 118) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K _{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
5	5.85 × 10 ⁻⁴	4	7.34	-10	11.93
15	1.22 × 10 ⁻³	11	12.81	0	11.23
25	2.07 × 10 ⁻³	18	21.79	10	10.64
35	3.31 × 10 ⁻³	25	36.2	20	10.08
		31	54.8	30	9.57
ln x = A -B/(T/K)		ln K _{AW} = -ΔH/RT + ΔS/R		ΔH _{OA} /(kJ mol ⁻¹) = 89.86	
eq. 1	x	A	15.8768	log K _{OA} = A + B/T	
A		B	5989.9	A	-5.924
B	ΔH _{sol} /R			B	4693
mp/°C	111–113	enthalpy, entropy change:			
ΔH _{sol} /(kJ mol ⁻¹)	= 37.4	ΔH/(kJ·mol ⁻¹) = 49.8 ± 5.8			
		ΔS/(J·mol ⁻¹ ·K ⁻¹) = 132 ± 18			

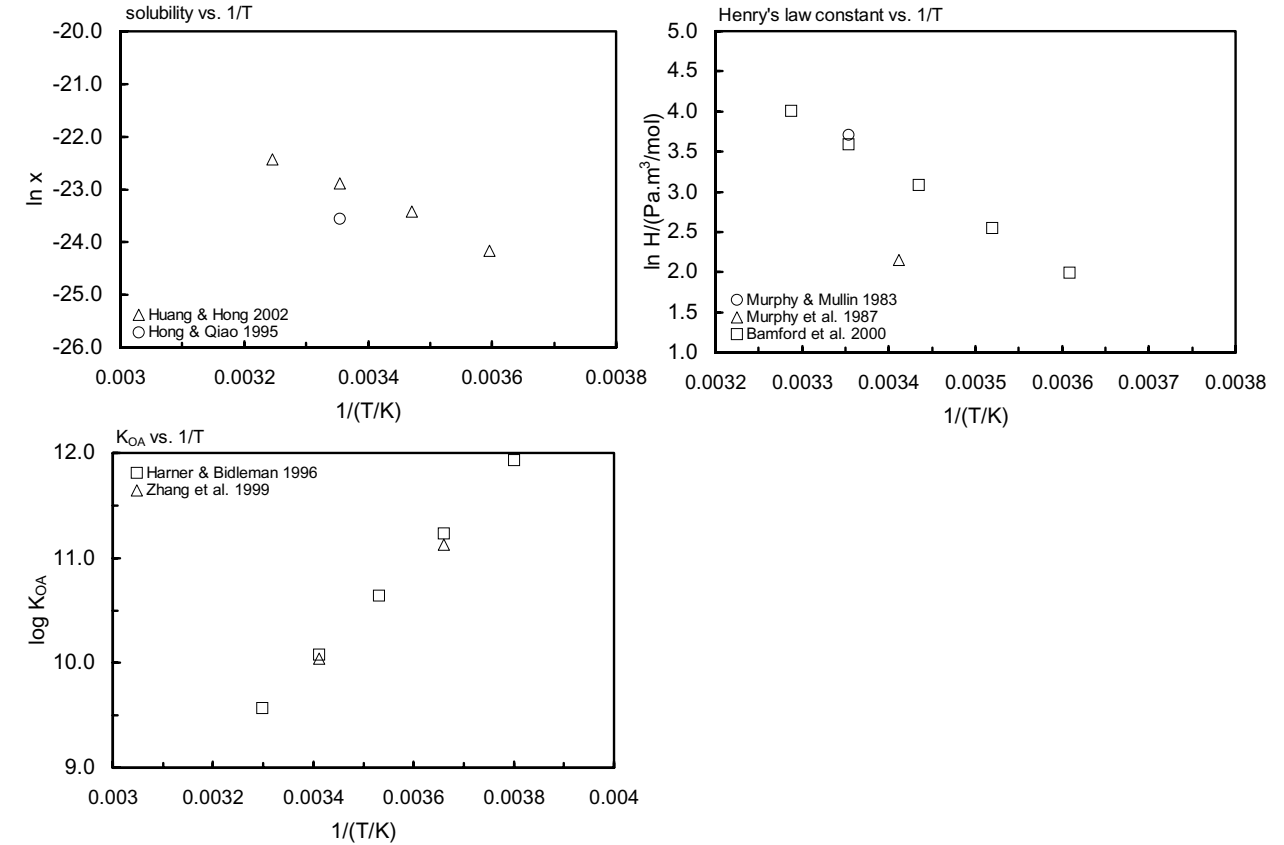
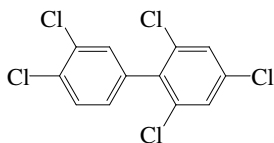


FIGURE 7.1.1.118.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,3',4,4',5-pentachlorobiphenyl (PCB-118).

7.1.1.119 2,3',4,4',6-Pentachlorobiphenyl (PCB-119)



Common Name: 2,3',4,4',6-Pentachlorobiphenyl

Synonym: PCB-119, 2,3',4,4',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3',4,4',6-pentachlorobiphenyl

CAS Registry No: 56558-17-9

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

81 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0353 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00326, 0.00375, 0.00411, 0.00529 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00651 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.48×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)

0.00735, 0.00269, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00288 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.61$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

22.90 (calculated-P/C, Burkhard 1984)

46.10 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

7.50 (wetted-wall column-GC/ECD, Brunner et al. 1990)

5.97 (calculated-QSPR, Achman et al. 1993)

31.46 (calculated-QSPR, Dunnivant et al. 1992)

31.8 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

50.0 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 20 \pm 5 kJ/mol$, $\Delta S_H = 0.03 \pm 0.02 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.36 (calculated-TSA, Burkhard 1984)

6.44, 6.49, 6.33, 6.35 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.58 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.40 (recommended, Sangster 1993)

8.7057 (calculated-UNIFAC group contribution, Chen et al. 1993)

6.4124 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.27 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.16 (suspended particulate matter, Burkhard 1984)

4.726 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

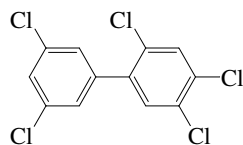
Ground water:

Sediment:

Soil:

Biota:

7.1.1.120 2,3',4,5,5'-Pentachlorobiphenyl (PCB-120)



Common Name: 2,3',4,5,5'-Pentachlorobiphenyl

Synonym: PCB-120, 2,3',4,5,5'-pentachloro-1,1'-biphenyl

Chemical Name: 2,3',4,5,5'-pentachlorobiphenyl

CAS Registry No: 68194-12-7

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

77 (Shiu & Mackay 1986)

77, 93 (exptl., estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F:

0.306 (assuming $\Delta S_{fus} = 56 J/mol K$, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0295 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.42×10^{-3} (P_L supercooled liquid, Burkhard et al. 1985a)

0.00735, 0.00155, 0.000352 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00197, 0.00203 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P/mmHg) = 11.0 - 4780/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

$\log(P_L/Pa) = -4688/(T/K) + 13.02$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

15.71 (calculated-P/C, Burkhard 1984)

40.94 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

6.57 (wetted wall column-GC/ECD, Brunner et al. 1990)

24.87 (calculated-QSPR, Dunnivant et al. 1992)

36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17 kJ/mol$, $\Delta S_H = 0.15 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.22, 5.68 (HPLC- k' correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

6.41 (calculated-TSA, Burkhard 1984)

5.68 (quoted, Sangster 1993)

6.79 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.772 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.87 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.32 (suspended particulate matter, Burkhard 1984)

4.862 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

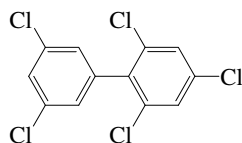
Ground water:

Sediment:

Soil:

Biota:

7.1.1.121 2,3',4,5',6-Pentachlorobiphenyl (PCB-121)



Common Name: 2,3',4,5',6-Pentachlorobiphenyl

Synonym: PCB-121, 2,3',4,5',6-pentachloro-1,1'-biphenyl

Chemical Name: 2,3',4,5',6-pentachlorobiphenyl

CAS Registry No: 56558-18-0

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

91 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0311 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00201, 0.00259, 0.00651, 0.00682 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00411 (calculated-TSA and mp., Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.68×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.00396, 0.000154 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

0.00483, 0.00608 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00501 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4522/(T/K) + 12.85$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

38.50 (calculated-P/C, Burkhard 1984)

75.39 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

56.59 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8$ kJ/mol, $\Delta S_H = 0.06 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.39 (calculated-TSA, Burkhard 1984)

6.63, 6.60, 6.19, 6.28 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.64 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.42 (recommended, Sangster 1993)

6.5572 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.84 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.19 (suspended particular matter, Burkhard 1984)
- 4.704 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h , calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d for pentachlorobiphenyls (Atkinson 1987);
calculated tropospheric lifetime of 16–48 d for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

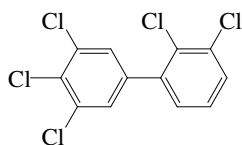
Ground water:

Sediment:

Soil:

Biota:

7.1.1.122 2,3,3',4',5'-Pentachlorobiphenyl (PCB-122)



Common Name: 2,3,3',4',5'-Pentachlorobiphenyl

Synonym: PCB-122

Chemical Name: 2,3,3',4',5'-pentachlorobiphenyl

CAS Registry No: 76842-07-4

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

111 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0128 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00259 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.76×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00735, 0.000854, 0.000804 (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

9.93×10^{-4} , 7.23×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.21×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P_L/Pa) = -4688/(T/K) + 12.72$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.21 (calculated-P/C, Burkhard 1984)

6.08 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

13.88 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

12.73 (calculated-QSPR, Dunnivant et al. 1992)

36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17\ kJ/mol$, $\Delta S_H = 0.15 \pm 0.01\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.29 (calculated-TSA, Burkhard 1984)

6.64 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.4986 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

6.09 (suspended particulate matter, Burkhard 1984)

4.906 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h , calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

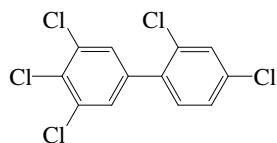
Ground water:

Sediment:

Soil:

Biota:

7.1.1.123 2,3',4,4',5'-Pentachlorobiphenyl (PCB-123)



Common Name: 2,3',4,4',5'-Pentachlorobiphenyl

Synonym: PCB-123, 2,3',4,4',5'-pentachloro-1,1'-biphenyl

Chemical Name: 2,3',4,4',5'-pentachlorobiphenyl

CAS Registry No: 65510-44-3

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

125 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00201, 0.00259, 0.00651, 0.00682 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.000424 (generator column-GC/ECD, Hong & Qiao 1995)

0.000899 (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see comment by van Noort 2004.

0.000299, 0.000512, 0.000899, 0.00155 ($5, 15, 25, 35^{\circ}C$, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

9.08×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00099 (P_L supercooled liquid values: GC-RI correlation, Burkhard et al. 1985b)

0.0013, 0.00095 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.000933 (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4688/(T/K) + 12.84$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

8.805 (calculated- P/C , Burkhard 1984)

26.55 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

17.65 (calculated-QSPR, Dunnivant et al. 1992)

36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.63, 6.60, 6.19, 6.28 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.74 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.64 (recommended, Sangster 1993)

6.4832 (calculated-molecular properties MNDO-AMI, Makino 1998)

6.50 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.83 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.16 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

4.884 (as $\log K_h$, association coefficient with marine humic substance, calculated- χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 15–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation half-life of 21.2 min when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).

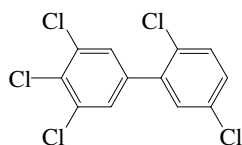
Ground water:

Sediment:

Soil:

Biota: reported biological half-lives for pentachlorobiphenyls: $t_{1/2} = 155$ to $> 1000 \text{ d}$ for trout, $t_{1/2} = 62\text{--}101 \text{ d}$ for trout muscle; $t_{1/2} = 73$ to $> 200 \text{ d}$ for carp (Niimi 1987)

7.1.1.124 2,3',4',5,5'-Pentachlorobiphenyl (PCB-124)



Common Name: 2,3',4',5,5'-Pentachlorobiphenyl

Synonym: PCB-124, 2',3,4,5,5'-pentachloro-1,1'-biphenyl, 2',3,4,5,5'-pentachlorobiphenyl

Chemical Name: 2,3',4',5,5'-pentachlorobiphenyl

CAS Registry No: 70424-70-3

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

99 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0336 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00158 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00326 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.01×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00112 (GC-RI correlation, Burkhard et al. 1985b)

2.60×10^{-4} ($20^{\circ}C$, supercooled liquid P_L , Murphy et al. 1987)

$\log(P_L/Pa) = -4688/(T/K) + 12.62$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

9.84 (calculated-P/C, Burkhard 1984)

5.37 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

19.76 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

5.70 (calculated-QSPR, Achman et al. 1993)

17.65 (calculated-QSPR, Dunnivant et al. 1992)

36.7 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 56 \pm 17$ kJ/mol, $\Delta S_H = 0.15 \pm 0.01$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.36 (calculated-TSA, Burkhard 1984)

6.73 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.6178 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.76 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.16 (suspended particulate matter, Burkhard 1984)
 4.884 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

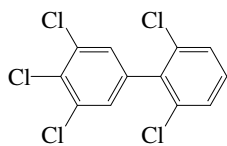
Ground water:

Sediment:

Soil:

Biota:

7.1.1.125 2,3',4',5',6-Pentachlorobiphenyl (PCB-125)



Common Name: 2,3',4',5',6-Pentachlorobiphenyl

Synonym: PCB-125

Chemical Name: 2,3',4',5',6-pentachlorobiphenyl

CAS Registry No: 74472-39-2

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

73 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0408 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.87×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00204 (GC-RI correlation, Burkhard et al. 1985b)

0.0020 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log (P_L/Pa) = -4255/(T/K) + 12.45$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

14.5 (calculated-P/C, Burkhard 1984)

33.23 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

29.16 (calculated-QSPR, Dunnivant et al. 1992)

44.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 29 \pm 8 kJ/mol$, $\Delta S_H = 0.06 \pm 0.01 kJ/mol \cdot K$ (Bamford et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.29 (calculated-TSA, Burkhard 1984)

6.51 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.2930 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.09 (suspended particulate matter, Burkhard 1984)
4.748 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2-0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60-120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3-0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16-48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

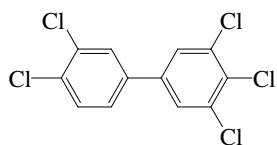
Ground water:

Sediment:

Soil:

Biota:

7.1.1.126 3,3',4,4',5-Pentachlorobiphenyl (PCB-126)



Common Name: 3,3',4,4',5-Pentachlorobiphenyl

Synonym: PCB-126

Chemical Name: 3,3',4,4',5-pentachlorobiphenyl

CAS Registry No: 57465-28-8

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

106 (Burkhard et al. 1985b; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F:

0.158 (assuming $\Delta S_{fus} = 56$ J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0321 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00103 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.000305 (generator column-GC/ECD, Hong & Qiao 1995)

0.00133* (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see comment by van Noort 2004

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.736×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

3.05×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

4.86×10^{-4} , 2.86×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.09×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4956/(T/K) + 13.31$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

2.51×10^{-4} (P_L , $20^{\circ}C$, from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.776 (calculated-P/C, Burkhard et al. 1985)

5.471 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

8.39 (calculated-QSAR, Dunnivant et al. 1992)

$21.02^* \pm 0.83$ (gas stripping-GC, measured range $4-31^{\circ}C$, Bamford et al. 2000)

$\ln K_{AW} = 35.001 - 11847.5/(T/K)$; temp range $4-31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(98.5/kJ \cdot mol^{-1})/RT] + (0.291/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314 J \cdot K^{-1} \cdot mol^{-1}$ and temp range: $4-31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

21.3 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 99 \pm 9$ kJ/mol, $\Delta S_H = 0.29 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.38 (calculated-TSA, Burkhard 1984)

- 6.57 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
 6.89 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
 6.6729 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
 6.56; 6.62 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
 7.00, 6.67 (calculated-MCI χ , calculated-MNDO-AMI method, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 10.61* (20°C, generator column-GC, measured range -10 to 30°C, Harner & Bidleman 1996)
 $\log K_{OA} = -5.98 + 4870/(T/K)$; temp range -10 to 30°C (generator column-GC, Harner & Bidleman 1996)
 11.77, 10.66; 10.61 (0, 20°C, GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 10.56 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.81, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor BSAF:

- 43 (trout, Niimi 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.18 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2-0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60-120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.3-0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16-48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 5 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2 = 0.05 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.0137 \text{ d}^{-1}$ with $t_{1/2} = 51 \text{ d}$ (newly contaminated oysters, Gardinali et al. 2004)

$k_2 = 0.0116 \text{ d}^{-1}$ with $t_{1/2} = 60 \text{ d}$ (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{1/2} = 304 \text{ min}$ when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996).

Ground water:

Sediment:

Soil:

Biota: reported biological half-lives for pentachlorobiphenyls: $t_{1/2} = 155$ to $> 1000 \text{ d}$ for trout, $t_{1/2} = 62-101 \text{ d}$ for trout muscle; $t_{1/2} = 73$ to $> 200 \text{ d}$ for carp (Niimi 1987);

elimination $t_{1/2} = 13 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

Depuration $t_{1/2} = 51 \text{ d}$ for newly contaminated oysters, and $t_{1/2} = 60 \text{ d}$ for chronically contaminated oysters (Gardinali et al. 2004)

TABLE 7.1.1.126.1

Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 3,3',4,4',5-pentachlorobiphenyl (PCB 126) at various temperatures and reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K _{OA}	
Huang & Hong 2002		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
5	6.30 × 10 ⁻⁴	4	0.958	-10	12.55
15	9.64 × 10 ⁻⁴	11	2.82	0	11.81
25	1.33 × 10 ⁻³	18	7.88	10	11.24
35	1.60 × 10 ⁻³	25	21.02	20	10.61
		31	47.0	30	10.10
$\ln x = A - B/(T/K)$		$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(kJ\ mol^{-1}) = 93.25$	
A	x	$\Delta S/R$	35.012	$\log K_{OA} = A + B/T$	
B	$\Delta H_{sol}/R$	$\Delta H/R$	11847.5	A	-5.979
mp/°C	160–161	enthalpy, entropy change:		B	4870
$\Delta H_{sol}/(kJ\ mol^{-1}) = 22.3$		$\Delta H/(kJ\cdot mol^{-1}) = 98.5 \pm 9.4$			
		$\Delta S/(J\cdot mol^{-1}\cdot K^{-1}) = 291 \pm 32$			

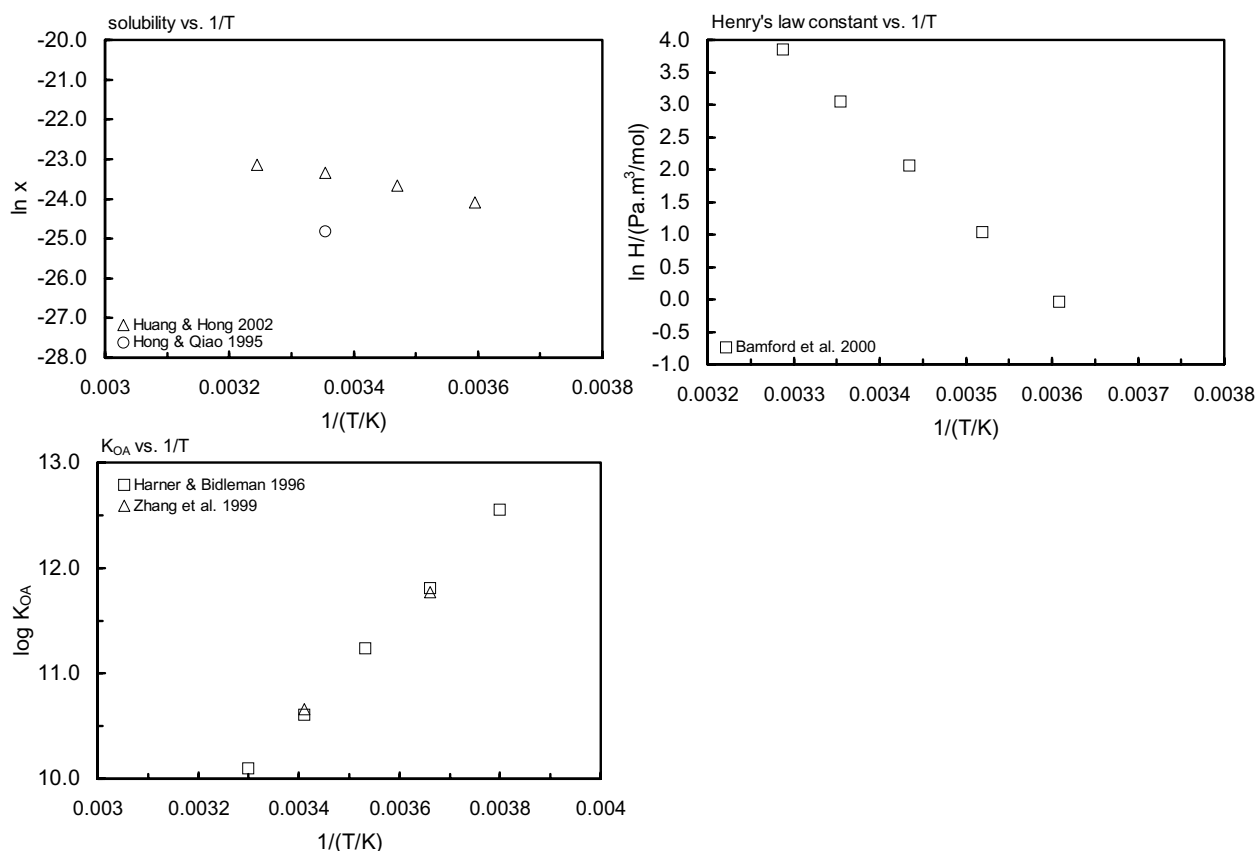
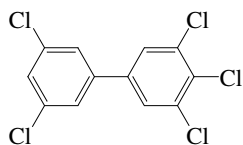


FIGURE 7.1.1.126.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 3,3',4,4',5-pentachlorobiphenyl (PCB-126).

7.1.1.127 3,3',4,5,5'-Pentachlorobiphenyl (PCB-127)



Common Name: 3,3',4,5,5'-Pentachlorobiphenyl

Synonym: PCB-127

Chemical Name: 3,3',4,5,5'-pentachlorobiphenyl

CAS Registry No: 39635-33-1

Molecular Formula: $C_{12}H_5Cl_5$

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

135 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

289.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0285 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.000651 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.04×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.000449 (GC-RI correlation, Burkhard et al. 1985b)

7.80×10^{-4} , 5.38×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4956/(T/K) + 13.51$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

4.64 (calculated-P/C, Burkhard 1984)

34.45 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

12.73 (calculated-QSPR, Dunnivant et al. 1992)

21.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 99 \pm 9$ kJ/mol, $\Delta S_H = 0.29 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.42 (calculated-TSA, Burkhard 1984)

6.95 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.8023 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.53 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.22 (suspended particulate matter, Burkhard 1984)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (0.2\text{--}0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 60\text{--}120 \text{ d}$, due to gas-phase loss process at room temp. (Atkinson 1987) $k_{OH}(\text{calc}) = (0.3\text{--}0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for pentachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 16\text{--}48 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radical for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 16–48 d based on the calculated rate constant for gas-phase reaction with OH radical for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

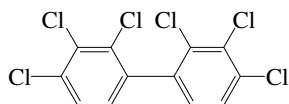
Ground water:

Sediment:

Soil:

Biota:

7.1.1.128 2,2',3,3',4,4'-Hexachlorobiphenyl (PCB-128)



Common Name: 2,2',3,3',4,4'-Hexachlorobiphenyl

Synonym: PCB-128, 2,2',3,3',4,4'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4'-hexachlorobiphenyl

CAS Registry No: 38380-07-3

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

151 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.3482

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.83 (Miller et al. 1984)

29.20 (Ruelle et al. 1993; Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

68.62 (Miller et al. 1984; Shiu & Mackay 1986)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.0582 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.40×10^{-4} (generator column-GC/ECD, Weil et al. 1974)

9.90×10^{-4} (shake flask-GC/ECD, Dexter & Pavlou 1978)

2.85×10^{-4} (generator column-GC/ECD, Miller et al. 1984,1985)

0.0067 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

2.74×10^{-3} , 2.17×10^{-3} , 9.07×10^{-4} , 1.54×10^{-3} (RP-HPLC- k' correlation, different stationary and mobile phase, Brodsky & Ballschmiter 1988)

0.0023 (generator column-GC, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.41×10^{-4} (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

3.59×10^{-4} (supercooled liquid P_L , Burkhard 1984)

2.31×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)

3.59×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

3.67×10^{-4} , 2.94×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

9.83×10^{-5} ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

3.67×10^{-4} , 2.94×10^{-4} , 3.41×10^{-4} (supercooled liquid P_L , GC-RT correlation, Foreman & Bidleman 1985)

$\log(P/mmHg) = 11.40 - 5020/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

1.78×10^{-4} , 3.31×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4881/(T/K) + 12.91$ (GC-RT correlation, Falconer & Bidleman 1994)

$(2.90 - 154.0) \times 10^{-6}$; $(9.80 - 35.9) \times 10^{-5}$ (literature solid P_s range; supercooled liquid P_L range, Delle Site 1997)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

50.66 (calculated, Murphy et al. 1983)

6.85 (calculated-P/C, Burkhard et al. 1985b)

11.91 (calculated-P/C, Shiu & Mackay 1986)

- 5.78 (20°C, calculated-P/C, Murphy et al. 1987)
 3.04 (gas stripping-GC/ECD, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
 50.5 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
 1.32 (wetted-wall column-GC/ECD, Brunner et al. 1990)
 10.51 (calculated-QSPR, Dunnivant et al. 1992)
 0.890, 3.224, 10.99, 35.40 \pm 1.5, 92.30 (4, 11, 18, 25, 31°C, gas stripping-GC, Bamford et al. 2000)
 $\ln K_{AW} = 43.30 - 14193/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford 2000)
 $K_{AW} = \exp[-(118.0/kJ\cdot mol^{-1})/RT] + (0.360/kJ\cdot mol^{-1}\cdot K^{-1})/R$; where $R = 8.314 J\cdot K^{-1}\cdot mol^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
 32.7 (exptl. data, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 118 \pm 8 kJ/mol$, $\Delta S_H = 0.36 \pm 0.03 kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.44 (RP-TLC-RT correlation, Bruggeman et al. 1982)
 6.98 (generator column-GC/ECD, Miller et al. 1984, 1985)
 6.14 (HPLC-RT correlation, Rapaport & Eisenreich 1984)
 6.28 (HPLC-RP/MS correlation, Burkhard et al. 1985c)
 6.50, 6.67, 6.83, 6.73 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 6.98 (generator column-GC/ECD, Doucette & Andren 1988)
 7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
 7.321 ± 0.027 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 6.98, 6.87; 6.92, 6.87 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
 6.71 (HPLC- k' correlation, Neogrohati & Hammers 1992)
 6.62 (generator column-GC, Larsen et al. 1992)
 6.96 (recommended, Sangster 1993)
 7.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.93 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 1.0 (poultry, Garten & Trabalka 1983)
 4.28 (worms, Oliver 1987c)
 5.77; 7.30 (22°C, zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)
 3.20–5.12 (various marine species, mean dry wt. BCF, Hope et al. 1998)
 4.90–6.03 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
 5.77, 7.31 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
 5.41, 7.48 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.05 (calculated-MCI, Koch 1983)
 6.42 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.06 (calculated-MCI, Bahnick & Doucette 1988)
 5.26 (marine humic substance, calculated-MCI χ , reported as $\log K_h$ at 5 mg/L DOC, Sabljic et al. 1989)
 6.28, 6.17, 6.01 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
 6.0 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 5.05 (soil, calculated-MCI, Sabljic et al. 1995)
 5.93 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioğlu 1996)
 6.50 (soil, calculated- K_{OW} , Girvin & Scott 1997)
 6.00; 5.10 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)

Sorption Partition Coefficient, $\log K_{OM}$:

5.05, 5.09 (quoted, calculated-MCI χ , Sabljic 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Photooxidation: calculated room temp. rate constant for hexachlorobiphenyls is $(0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas-phase reaction with OH radicals, the tropospheric lifetime is calculated to be $29\text{--}60 \text{ d}$ (Kwok et al. 1996).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 4970 \text{ d}^{-1}$; $k_2 = 0.00843 \text{ d}^{-1}$ (22°C , zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 75 \text{ d}$ and $k_2 = 0.012 \text{ d}^{-1}$ with $t_{1/2} = 59 \text{ d}$ for food concn of 8 ng/g and 99 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 146 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 205 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of $29\text{--}90 \text{ d}$ based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

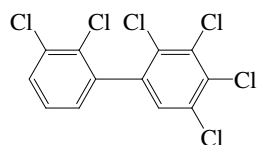
Soil:

Biota: $t_{1/2} > 1000 \text{ d}$ in rainbow trout, and $t_{1/2} = 89 \text{ d}$ in its muscle (Niimi & Oliver 1983).

Depuration $t_{1/2} = 59\text{--}75 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 146 \text{ d}$ for high-dose treatment, $t_{1/2} = 205 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

7.1.1.129 2,2',3,3',4,5-Hexachlorobiphenyl (PCB-129)



Common Name: 2,2',3,3',4,5-Hexachlorobiphenyl

Synonym: PCB-129, 2,2',3,3',4,5-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5-hexachlorobiphenyl

CAS Registry No: 55215-18-4

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

85 (Mackay et al. 1980; Bruggeman et al. 1982; Burkhard et al. 1985a; Opperhuizen et al. 1988; Brodsky & Ballschmiter 1988; Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.3482

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point,)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.256 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00085 (generator column-GC/ECD, Weil et al. 1974)

0.0117 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00150, 0.00198, 0.000688, 0.00169 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00582 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.76×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)

0.00208 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

4.68×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4816/(T/K) + 12.80$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

39.52 (calculated-P/C, Burkhard et al. 1985b)

8.61 (calculated-MCI χ , Sabljic & Güsten 1989)

2.94 (wetted-wall column-GC, Brunner et al. 1990)

14.18 (calculated-QSPR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18\ kJ/mol$, $\Delta S_H = 0.23 \pm 0.06\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.50 (HPLC-RT correlation, Rapaport & Eisenreich 1984)

6.71, 6.71, 6.90, 6.71 (RP-HPLC- k' correlations, Brodsky & Ballschmiter 1988)

6.94, 6.70; 6.81, 6.83 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

- 6.76 (recommended, Sangster 1993)
 7.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.80 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.42 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.259 (marine humic substance, calculated-MCI χ , reported as association coefficient $\log K_h$ at 5 mg/L DOC, Sabljic 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 156 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 166 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

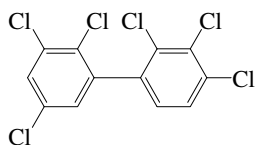
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 156 \text{ d}$ for high-dose treatment, $t_{1/2} = 166 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.130 2,2',3,3',4,5'-Hexachlorobiphenyl (PCB-130)



Common Name: 2,2',3,3',4,5'-Hexachlorobiphenyl

Synonym: PCB-130, 2,2',3,3',4,5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5'-hexachlorobiphenyl

CAS Registry No: 52663-66-8

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

96 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0168 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00569 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

5.35×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

5.92×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

1.61×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

4.17×10^{-4} , 5.75×10^{-4} (supercooled liquid P_L ; GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4816/(T/K) + 12.89$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

11.55 (calculated-P/C, Burkhard 1984)

10.84 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

19.45 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

3.75 (wetted wall column-GC/ECD, Brunner et al. 1990)

15.44 (calculated-QSPR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18\ kJ/mol$, $\Delta S_H = 0.23 \pm 0.06\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.57, 7.39 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapport & Eisenreich 1984)

6.98, 7.15; 6.79, 6.78 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.12 (recommended, Sangster 1993)

7.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.98 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.47 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 184 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 153 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

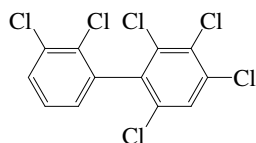
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 184 \text{ d}$ for high-dose treatment, $t_{1/2} = 153 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.131 2,2',3,3',4,6-Hexachlorobiphenyl (PCB-131)



Common Name: 2,2',3,3',4,6-Hexachlorobiphenyl

Synonym: PCB-131, 2,2',3,3',4,6-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,6-hexachlorobiphenyl

CAS Registry No: 61798-70-7

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

122 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0151 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.01212 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00120 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.62×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00285 (GC-RI correlation, Burkhard et al. 1985b)

0.00126, 0.0107 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.63×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

6.92×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4681/(T/K) + 12.80$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

62.82 (calculated-P/C, Burkhard 1984)

6.59 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

26.24 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

3.95 (wetted wall column-GC/ECD, Brunner et al. 1990; quoted, Achman et al. 1993)

24.53 (calculated-QSPR, Dunnivant et al. 1992)

68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.78 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.97, 6.38; 6.41, 6.44 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.78 (recommended, Sangster 1993)

6.82 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.92, 9.83 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)

10.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.51 (suspended particulate matter, Burkhard 1984)

5.100 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

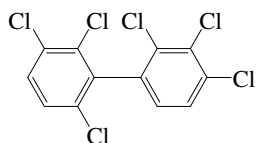
Ground water:

Sediment:

Soil:

Biota:

7.1.1.132 2,2',3,3',4,6'-Hexachlorobiphenyl (PCB-132)



Common Name: 2,2',3,3',4,6'-Hexachlorobiphenyl

Synonym: PCB-132, 2,2',3,3',4,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,6'-hexachlorobiphenyl

CAS Registry No: 38380-05-1

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

81 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0149 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00808 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00720 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.155×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.27×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

7.58×10^{-4} , 9.08×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

5.62×10^{-4} , 1.0×10^{-3} (supercooled liquid P_L : GC-RI correlations, different stationary phase, Fischer et al. 1992)

$\log(P_L/Pa) = -4681/(T/K) + 12.5$, (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

27.97 (calculated-P/C, Burkhard 1984)

16.31 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

4.46 (wetted wall column-GC/ECD, Brunner et al. 1990)

2.42 (calculated-QSPR, Achman et al. 1993)

20.55 (calculated-QSPR, Dunnivant et al. 1992)

16.6 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

59.4 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 61 \pm 7\ kJ/mol$, $\Delta S_H = 0.17 \pm 0.02\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.70 (HPLC-RT correlation, Shaw & Connell 1982)

6.20 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.09, 6.77; 6.63, 6.58 (multi-column-HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.20 (recommended, Sangster 1993)

7.04 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

11.16, 10.07; 9.96 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
9.76 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.52 (suspended particulate matter, Burkhard 1984)
5.10 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 136 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 147 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29-90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

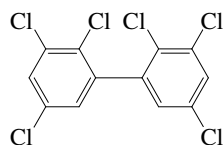
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 136 \text{ d}$ for high-dose treatment, $t_{1/2} = 147 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.133 2,2',3,3',5,5'-Hexachlorobiphenyl (PCB-133)



Common Name: 2,2',3,3',5,5'-Hexachlorobiphenyl

Synonym: PCB-133, 2,2',3,3',5,5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',5,5'-hexachlorobiphenyl

CAS Registry No: 35694-04-3

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

129 (Burkhard et al. 1985b)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0954 (mp at $129^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0149 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

4.37×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.98×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

8.24×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)

8.43×10^{-4} , 0.00110 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4816/(T/K) + 13.08$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

19.25 (calculated-P/C, Burkhard 1984)

33.84 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

20.64 (calculated-QSPR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.72 (calculated-TSA, Burkhard 1984)

6.86 (calculated-TSA, Hawker & Connell 1988a)

6.97, 7.02; 6.66, 6.60 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.63, 7.00 (quoted average values of GC-RV and HPLC- k' correlations of Risby et al. 1990, Sangster 1993)

7.07 (recommended, Hansch et al. 1995)

6.7470 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

7.69 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.57 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.52 (suspended particulate matter, Burkhard 1984)

5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

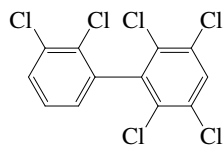
Ground water:

Sediment:

Soil:

Biota:

7.1.1.134 2,2',3,3',5,6-Hexachlorobiphenyl (PCB-134)



Common Name: 2,2',3,3',5,6-Hexachlorobiphenyl

Synonym: PCB-134, 2,2',3,3',5,6-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',5,6-hexachlorobiphenyl

CAS Registry No: 52704-70-8

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

100 (Mackay et al. 1980; Burkhard et al. 1985a; Kühne et al. 1995; Ruelle & Kesselring 1997)

132 (Ran et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.3482

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.181 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00091 (generator column-GC/ECD, Weil et al. 1973)

0.0081 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.46×10^{-4} (calculated-S \times HLC, Burkhard et al. 1985a)

0.00246 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

4.83×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)

0.00127, 0.00185 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.60×10^{-4} ($20^{\circ}C$, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log(P/mmHg) = 11.30 - 4940/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

7.41×10^{-4} , 1.32×10^{-3} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4681/(T/K) + 12.79$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

57.76 (Murphy et al. 1983)

55.53 (calculated-P/C, Burkhard et al. 1985b)

9.83 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

20.67 (calculated-QSPR MCI χ , Sabljic & Güsten 1989)

4.96 (wetted-wall column-GC/ECD, Brunner et al. 1990)

32.27 (calculated-QSPR, Dunnivant et al. 1992)

25.6 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

68.0 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 6\ kJ/mol$, $\Delta S_H = 0.13 \pm 0.02\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.81 (generator column-GC/ECD, Doucette & Andren 1987)
- 6.20 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
- 6.22, 6.43; 6.40, 6.44 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.20 (recommended, Sangster 1993)
- 6.91 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.80, 9.71 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
- 9.72 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:Sorption Partition Coefficient, $\log K_{OC}$:

- 6.49 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 5.18, 5.16, 5.15, 4.41 (humic substances, in concentrations of 5, 10, 20, 40 mg C/L, reported as $\log K_h$, Lara & Ernst 1989)
- 5.18, 5.10 (marine humic substances, quoted, calculated-MCI χ , reported as $\log K_h$ at 5 mg/L DOC, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, and Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

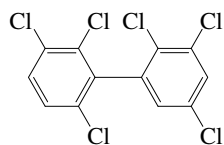
Groundwater:

Sediment:

Soil:

Biota:

7.1.1.135 2,2',3,3',5,6'-Hexachlorobiphenyl (PCB-135)



Common Name: 2,2',3,3',5,6'-Hexachlorobiphenyl

Synonym: PCB-135, 2,2',3,3',5,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',5,6'-hexachlorobiphenyl

CAS Registry No: 52744-13-5

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

102 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0133 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.01294 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00546 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00361 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00188 (GC-RI correlation, Burkhard et al. 1985b)

0.00115, 0.00184 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

5.07×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.000741, 0.00132 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4861/(T/K) + 12.76$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

46.81 (calculated-P/C, Burkhard 1984)

14.19 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

30.8 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

5.67 (wetted wall column-GC/ECD, Brunner et al. 1990)

27.21 (calculated-QSPR, Dunnivant et al. 1992)

26.8 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

69.0 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 45 \pm 3$ kJ/mol, $\Delta S_H = 0.12 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.94, 7.15 (RP-HPLC- k' correlation: uncorrected; with ortho correction, Rapaport & Eisenreich 1984)

6.32 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.97, 6.95; 6.41, 6.40 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

- 6.32 (recommended, Sangster 1993)
 7.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.78, 9.69 (0, 20°C, multicolumn GC-k' correlation, Zhang et al. 1999)
 9.71 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.57 (suspended particulate matter, Burkhard 1984)
 5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 159 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 192 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

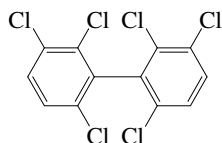
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 159 \text{ d}$ for high-dose treatment, $t_{1/2} = 192 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.136 2,2',3,3',6,6'-Hexachlorobiphenyl (PCB-136)



Common Name: 2,2',3,3',6,6'-Hexachlorobiphenyl

Synonym: PCB-136, 2,2',3,3',6,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',6,6'-hexachlorobiphenyl

CAS Registry No: 38411-22-2

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

112.05 (differential scanning calorimetry, Miller et al. 1984)

114.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.21 (differential scanning calorimetry, Miller et al. 1984)

21.10 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

54.81 (Miller et al. 1984)

Fugacity Ratio at $25^{\circ}C$, F :

0.138 (calculated, assuming $\Delta S_{fus} = 56\ J/mol\ K$, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00099 (shake flask-GC/ECD, Dexter & Pavlou 1978)

0.00603 (generator column-GC/ECD, Miller et al. 1984)

0.00451* (generator column-GC/ECD, measured range $4-32^{\circ}C$, Dickhut et al. 1986)

1.10×10^{-3} , 3.25×10^{-3} , 4.51×10^{-3} , 6.68×10^{-3} ($4, 20, 25, 32^{\circ}C$, generator column-GC/ECD, Dickhut et al. 1986)

$\ln x = -5484.72/(T/K) - 3.8682$; temp range $4-32^{\circ}C$, $\Delta H_{ss} = 45.6\ kJ/mol$ (generator column-GC/ECD, Dickhut et al. 1986)

$\log x = -2378/(T/K) - 1.679$, $\Delta H_{ss} = 45.5\ kJ/mol$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or

$S/(mol/L) = 2.39 \times 10^{-9} \exp(0.065 \cdot t/^{\circ}C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)

0.0202 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\ln x = -3.880235 - 5471.2/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.000531 (GC-RI correlation, Burkhard et al. 1985a)

0.00374 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

0.00156, 0.00292 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

0.00127 ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00158, 0.00331 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = -4303/(T/K) + 11.63$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

- 93.22 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)
- 22.79 (20°C, calculated-P/C, Murphy et al. 1987)
- 25.54 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
- 8.92 (wetted-wall column-GC/ECD, Brunner et al. 1990)
- 32.64 (calculated-QSPR, Dunnivant et al. 1992)
- 45.4 (11°C, gas stripping-GC/ECD, Bamford et al. 2002)
- 81.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
- $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, log K_{OW}:

- 8.35 (Hansch & Leo 1979)
- 6.81 (generator column-HPLC, Woodburn et al. 1984)
- 6.63 (generator column-GC/ECD, Miller et al. 1984)
- 4.91 (RP-HPLC-RT correlation, Rapaport & Eisenreich 1984)
- 5.48 (HPLC-RP/MS correlation, Burkhard et al. 1985c)
- 6.81 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
- 5.76 (generator column-GC/ECD, Hawker & Connell 1988a)
- 7.118 ± 0.034 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens)
- 7.18 (calculated- π const., De Bruijn et al. 1989)
- 6.63, 6.30; 6.30, 6.24 (multi-column HPLC-k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 7.50 (calculated-UNIFAC activity coefficient, Dallos et al. 1993)
- 6.54 (recommended, Sangster 1993)
- 7.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

- 10.59, 9.53; 9.58 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- 9.51 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF at 25°C or as indicated:

- 0.86 (poultry, Garten & Trabalka 1983)
- 5.43; 6.96 (22°C, zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
- 5.43, 6.96 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC}:

- 6.53 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
- 6.53 (suspended solids, 0.7 mg/L, 43.2% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
- 5.68 (suspended solids, 6.5 mg/L, 14.8% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
- 4.95, 5.05, 4.95, 4.27 (marine humic substances in concentrations of 5, 10, 20, 40 mg L of DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
- 4.952, 4.942 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h. Observed; calculated-MCI χ , Sabljic et al. 1989)
- 6.01, 6.06, 5.90 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
- 6.04 (5.73–6.35) (sediment: organic carbon OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: 18% at 24 h and 33% degradation at 72 h in one of the PCB mixture including congeners ranging from di- to hexa-PCBs with several structure classes, by microorganism *Alcaligenes eutrophus* H850 (Bedard et al. 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 4390 \text{ d}^{-1}$; $k_2 = 0.0181 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 132 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 144 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{1/2} = 15.0 \text{ min}$ when irradiated in a TiO_2 semiconductor aqueous suspensions with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996)

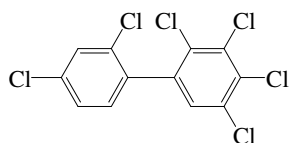
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 132 \text{ d}$ for high-dose treatment, $t_{1/2} = 144 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.137 2,2',3,4,4',5-Hexachlorobiphenyl (PCB-137)



Common Name: 2,2',3,4,4',5-Hexachlorobiphenyl

Synonym: PCB-137, 2,2',3,4,4',5-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',5-hexachlorobiphenyl

CAS Registry No: 35694-06-5

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

78.0 (Burkhard et al. 1985b)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.302 (mp at $78^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0158 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0084 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

9.94×10^{-4} , 1.12×10^{-3} , 7.54×10^{-4} , 1.69×10^{-3} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

1.71×10^{-3} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.41×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

7.83×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

1.50×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

3.80×10^{-4} , 3.02×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4816/(T/K) + 12.61$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

55.02 (calculated-P/C, Burkhard 1984)

6.89 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

21.08 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

18.82 (calculated-QSPR, Dunnivant et al. 1992)

3.13 (calculated-QSPR, Achman et al. 1993)

13.0 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

55.0 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 69 \pm 8$ kJ/mol, $\Delta S_H = 0.20 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

> 6.89, > 7.71 (RP-HPLC- k' correlation; uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

7.46 (HPLC-RT correlation, De Kock & Lord 1987)

- 6.84, 6.87, 6.88, 6.71 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 6.97, 7.06; 6.82, 6.78 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
 6.83 (recommended, Sangster 1993)
 7.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.89 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.49 (suspended particulate matter, Burkhard 1984)
 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)
 6.30 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 5.94 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 186 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 191 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

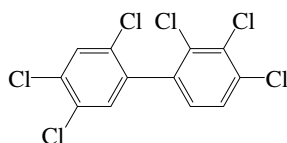
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 186 \text{ d}$ for high-dose treatment, $t_{1/2} = 191 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.138 2,2',3,4,4',5'-Hexachlorobiphenyl (PCB-138)



Common Name: 2,2',3,4,4',5'-Hexachlorobiphenyl

Synonym: PCB-138, 2,2',3,4,4',5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',5'-hexachlorobiphenyl

CAS Registry No: 35065-28-2

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

79 (Hutzinger et al. 1974; Brodsky & Ballschmiter 1988)

80.5 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986)

247.4 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.286 (calculated, assuming $\Delta S_{fus} = 56\ J/mol\ K$, Mackay et al. 1992)

0.285 (calculated- ΔS_{fus} and mp, Passivirta et al. 1995)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0159 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.00729 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00173, 0.00158, 0.00122, 0.0015 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00181 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.0024 (calculated-MCI χ , Patil 1991)

0.00151 (calculated-QSPR, Dunnivant et al. 1992)

0.00268 (calculated-group contribution method, Kühne et al. 1995)

0.00268, 0.0072 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

$\log [S_L/(mol/L)] = -1.12 + 1403/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

6.57×10^{-3} (calculated-mp and K_{ow} , Ran et al. 2002)

7.51×10^{-3} ; 6.75×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)

$\log [S_L/(mol\ m^{-3})] = -1437/(T/K) + 0.093$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

5.06×10^{-4} , 5.65×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Bidleman 1984)

1.58×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)

4.87×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

5.10×10^{-4} , 4.96×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

5.33×10^{-4} (quoted average value from Bidleman 1984, Erickson 1986)

1.47×10^{-4} ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

$\log (P/mmHg) = 11.60 - 5040/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

3.31×10^{-4} , 4.90×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)
 $\log (P_L/Pa) = -4800/(T/K) + 12.81$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)
 3.63×10^{-4} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
 1.47×10^{-4} ; 5.14×10^{-4} (solid, supercooled liquid, Passivirta et al. 1999)
 $\log (P_S/Pa) = 15.76 - 5842/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/Pa) = 12.81 - 4800/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 5.37×10^{-4} ; 5.62×10^{-4} (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log (P_L/Pa) = -5034/(T/K) + 13.62$ (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
 $\log (P_L/Pa) = -4770/(T/K) + 12.75$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

48.64 (calculated-P/C, Murphy et al. 1983)
 11.04 (calculated-P/C, Burkhard et al. 1985b)
 7.60 (20°C, calculated-P/C, Murphy et al. 1987)
 10.84 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)
 2.13 (wetted-wall column-GC, Brunner et al. 1990)
 69.0 (Wittlinger & Ballschmiter 1990)
 13.17 (calculated-QSPR, Dunnivant et al. 1992)
 $\log [H/(Pa \text{ m}^3/\text{mol})] = 13.93 - 3757/(T/K)$ (Passivirta et al. 1999)
 44.6* ± 1.7 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
 $\ln K_{AW} = 31.152 - 10476.3/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
 $K_{AW} = \exp[-(87.1/\text{kJ}\cdot\text{mol}^{-1})/RT + (0.259/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R]$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
 45.2 (from 11°C exptl. data and compensation point, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 87 \pm 7 \text{ kJ/mol}$, $\Delta S_H = 0.26 \pm 0.03 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004
 39.81, 30.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
 $\log [H/(Pa \text{ m}^3/\text{mol})] = -4672/(T/K) + 17.27$ (LDV linear regression of literature data, Li et al. 2003)
 $\log [H/(Pa \text{ m}^3/\text{mol})] = -3332/(T/K) + 12.66$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.90 (HPLC-RT correlation, Shaw & Connell 1982)
 6.62, 7.44 (RP-HPLC-RT correlation Rapaport & Eisenreich 1984)
 6.67, 6.77, 6.73, 6.74 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 7.04, 6.80; 6.84, 6.79 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
 6.42 (average, generator column-GC, Larsen et al. 1992)
 6.92 (recommended, Sangster 1993)
 7.25 (recommended, Hansch et al. 1995)
 7.00, 7.22 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

10.09* (20°C, generator column-GC, measured range -10 to 30°C, Harner & Bidleman 1996)
 $\log K_{OA} = -5.57 + 4584/(T/K)$; temp range -10 to 30°C (generator column-GC, Harner & Bidleman 1996)
 9.51; 9.12 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
 $\log K_{OA} = -5.17 + 4380/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
 10.62 (10°C, estimated, Thomas et al. 1998)
 11.34, 10.20; 10.18 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 10.09 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
 9.76, 9.66 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log K_{OA} = 4509/(T/K) - 5.37$ (LDV linear regression of literature data, Li et al. 2003)

$\log K_{OA} = 4510/(T/K) - 5.47$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF:

5.88; 7.41 (zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)

3.31–5.47 (various marine species, mean dry wt. BCF, Hope et al. 1998)

4.79–5.96 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

5.88, 7.42 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

5.42, 7.48 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Partition Coefficient between particulate and dissolved contaminant concentrations, log K_p or log K_d

5.80, 5.30 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

5.70 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

5.52–5.89 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

6.49 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)

5.8–7.3, 6.6 (suspended sediment, average, Oliver 1987a)

7.60 (algae > 50 µm, Oliver 1987a)

6.65 (Lake Michigan water column, Swackhamer & Armstrong 1987)

5.21, 5.22, 5.17, 4.60 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)

5.207, 5.241 (marine humic substances, quoted, calculated-MCI χ, reported as log K_h at 5 mg/L DOC, Sabljic et al. 1989)

5.93 (soil from Ispra, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)

6.50 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

6.50 (soil, calculated-K_{OW}, Girvin & Scott 1997)

6.04–7.28; 5.80–7.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)

5.51; 6.28, 6.78, 6.41 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

6.27–7.44 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: photodegradation rate constant k = (0.08 ± 0.01) h⁻¹ with t_{1/2} = 8.2 h in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO₃ radical and k_{O3} with O₃ or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (0.16–0.5) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime τ(calc) = 29–60 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

k₁ = 0.049 h⁻¹; k₂ = 0.008 h⁻¹ (mayfly-sediment model II, Gobas et al. 1989)

k₁ = 4770 d⁻¹; k₂ = 0.00624 d⁻¹ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

k₂ = 0.0344 d⁻¹ with an elimination t_{1/2} = 20.2 d (earthworm, Belfroid et al. 1995)

k₂ = 0.005 d⁻¹ with t_{1/2} = 139 d and k₂ = 0.011 d⁻¹ with t_{1/2} = 64 d for food concn of 31 ng/g and 176 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

k₁ = 0.00226 h⁻¹; k₂ = 0.145 h⁻¹ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_1(\text{calc}) = 5 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2(\text{calc}) = 0.05 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 186 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 191 \text{ d}$ (8°C , juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995);

$t_{1/2} = 6000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photodegradation $t_{1/2} = (8.2 \pm 0.3) \text{ h}$ in aqueous solution with the presence of diethylamine after exposure to simulated sunlight (Lin et al. 1995);

$t_{1/2} = 120000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{1/2} = 19\text{--}25 \text{ yr}$ (Geyer et al. 2000)

$t_{1/2} = 165000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2} = 165000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2}$ = of 20.d from earthworm (Belfroid et al. 1995)

Depuration $t_{1/2} = 64\text{--}139 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$t_{1/2} = 4.8 \text{ h}$ in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination $t_{1/2} = 13 \text{ d}$ in earthworm given contaminated food (predicted, Wågman et al. 2001)

depuration $t_{1/2} = 186 \text{ d}$ for high-dose treatment, $t_{1/2} = 191 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C , juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.138.1
Reported Henry's law constants and octanol-air partition coefficients of 2,2',3,4,4',5'-hexachlorobiphenyl (PCB-138) at various temperatures and temperature dependence equations

Henry's law constant		log K _{OA}					
Bamford et al. 2000		Harner & Bidleman 1996		Kömp & McLachlan 1997		Zhang et al. 1999	
gas stripping-GC/MS		generator column-GC		fugacity meter-GC/MS		multicolumn-GC-k' correlation	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}	t/°C	log K _{OA}	t/°C	log K _{OA}
4	2.88	−10	11.81	25	9.51	0	11.34
11	7.50	0	11.27			20	10.20
18	18.68	10	10.61				
25	44.6	20	10.09	log K _{OA} = A + B/T			
31	91.1	30	9.53	A	−5.17		
				B	4380		
				temp range 10–43°C			
enthalpy, entropy change:		ΔH _{OA} /(kJ mol ^{−1}) = 87.77					
ΔH/(kJ·mol ^{−1}) = 87.1 ± 7.4		log K _{OA} = A + B/T					
ΔS/(J·mol ^{−1} ·K ^{−1}) = 259 ± 26		A	−5.568				
		B	4584				
ln K _{AW} = −ΔH/RT + ΔS/R							
eq. 1	K _{AW}						
A	31.1523						
B	10476						

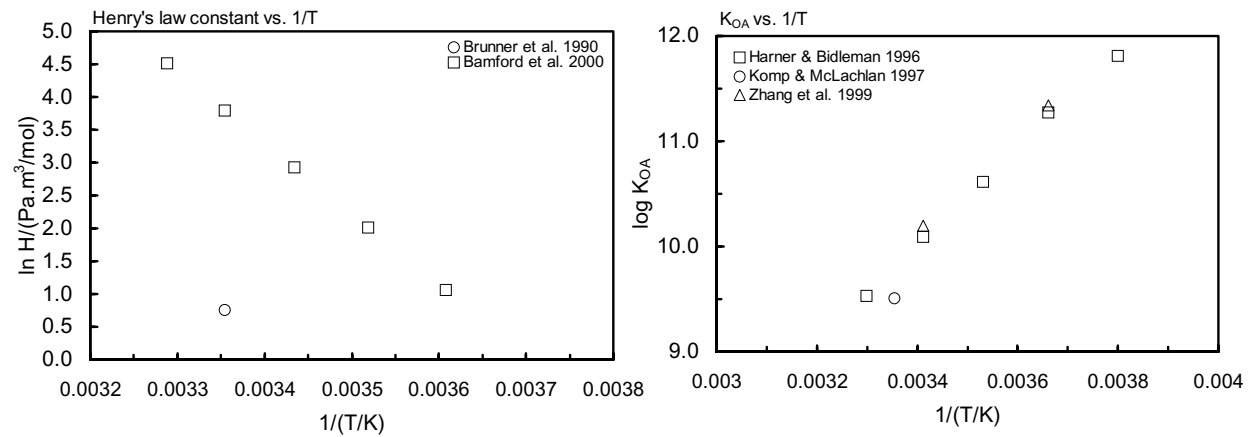
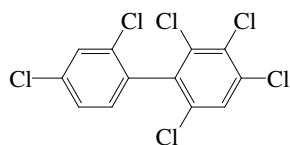


FIGURE 7.1.1.138.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,2',3,4,4',5'-hexachlorobiphenyl (PCB-138).

7.1.1.139 2,2',3,4,4',6-Hexachlorobiphenyl (PCB-139)



Common Name: 2,2',3,4,4',6-Hexachlorobiphenyl

Synonym: PCB-139

Chemical Name: 2,2',3,4,4',6-hexachlorobiphenyl

CAS Registry No: 56030-56-9

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

123 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0126 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.05×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

2.65×10^{-3} , 3.30×10^{-3} , 2.33×10^{-4} (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

1.26×10^{-3} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4681/(T/K) + 12.78$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

87.24 (calculated-P/C, Burkhard 1984)

38.60 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

33.32 (calculated-QSPR, Dunnivant et al. 1992)

68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.79 (calculated-TSA, Burkhard 1984)

6.67 (calculated-TSA, Hawker & Connell 1988a)

7.12, 6.68; 6.54, 6.50 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.70 (recommended, Sangster 1993)

6.95 (recommended, Hansch et al. 1995)

6.6419 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.17 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

6.59 (suspended particulate matter, Burkhard 1984)

5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

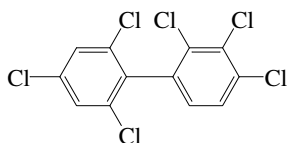
Ground water:

Sediment:

Soil:

Biota:

7.1.1.140 2,2',3,4,4',6'-Hexachlorobiphenyl (PCB-140)



Common Name: 2,2',3,4,4',6'-Hexachlorobiphenyl

Synonym: PCB-140, 2,2',3,4,4',6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',6'-hexachlorobiphenyl

CAS Registry No: 59291-64-4

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

123 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0125 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00314, 0.00203, 0.0015, 0.00194 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00325 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$):

1.26×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00138 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa- m^3/mol at $25^{\circ}C$):

36.38 (calculated-P/C, Burkhard 1984)

43.06 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

31.17 (calculated-QSAR, Dunnivant et al. 1992)

68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.79 (calculated-TSA, Burkhard 1984)

6.48, 6.70, 6.47, 6.66 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.67 (calculated-TSA, Hawker & Connell 1988a)

7.01, 6.86; 6.56, 6.51 (multicolumn HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.58 (recommended, Sangster 1993).

6.97 (recommended, Hansch et al. 1995)

6.4851 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

6.59 (suspended particulate matter, Burkhard 1984)

5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calc-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

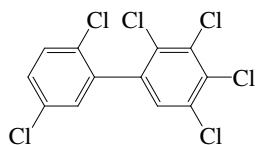
Ground water:

Sediment:

Soil:

Biota:

7.1.1.141 2,2',3,4,5,5'-Hexachlorobiphenyl (PCB-141)



Common Name: 2,2',3,4,5,5'-Hexachlorobiphenyl

Synonym: PCB-141, 2,2',3,4,5,5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,5,5'-hexachlorobiphenyl

CAS Registry No: 52712-04-6

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

85 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.258 (mp at $85^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0160 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00755 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00109, 0.00150, 0.00134, 0.00165 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.0025 (calculated-group contribution method, Kühne et al. 1995)

0.00244, 0.00642 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.73×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00295 (GC-RI correlation, Burkhard et al. 1985b)

2.05×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 11.50 - 5080/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

5.01×10^{-4} , 6.46×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4816/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

61.5 (calculated-P/C, Burkhard 1984)

9.83 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

14.49 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

2.33 (wetted wall column-GC/ECD, Brunner et al. 1990)

17.61 (calculated-QSPR, Dunnivant et al. 1992)

6.54 (calculated-QSPR, Achman et al. 1993)

12.7 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

54.5 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 70 \pm 7$ kJ/mol, $\Delta S_H = 0.20 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 6.69 (calculated-TSA, Burkhard 1984)
- 6.80, 6.79, 6.79, 6.71 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.82 (calculated-TSA, Hawker & Connell 1988a)
- 6.98, 7.02; 6.78, 6.73 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.75 (recommended, Sangster 1993)
- 9.538 (calculated-UNIFAC group contribution, Chen et al. 1993)
- 7.19 (recommended, Hansch et al. 1995)
- 7.10, 6.64–6.89 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
- 6.70 (estimated, Girvin & Scott 1997)
- 6.8226 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.55 (10°C, estimated, Thomas et al. 1998)
- 11.18, 10.07; 10.13 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 9.87 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.81; 7.34 (zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.80, 5.10 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.49 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.05 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
- 6.20 (soil-organic carbon, calculated- K_{ow} , Girvin & Scott 1997)
- 6.02 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_1 = 4910 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
- $k_2 = 0.00764 \text{ d}^{-1}$ (22°C, zebrafish, 30-d clearance, Fox et al. 1994)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 171 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 198 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

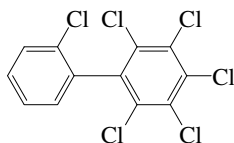
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 171$ d for high-dose treatment, $t_{1/2} = 198$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.142 2,2',3,4,5,6-Hexachlorobiphenyl (PCB-142)



Common Name: 2,2',3,4,5,6-Hexachlorobiphenyl

Synonym: PCB-142, 2,2',3,4,5,6-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,5,6-hexachlorobiphenyl

CAS Registry No: 41411-61-4

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

136.0 (Burkhard et al. 1985b)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0815 (mp at $136^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0171 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00361 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00138 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$):

3.41×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.000293 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

71.74 (calculated-P/C, Burkhard 1984)

21.18 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

31.89 (calculated-QSPR, Dunnivant et al. 1992)

68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.66 (calculated-TSA, Burkhard 1984)

6.51 (calculated-TSA, Hawker & Connell 1988)

6.94, 6.75; 6.56, 6.41 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.85 (recommended, Sangster 1993)

6.97 (recommended, Hansch et al. 1995)

6.5729 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.84 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.46 (suspended particulate matter, Burkhard 1984)
5.119 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16-0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

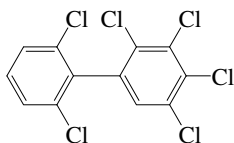
Ground water:

Sediment:

Soil:

Biota:

7.1.1.143 2,2',3,4,5,6'-Hexachlorobiphenyl (PCB-143)



Common Name: 2,2',3,4,5,6'-Hexachlorobiphenyl

Synonym: PCB-143, 2,2',3,4,5,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,5,6'-hexachlorobiphenyl

CAS Registry No: 68194-15-0

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

116 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0143 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00287, 0.00238, 0.00250, 0.00293 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.046×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

5.41×10^{-3} (P_L supercooled liquid values: GC-RI correlation, Burkhard et al. 1985b)

9.014×10^{-4} , 9.59×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

7.41×10^{-4} , 1.35×10^{-3} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4681/(T/K) + 12.65$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

127.7 (calculated-P/C, Burkhard 1984)

25.94 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

3.95 (wetted wall column-GC/ECD, Brunner et al. 1990)

29.83 (calculated-QSPR, Dunnivant et al. 1992)

68.8 (Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 9$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.74 (calculated-TSA, Burkhard 1984)

6.52, 6.65, 6.51, 6.55 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.60 (calculated-TSA, Hawker & Connell 1988)

6.89, 6.63; 6.51, 6.48 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

- 6.56 (recommended, Sangster 1993)
6.92 (recommended, Hansch et al. 1995)
6.545 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.64 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.54 (suspended particulate matter, Burkhard 1984)
5.100 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 3 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2 = 0.07 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

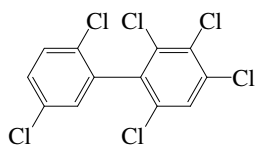
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 10 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.144 2,2',3,4,5',6-Hexachlorobiphenyl (PCB-144)



Common Name: 2,2',3,4,5',6-Hexachlorobiphenyl

Synonym: PCB-144, 2,2',3,4,5',6-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,5',6-hexachlorobiphenyl

CAS Registry No: 68194-14-9

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

110 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0126 (P_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.01294 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00353 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.45×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00371 (GC-RI correlation, Burkhard et al. 1985b)

5.07×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00166, 0.00105 (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4681/(T/K) + 12.70$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

98.23 (calculated-P/C, Burkhard 1984)

14.19 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

32.22 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

5.70 (calculated-QSPR, Achman et al. 1993)

29.97 (calculated-QSPR, Dunnivant et al. 1992)

68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.79 (calculated-TSA, Burkhard 1984)

6.45 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.67 (calculated-TSA, Hawker & Connell 1988a, 1990)

6.96, 6.68; 6.38, 6.29 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.45 (recommended, Sangster 1993)

6.79 (recommended, Hansch et al. 1995)

- 6.70 (estimated, Girvin & Scott 1997)
6.6482 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.73, 9.62; 9.62 (0, 20°C, multi-column GC-k' correlation; calc at 20°C, Zhang et al. 1999)
10.15 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.59 (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)
6.20 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 137 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 184 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

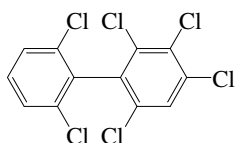
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 137 \text{ d}$ for high-dose treatment, $t_{1/2} = 184 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.145 2,2',3,4,6,6'-Hexachlorobiphenyl (PCB-145)



Common Name: 2,2',3,4,6,6'-Hexachlorobiphenyl

Synonym: PCB-145, 2,2',3,4,6,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,6,6'-hexachlorobiphenyl

CAS Registry No: 74472-40-5

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

84 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0137 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.36×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00681 (GC-RI correlation, Burkhard et al. 1985b)

0.00309 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4303/T + 11.90$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

168.2 (calculated-P/C, Burkhard 1984)

41.34 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

46.61 (calculated-QSPR, Dunnivant et al. 1992)

81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5\ kJ/mol$, $\Delta S_H = 0.06 \pm 0.02\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.76 (calculated-TSA, Burkhard 1984)

6.25 (calculated-TSA, Hawker & Connell 1988a)

6.92, 6.59; 6.30, 6.26 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phase, Risby et al. 1990)

6.28, 6.78 (quoted average values of Risby et al. 1990, Sangster 1993)

6.71 (recommended, Hansch et al. 1995)

6.2606 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.94 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.56 (suspended particulate matter, Burkhard 1984)
4.942 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

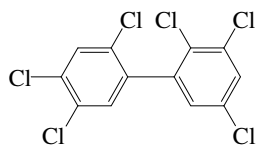
Ground water:

Sediment:

Soil:

Biota:

7.1.1.146 2,2',3,4',5,5'-Hexachlorobiphenyl (PCB-146)



Common Name: 2,2',3,4',5,5'-Hexachlorobiphenyl

Synonym: PCB-146, 2,2',3,4',5,5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',5,5'-hexachlorobiphenyl

CAS Registry No: 51908-16-8

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

90 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00759 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00095 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00228 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.28×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.000801 (GC-RT correlation, Burkhard et al. 1985b)

7.73×10^{-4} , 9.614×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.87×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

6.31×10^{-4} , 8.51×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4816/(T/K) + 13.04$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

18.54 (calculated-P/C, Burkhard 1984)

8.92 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

25.23 (calculated-QSAR- MCI χ , Sabljic & Güsten 1989)

2.53 (wetted wall column-GC/ECD, Brunner et al. 1990; quoted, Achman et al. 1993)

19.0 (calculated-QSPR, Dunnivant et al. 1992)

17.8 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

60.7 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 59 \pm 7$ kJ/mol, $\Delta S_H = 0.17 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.74 (calculated-TSA, Burkhard 1984)

6.85 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.89 (calculated-TSA, Hawker & Connell 1988a)

- 7.02, 7.08; 6.71, 6.71 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
 6.57 (generator column-GC, Larsen et al. 1992)
 6.85 (recommended, Sangster 1993)
 7.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.96, 9.84 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 9.97 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Partition Coefficient between particulate and dissolved contaminant concentrations, $\log K_p$ or $\log K_d$

- 5.80, 5.30 (Lake Superior suspended solids, concn ratio-GC/ECD, Baker et al. 1986)
 5.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.54 (suspended particulate matter, Burkhard 1984)
 5.40 (Lake Superior suspended solids, GC/ECD, Baker et al. 1986)
 5.18, 5.22, 5.14, 4.58 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
 5.18; 5.22 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)
 5.87 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
 6.20 (colloids and micro-particulates from precipitation events, Murray & Andren 1992)
 6.20 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)
 6.01 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 166 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 216 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

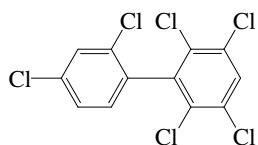
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 166 \text{ d}$ for high-dose treatment, $t_{1/2} = 216 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.147 2,2',3,4',5,6-Hexachlorobiphenyl (PCB-147)



Common Name: 2,2',3,4',5,6-Hexachlorobiphenyl

Synonym: PCB-147, 2,2',3,4',5,6-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',5,6-hexachlorobiphenyl

CAS Registry No: 68194-13-8

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

116 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0134 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.86×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00309 (GC-RI correlation, Burkhard et al. 1985b)

$\log(P/mmHg) = 11.20 - 4910/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

77.21 (calculated-P/C, Burkhard 1984)

32.63 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

5.17 (wetted wall column-GC/ECD, Brunner et al. 1990)

31.97 (calculated-QSPR, Dunnivant et al. 1992)

5.70 (calculated-QSPR, Achman et al. 1993)

68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8\ kJ/mol$, $\Delta S_H = 0.13 \pm 0.02\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.77 (calculated-TSA, Burkhard 1984)

6.64 (calculated-TSA, Hawker & Connell 1988a)

7.07, 6.73, 6.52, 6.51 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.52, 6.90 (quoted average values of Risby et al. 1990, Sangster 1993)

6.93 (recommended, Hansch et al. 1995)

6.6069 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

10.79, 9.672 (0, $20^{\circ}C$, multi-column GC- k' correlation, Zhang et al. 1999)

9.70 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.57 (suspended particulate matter, Burkhard 1984)
5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 194 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.002 \text{ d}^{-1}$ with $t_{1/2} = 283 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

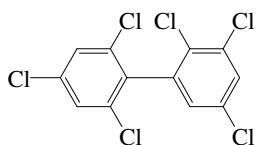
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 194 \text{ d}$ for high-dose treatment, $t_{1/2} = 283 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.148 2,2',3,4',5,6'-Hexachlorobiphenyl (PCB-148)



Common Name: 2,2',3,4',5,6'-Hexachlorobiphenyl

Synonym: PCB-148, 2,2',3,4',5,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',5,6'-hexachlorobiphenyl

CAS Registry No: 74472-42-7

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

104 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0112 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0369 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00287 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.87×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00204 (GC-RI correlation, Burkhard et al. 1985b)

0.00190, 0.00277 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4681/(T/K) + 12.98$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

60.69 (calculated-P/C, Burkhard 1984)

57.65 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

43.52 (calculated-QSPR, Dunnivant et al. 1992)

68.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 47 \pm 8$ kJ/mol, $\Delta S_H = 0.13 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.84 (calculated-TSA, Burkhard 1984)

5.74 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.73 (calculated-TSA, Hawker & Connell 1988a)

7.04, 6.74; 6.46, 6.44 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

5.74 (recommended, Sangster 1993)

6.87 (recommended, Hansch et al. 1995)

6.6291 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.51 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.64 (suspended particulate matter, Burkhard 1984)

5.064 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

5.707 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

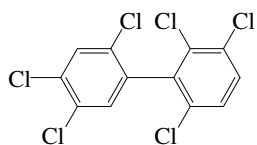
Ground water:

Sediment:

Soil:

Biota:

7.1.1.149 2,2',3,4',5',6-Hexachlorobiphenyl (PCB-149)



Common Name: 2,2',3,4',5',6-Hexachlorobiphenyl

Synonym: PCB-149, 2,2',3,4',5',6-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',5',6-hexachlorobiphenyl

CAS Registry No: 38380-04-0

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 369.9

Melting Point ($^{\circ}C$):

oil (Erickson 1986)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0127 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.01217 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00414 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00454 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.124×10^{-3} , 1.83×10^{-3} (P_L supercooled liquid, GC-RT correlation, different stationary phases, Bidleman 1984)

1.57×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.72×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

0.00105, 0.00158 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.47×10^{-3} (P_L supercooled liquid, quoted average value of Bidleman 1984, Erickson 1986)

4.96×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

8.51×10^{-4} , 1.48×10^{-3} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4689/(T/K) + 12.78$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

44.79 (calculated-P/C, Burkhard 1984)

15.0 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

22.09 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

4.32 (calculated-QSPR, Achman et al. 1993)

24.03 (calculated-QSPR, Dunnivant et al. 1992)

0.682; 1.994 (0, $15^{\circ}C$, Hornbuckle et al. 1994)

25.9 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

68.4 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 7$ kJ/mol, $\Delta S_H = 0.12 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.70 (HPLC-RT correlation, Shaw & Connell 1982)

6.14, 7.28 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

- 6.79 (calculated-TSA, Burkhard 1984)
- 6.41 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
- 6.67 (calculated-TSA, Hawker & Connell 1988a)
- 7.02, 7.0; 6.45, 6.47 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.54 (generator column-GC, Larsen et al. 1992)
- 6.41 (recommended, Sangster 1993)
- 6.86 (recommended, Hansch et al. 1995)
- 6.4731 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

- 9.27; 8.68 (generator column; calculated- K_{OW}/K_{AW} , Kömp & McLachlan 1997a)
- $\log K_{OA} = -6.50 + 4700/(T/K)$, temp range 10–43°C (Kömp & McLachlan 1997a)
- 9.27 (quoted, Kömp & McLachlan 1997b)
- 10.83, 9.74; 9.80 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 9.78 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Biota Sediment Accumulation Factor, BSAF:

- 105 (trout, Niimi 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.59 (suspended particulate matter, Burkhard 1984)
- 5.083 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)
- 5.79 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
- 6.10 (colloids and micro-particulates from precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 0.00097 \text{ h}^{-1}$; $k_2 = 0.240 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 162 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 199 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

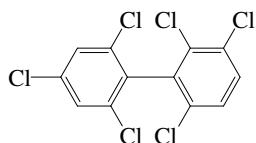
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 162 \text{ d}$ for high-dose treatment, $t_{1/2} = 199 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.150 2,2',3,4',6,6'-Hexachlorobiphenyl (PCB-150)



Common Name: 2,2',3,4',6,6'-Hexachlorobiphenyl

Synonym: PCB-150, 2,2',3,4',6,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',6,6'-hexachlorobiphenyl

CAS Registry No: 68194-08-1

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

104 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0121 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00907 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

4.07×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00438 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

121.6 (calculated-P/C, Burkhard 1984)

52.18 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

51.25 (calculated-QSPR, Dunnivant et al. 1992)

81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5$ kJ/mol, $\Delta S_H = 0.06 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.81 (calculated-TSA, Burkhard 1984)

6.32 (calculated-TSA, Hawker & Connell 1988a)

6.69; 6.59; 6.34, 6.27 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.64, 6.31 (quoted average values of Risby et al. 1990, Sangster 1993)

6.75 (recommended, Hansch et al. 1995)

6.1643 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.65 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.61 (suspended particulate matter, Burkhard 1984)
4.924 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

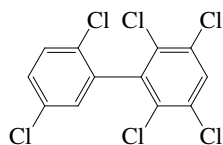
Ground water:

Sediment:

Soil:

Biota:

7.1.1.151 2,2',3,5,5',6-Hexachlorobiphenyl (PCB-151)



Common Name: 2,2',3,5,5',6-Hexachlorobiphenyl

Synonym: PCB-151, 2,2',3,5,5',6-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,5,5',6-hexachlorobiphenyl

CAS Registry No: 52663-63-5

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

101 (Burkhard et al. 1985b)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.180 (mp at $101^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0134 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.01355 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00454, 0.00414, 0.00487, 0.00337 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00720 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00223 (calculated-QSPR, Dunnivant et al. 1992)

0.00203 (calculated-group contribution method, Kühne et al. 1995)

0.00173, 0.00454 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.00559 (calculated-mp and K_{ow} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.32×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.16×10^{-3} , 1.67×10^{-4} , 2.23×10^{-4} (calculated-MW, GC-RI correlation, MCI χ , Burkhard et al. 1985b)

0.00177, 0.00255 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

5.97×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 11.30 - 4910/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

1.91×10^{-3} (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4681/(T/K) + 12.95$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

86.94 (calculated-P/C, Burkhard 1984)

15.91 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

52.18 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

5.98 (wetted wall column-GC/ECD, Brunner et al. 1990)

28.69 (calculated-QSPR, Dunnivant et al. 1992)

33.4 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

73.5 (from 11°C exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 37 \pm 5$ kJ/mol, $\Delta S_H = 0.10 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.76 (calculated-TSA, Burkhard 1984)

6.38, 6.49, 6.32, 6.51 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.64 (calculated-TSA, Hawker & Connell 1988a)

6.95, 7.35; 6.44, 6.43 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.45 (generator column-GC, Larsen et al. 1992)

6.43 (recommended, Sangster 1993)

6.85 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

10.08 (10°C, estimated, Thomas et al. 1998)

10.68, 9.58 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)

9.68 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

5.54; 7.07 (zebrafish: $\log BCF_W$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, $\log K_{OC}$:

6.56 (suspended particulate matter, Burkhard 1984)

5.03, 5.11, 5.09, 4.41 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)

5.031; 5.083 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, observed; calculated-MCI χ , Sabljic et al. 1989)

6.05, 6.05, 5.93 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

5.79 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)

4.99, 4.82; 4.85 (sediments from Brown's Lake, Helmet City Lake; WES reference soil, shake flask-HPLC/fluorescence, Brannon et al. 1995)

6.20 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

5.75 (4.96–6.18) (sediment: organic carbon OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60$ d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 4220$ d⁻¹; $k_2 = 0.0121$ d⁻¹ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.004$ d⁻¹ with $t_{1/2} = 174$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d⁻¹ with $t_{1/2} = 196$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

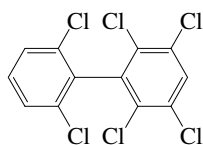
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 174$ d for high-dose treatment, $t_{1/2} = 196$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.152 2,2',3,5,6,6'-Hexachlorobiphenyl (PCB-152)



Common Name: 2,2',3,5,6,6'-Hexachlorobiphenyl

Synonym: PCB-152, 2,2',3,5,6,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',3,5,6,6'-hexachlorobiphenyl

CAS Registry No: 68914-09-2

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

111 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0145 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.0114 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

5.95×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00638 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

147.9 (calculated-P/C, Burkhard 1984)

35.57 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

43.32 (calculated-QSPR, Dunnivant et al. 1992)

81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5\ kJ/mol$, $\Delta S_H = 0.06 \pm 0.02\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.73 (calculated-TSA, Burkhard 1984)

6.22 (calculated-TSA, Hawker & Connell 1988a;)

6.86, 6.36; 6.10, 6.09 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.61, 6.10 (average values of Risby et al. 1990, Sangster 1993)

6.51 (recommended, Hansch et al. 1995)

6.2295 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.44 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.53 (suspended particulate matter, Burkhard 1984)
4.942 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16-0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

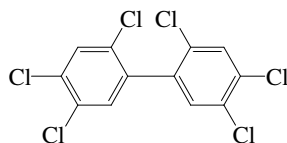
Ground water:

Sediment:

Soil:

Biota:

7.1.1.153 2,2',4,4',5,5'-Hexachlorobiphenyl (PCB-153)



Common Name: 2,2',4,4',5,5'-Hexachlorobiphenyl

Synonym: PCB-153, 2,2',4,4',5,5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',4,4',5,5'-hexachlorobiphenyl

CAS Registry No: 35065-27-1

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

103.5 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.90 (Opperhuizen et al. 1987; Ruelle et al. 1993)

17.50 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F :

0.169 (calculated, assuming $\Delta S_{fus} = 56\ J/mol\ K$, Mackay et al. 1980; Shiu & Mackay 1986)

0.167 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0088 (shake flask-GC/ECD, Wallnöfer et al. 1973)

0.0012 (generator column-GC/ECD, Weil et al. 1974)

9.53×10^{-4} (shake flask-GC/ECD, Haque & Schmedding 1975)

9.50×10^{-4} ($24^{\circ}C$, shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977)

0.00105 ($16.5^{\circ}C$, shake flask-GC/ECD, Wiese & Griffin 1978)

6.9×10^{-5} (calculated-UNIFAC activity coefficients, Banerjee 1985)

0.00914 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

8.86×10^{-4} , 9.4×10^{-4} , 1.34×10^{-3} , 1.5×10^{-3} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

5.28×10^{-5} (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)

6.60×10^{-4} (generator column-GC/ECD, Dunnivant & Elzerman 1988)

$8.45 \times 10^{-3*}$ (generator column-GC/ECD, measured range $4-40^{\circ}C$, Doucette & Andren 1988)

4.62×10^{-3} , 8.45×10^{-3} , 1.28×10^{-2} ($4, 25, 40^{\circ}C$, generator column-GC/ECD, Doucette & Andren 1988)

$S/(mol/L) = 1.15 \times 10^{-8} \exp(0.028 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range $4-40^{\circ}C$, Doucette & Andren 1988a); or

$\log x = -1059/(T/K) - 5.819$, temp range $4-40^{\circ}C$, $\Delta H_{ss} = 20.3\ kJ/mol$ (generator column-GC/ECD, Doucette & Andren 1988a)

0.00115 ($22^{\circ}C$, generator column-GC/ECD, Opperhuizen et al. 1988)

$\log [S_L/(mol/L)] = -1.20 - 1113/(T/K)$ (supercooled liquid S_L , Passivirta et al. 1999)

$\ln x = -13.37313 - 2445.3/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.0136, 0.0111 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Li et al. 2003)

$\log [S_L/(mol\ m^{-3})] = -1305/(T/K) + 0.14$ (supercooled liquid S_L , FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

- 6.80×10^{-4} , 7.19×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Bidleman 1984)
- 6.63×10^{-3} (supercooled liquid P_L , GC-RT correlation Burkhard 1984)
- 1.24×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)
- 6.63×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)
- 7.08×10^{-4} , 8.13×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
- 4.57×10^{-4} (supercooled liquid P_L , GC-RT correlation, Burkhard et al. 1985b)
- 1.19×10^{-4} ; 7.0×10^{-4} (selected values: solid P_S ; supercooled liquid P_L , Shiu & Mackay 1986)
- 2.53×10^{-4} (20°C, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)
- $\log(P/\text{mmHg}) = 11.40 - 5040/(T/K)$ (GC-RT correlation, Tateya et al. 1988)
- 7.0×10^{-4} (supercooled liquid P_L , Dunnivant & Elzerman 1988)
- 5.60×10^{-4} (Wittlinger & Ballschmiter 1990)
- 5.62×10^{-4} , 7.24×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)
- $\log(P_L/\text{Pa}) = -4775/(T/K) + 12.85$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)
- 3.63×10^{-4} (20°C, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
- 1.39×10^{-4} ; 8.34×10^{-4} (solid; supercooled liquid, Passivirta et al. 1999)
- $\log(P_S/\text{Pa}) = 15.80 - 5887/(T/K)$ (solid, Passivirta et al. 1999)
- $\log(P_L/\text{Pa}) = 12.85 - 4775/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
- $(3.20 - 124.0) \times 10^{-5}$; $(1.80 - 66.3) \times 10^{-4}$ (literature P_S range; literature P_L range, Delle Site 1997)
- 7.75×10^{-5} (estimated-EPIWIN v3.04, Hardy 2002)
- 5.25×10^{-4} ; 6.03×10^{-4} (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)
- $\log P_L/\text{Pa} = -4923/(T/K) + 13.24$ (supercooled liquid, linear regression of literature data, Li et al. 2003)
- $\log P_L/\text{Pa} = -4712/(T/K) + 12.59$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):

- 35.46 (calculated, Murphy et al. 1983)
- 12.46 (gas stripping-GC, Coates 1984)
- 17.93 (calculated-P/C, Burkhard et al. 1985b)
- 6.08 (20°C, batch stripping-GC, Oliver 1985)
- 42.9 (calculated-P/C, Shiu & Mackay 1986)
- 10.03 (20°C, calculated-P/C, Murphy et al. 1987)
- 13.37 (gas stripping-GC, Dunnivant & Elzerman 1988; Dunnivant et al. 1988)
- 50.34 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
- 2.33 (wetted-wall column-GC/ECD, Brunner et al. 1990)
- 16.70 (calculated-QSPR, Dunnivant et al. 1992)
- 13.98 ± 1.5 , 13.48 ± 1.2 (gas stripping-GC/ECD, purge vessel's height at 26-cm; 67-cm; Girvin et al. 1997)
- $\log[H/(\text{Pa m}^3/\text{mol})] = 14.05 - 3662/(T/K)$ (Passivirta et al. 1999)
- $52.8^* \pm 1.6$ (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
- $\ln K_{AW} = 22.853 - 7950.45/(T/K)$; temp range 4–31°C (gas stripping-GC, Bamford et al. 2000)
- $K_{AW} = \exp\{-[66.1/(\text{kJ mol}^{-1})]/RT\} + [0.190/(\text{kJ mol}^{-1} \text{K}^{-1})/R]$; where $R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
- 54.0 (exptl. data, Bamford et al. 2002)
- $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 66 \pm 5 \text{ kJ/mol}$, $\Delta S_H = 0.19 \pm 0.02 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004
- 6.94 (estimated-bond method EPIWIN v3.04, Hardy 2002)
- 25.12, 19.95 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
- $\log H/(\text{Pa m}^3/\text{mol}) = -2584/(T/K) + 10.07$ (LDV linear regression of literature data, Li et al. 2003)
- $\log H/(\text{Pa m}^3/\text{mol}) = -3407/(T/K) + 12.72$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.72 (shake flask-GC/ECD, Chiou et al. 1977; Freed et al. 1977; Chiou et al. 1982)
- 8.35 (Hansch & Leo 1979)

- 6.34 (shake flask-GC/ECD, Karickhoff et al. 1979)
- 7.44 (RP-TLC- k' correlation, Bruggeman et al. 1982; 1984)
- 6.93, 7.75 (RP-HPLC-RT correlation, uncorrected, with ortho correction, Rapaport & Eisenreich 1984)
- 6.90 (generator column-HPLC, Woodburn et al. 1984)
- 6.68 (HPLC/MS correlation, Burkhard et al. 1985c)
- 7.69, 7.71 (HPLC- k' correlation, calculated, De Kock & Lord 1987)
- 6.90 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
- 7.69 (HPLC-RT correlation, De Kock & Lord 1987)
- 7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
- 6.84, 6.90, 6.71, 6.74 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 6.82, 6.85 (RP-HPLC- k' correlation, different stationary phases, Sherbolm & Eganhouse 1988)
- 7.00 (RP-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
- 7.07, 7.12; 6.75, 6.72 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.81 (HPLC- k' correlation, Noegrohati & Hammers 1992)
- 6.51 (average, generator column-GC, Larsen et al. 1992)
- 6.80 (recommended, Sangster 1993)
- 7.50 (recommended, Hansch et al. 1995)
- 6.58 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)
- 6.71, 6.87 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 8.50 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
- 10.04* (20°C, generator column-GC, measured range -10 to 30°C, Harner & Bidleman 1996)
- $\log K_{OA} = -6.02 + 4696/(T/K)$; temp range -10 to +30°C (generator column-GC, Harner & Bidleman 1996)
- 9.37; 9.09 (fugacity meter/generator column-GC; measured range 10–43°C, calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -5.49 + 4430/(T/K)$; temp range 10–43°C (fugacity meter, Kömp & McLachlan 1997a)
- 10.50 (10°C, estimated, Thomas et al. 1998)
- 11.03, 9.99; 10.02 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 10.08 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
- 9.80; 9.65 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
- 9.52, 9.44 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
- $\log K_{OA} = 4966/(T/K) - 7.14$ (LDV linear regression of literature data, Li et al. 2003)
- $\log K_{OA} = 3785/(T/K) - 7.00$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

- 4.68 (oyster, Vreeland 1974)
- 4.66 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
- 4.48, 5.23 (calculated-S, K_{OC} , Kenaga 1980)
- 5.23, 3.76 (amphipods, clams, Lynch et al. 1982)
- 5.03, 4.88, 4.65 (algae, snail, aquatic earthworm, Lynch et al. 1982)
- 4.82, 4.63 (crayfish, fish, Lynch et al. 1982)
- 4.00, 4.72, 3.77 (calculated-S, calculated-C, calculated- K_{OW} , Lynch et al. 1982)
- 0.99 (poultry, Garten & Trabalka 1983)
- 6.78 (guppy, 3.5% lipid, Bruggeman et al. 1982, 1984)
- 4.84 (rainbow trout, ratio of uptake and depuration rate constants, Muir et al. 1985)
- 5.87; 6.00 (rainbow trout: laboratory studies; Lake Ontario field data, Oliver & Niimi 1985)
- 2.60, 2.48 (human fat of lipid, wet wt. basis, calculated- K_{OW} , Geyer et al. 1987)
- 5.32 (guppy, Gobas et al. 1987)
- 4.57 (*Selenastrum capricornutum*, Mailhot 1987)
- 4.48 (worms, Oliver 1987c)
- 4.84, 5.32 (fish, calculated- C_B/C_W or k_1/k_2 , Connell & Hawker 1988; Hawker 1990)

- 3.85 (*Hexagenia limbata*, 4°C, rate const. ratio: uptake and depuration k_1/k_2 , Landrum & Poore 1988)
 4.94–5.28 (*Hexagenia limbata*, May–November, calculated-lipid-normalized, Landrum & Poore 1988)
 5.01 (*Pontoporeia hoyi*, calculated, Evans & Landrum 1989)
 5.06 (guppy, estimated, Banerjee & Baughman 1991)
 5.65; 7.18 (22°C, zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
 3.31–5.57 (various marine species, mean dry wt. BCF, Hope et al. 1998)
 5.11–6.96 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
 5.32 (Baltic Sea blue mussels, flow-through exptl, dry wt., Gustafsson et al. 1999)
 4.68, 5.93 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
 5.48, 7.40 (mussel: wet wt basis, lipid wt basis, Geyer et al. 2000)
 5.63, 6.99 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
 5.65, 7.19 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.95; 3.95 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)
 4.40 (estimated-EPIWIN v3.04, Hardy 2002)

Sorption Partition Coefficient, log K_p:

- 3.95–4.17 (Saginaw Bay sediment, sorption isotherm, Horzempa & Di Toro 1983)
 4.12–4.55 (Saginaw Bay suspended solids, sorption isotherm, Horzempa & Di Toro 1983)
 5.30 (Lake Superior suspended solids, field measurement-GC/ECD, Baker et al. 1986)
 5.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 5.65–5.91 (field-generated particulates, New Bedford Harbor, Bergen et al. 1993)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 5.62 (soil/sediment, batch equilibrium-sorption isotherm, Haque & Schmedding 1976)
 5.34 (soil, batch equilibrium-sorption isotherm measurement, Chiou et al. 1979)
 6.51 (soil, calculated-K_{OW}, Karickhoff et al. 1979)
 6.08 (soil, quoted experimental value, Kenaga 1980)
 5.33 (calculated-K_{OW}, Schwarzenbach & Westall 1981)
 6.51 (calculated-K_{OW}, Schwarzenbach & Westall 1981 from Karickhoff 1981)
 6.43, 6.42, 5.33 (calculated-K_{OW}, calculated-C_L, calculated-C_S, Karickhoff 1981)
 6.51 (sediment, calculated-K_{OW}, Lynch et al. 1982)
 6.57 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
 5.60; 5.50; 7.30 (field data of sediment trap material; Niagara River-org. matter; calculated-K_{OW}, Oliver & Charlton 1984)
 6.61 (sediment/pore water-Saginaw Bay, dual radio-tag experiment, Di Toro et al. 1985)
 5.51 (Aldrich humic acid, reversed phase separation, Landrum et al. 1985)
 5.40, 5.70, 6.10 (Offshore Grand Haven sediment, nearshore Grand Haven sediment, Benton Harbor sediment, by batch equilibrium-sorption isotherm, Voice & Weber 1985)
 7.56, 7.68 (river sediment, Coates & Elzerman 1986)
 5.575 (correlated literature values in soils, Sklarew & Girvin 1987)
 5.8–7.3, 6.60; 7.20 (suspended sediment, average; algae > 50 µm, Oliver 1987a)
 6.60 (river sediment 7–13% OC, batch equilibrium, Oliver 1987)
 6.48 (Lake Michigan water column, Swackhamer & Armstrong 1987)
 4.75 (12 lakes/streams in southern Ontario at 1.6–26.5 mg/L DOC, Evans 1988)
 5.26, 5.25, 5.19, 4.62 (humic substances, in concentration of 5, 10, 20, 40 mg/L DOC, reported as log K_h, Lara & Ernst 1989)
 5.258, 5.222 (marine humic substances, calculated-MCI χ , reported as log K_h at concentration of 5 mg/L DOC, Sabljic et al. 1989)
 6.76, 4.42 (Great Lake suspended matter, Great Lake DOC: reversed phase separation, Eadie et al. 1990)
 6.18, 6.13, 5.99 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
 5.86 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991; quoted, Baker et al. 2000)
 6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
 5.54 (Red Hood sediment, batch equilibrium, Brannon et al. 1995)

- 5.65 (soil, calculated-MCI χ , Sabljic et al. 1995)
 6.02 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)
 6.42–6.48 (Catlin silt loam, $f_{OC} = 0.0226$, depth 0–15 cm, batch equilibrium-GC, Girvin & Scott 1997)
 6.77–6.84 (Cloudland loam, $f_{OC} = 0.0024$, depth 15–30 cm, batch equilibrium-GC, Girvin & Scott 1997)
 6.43–6.52 (Kenoma silt loam, $f_{OC} = 0.0153$, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
 6.51–6.57 (Kenoma silt loam, $f_{OC} = 0.0092$, depth 58–82 cm, batch equilibrium-GC, Girvin & Scott 1997)
 6.19–6.28 (Norborne silt loam, $f_{OC} = 0.0137$, depth 0–20 cm, batch equilibrium-GC, Girvin & Scott 1997)
 6.55 (Norborne silt loam, $f_{OC} = 0.009$, depth 33–65 cm, batch equilibrium-GC, Girvin & Scott 1997)
 6.41–6.59 (Norborne silt loam, $f_{OC} = 0.0057$, depth 65–85 cm, batch equilibrium-GC, Girvin & Scott 1997)
 6.40 (soil, calculated- K_{OW} , Girvin & Scott 1997)
 6.20; 5.60 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
 5.86, 5.81 (sediments: organic carbon OC –0.1%, OC –0.5%, average, Delle Site 2001)
 6.05–7.27; 5.30–7.60 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
 5.55; 6.17, 6.96, 6.50 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
 5.088 (estimated-EPIWIN v3.04, Hardy 2002)
 6.20–7.20 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Sorption Partition Coefficient, log K_{OM} :

- 4.42 (natural sediment, Eadie et al. 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: depletion rate constant $k = 17 \text{ d}^{-1}$ from a 26-cm or 67-cm high purge vessel (Girvin et al. 1997);
 $t_{1/2} = 2.096 \text{ d}$ from river, $t_{1/2} = 29.5 \text{ d}$ from lake (estimated-EPIWIN v3.04, Hardy 2002).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16\text{--}0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_1 = 29.5 \text{ d}^{-1}$ in pond, $k_1 = 14.6 \text{ d}^{-1}$ in river, $k_1 = 36.8 \text{ d}^{-1}$ in sand by *Chironomus tentans* larvae (Muir et al. 1983)
 $k_2 = 0.0029 \text{ d}^{-1}$ with elimination $t_{1/2} = 241 \text{ h}$ in pond-sediment, $k_2 = 0.0059 \text{ d}^{-1}$ with $t_{1/2} = 117 \text{ h}$ in river water, $k_2 = 0.0034 \text{ d}^{-1}$ with $t_{1/2} = 203 \text{ h}$ in river sediment and $k_2 = 0.0030 \text{ d}^{-1}$ with $t_{1/2} = 230 \text{ h}$ in sand-sediment by *Chironomus tentans* larvae (Muir et al. 1983)
 $k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
 $k_1 = 800 \text{ d}^{-1}$; $k_2 = 0.004 \text{ d}^{-1}$ (guppy, Bruggeman et al. 1984)
 $k_1 = 461 \text{ d}^{-1}$; $k_2 = 0.008 \text{ d}^{-1}$ (rainbow trout, total ^{14}C in whole fish-wet weight, Muir et al. 1985)
 $k_1 = 1100 \text{ d}^{-1}$ (guppy, Opperhuizen 1986)
 $k_1 = 63.2 \text{ h}^{-1}$; $k_2 = 0.009 \text{ h}^{-1}$ (10–20°C, *Hexagenia limbata*, Landrum & Poore 1988)
 $k_s = 0.049 \text{ h}^{-1}$; $k_t = 0.009 \text{ h}^{-1}$ (uptake, depuration of mayfly-sediment model II, Gobas et al. 1989)
 $\log k_1 = 2.90, 2.66 \text{ d}^{-1}$; $\log 1/k_2 = 2.39, 2.10 \text{ d}$ (fish, quoted, Connell & Hawker 1990)
 $k_1 = 4660 \text{ d}^{-1}$; $k_2 = 0.0104 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 $k_2 = 0.044 \text{ d}^{-1}$ with an elimination half-life of 15.9 d (earthworm, Belfroid et al. 1995)
 $k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 224 \text{ d}$ and $k_2 = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 69 \text{ d}$ for food concn of 22 ng/g and 124 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
 $k_1 = 5.7 \text{ L d}^{-1} \text{ g}^{-1}$; $k_2 = 0.027 \text{ d}^{-1}$ (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999)
 $k_1 = 0.00231 \text{ h}^{-1}$; $k_2 = 0.137 \text{ h}^{-1}$ (in blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_1 = 5$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.04$ d⁻¹ (earthworm, Wågman et al. 2001)
 $k_2 = 0.004$ d⁻¹ with $t_{1/2} = 177$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.003$ d⁻¹ with $t_{1/2} = 219$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)
 $k_2 = 0.015$ d⁻¹ with $t_{1/2} = 46.2$ d (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radical for hexachlorobiphenyls (Kwok et al. 1995);

$t_{1/2} = 6000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: 25–53 min in aqueous solution purged at a flow rate of 1 L/min (Coates 1984);

$t_{1/2} = 123000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000); volatilization $t_{1/2} = 2.096$ d from river, 29.5 d from lake (estimated-EPIWIN v3.04, Hardy 2002).

Groundwater:

Sediment: uptake clearance from sediment was (0.0021 ± 0.001) g of dry sediment·g⁻¹ of organism·h⁻¹ for amphipod, *P. hoyi* in Lake Michigan sediments at 4°C (Landrum 1989);

$k(\text{exptl}) < 0.9$ M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 2.7–6.3, with $t_{1/2} > 7$ h at pH 7 and 23 ± 2 °C (Yao & Haag 1991).

$t_{1/2} = 165000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2} = 165000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: half-life in rainbow trout, > 1000 d and its muscle, 77 d (Niimi & Oliver 1983);

$t_{1/2} = 170$ d in worms at 8°C (Oliver 1987c);

$t_{1/2} = 175$ d in guppy (Bruggeman et al. 1984);

$t_{1/2} = 45.6$ d in *Pontoporeia hoyi* (Evans & Landrum 1989);

elimination $t_{1/2} = 15.9$ d from earthworm (Belfroid et al. 1995)

Depuration $t_{1/2} = 69$ –224 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

theoretical $t_{1/2} = 25.7$ d to reach 90% steady-state tissue concn (Baltic Sea blue mussels, flow-through expt., Gustafsson et al. 1999);

$t_{1/2} = 5.1$ h in blood plasma (ring doves, Drouillard & Norstrom 2000);

elimination $t_{1/2} = 18$ d in earthworm given contaminated food (Wågman et al. 2001).

depuration $t_{1/2} = 177$ d for high-dose treatment, $t_{1/2} = 219$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

depuration $t_{1/2} = 46.2$ d (juvenile carp in 100-d experiment Stapleton et al. 2004)

TABLE 7.1.1.153.1

Reported aqueous solubilities, Henry's law constants and octanol-air partition coefficients of 2,2',4,4',5,5'-hexachlorobiphenyl (PCB-153) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Henry's law constant		log K_{OA}	
Doucette & Andren 1988		Bamford et al. 2000		Harner & Bidleman 1996	
generator column-GC/ECD		gas stripping-GC/MS		generator column-GC	
t/°C	S/g·m ⁻³	t/°C	H/(Pa·m ³ /mol)	t/°C	log K_{OA}
4	0.00462	4	6.50	-10	11.73
25	0.00845	11	13.52	0	11.25
40	0.0128	18	27.2	10	10.62
		25	52.8	20	10.04
		31	91.2	30	9.39
$S/(\text{mol/L}) = A \cdot \exp[B \cdot (t/^\circ\text{C})]$		$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 89.90$	
A	1.15×10^{-8}	A	22.8530	$\log K_{OA} = A + B/T$	
B	0.028	B	7950.45	A	-6.015
$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 20.3$		enthalpy, entropy change:		B	4695
for 4–40°C		$\Delta H/(\text{kJ mol}^{-1}) = 66.1 \pm 5.4$			
		$\Delta S/(\text{J mol}^{-1} \cdot \text{K}^{-1}) = 190 \pm 18$			

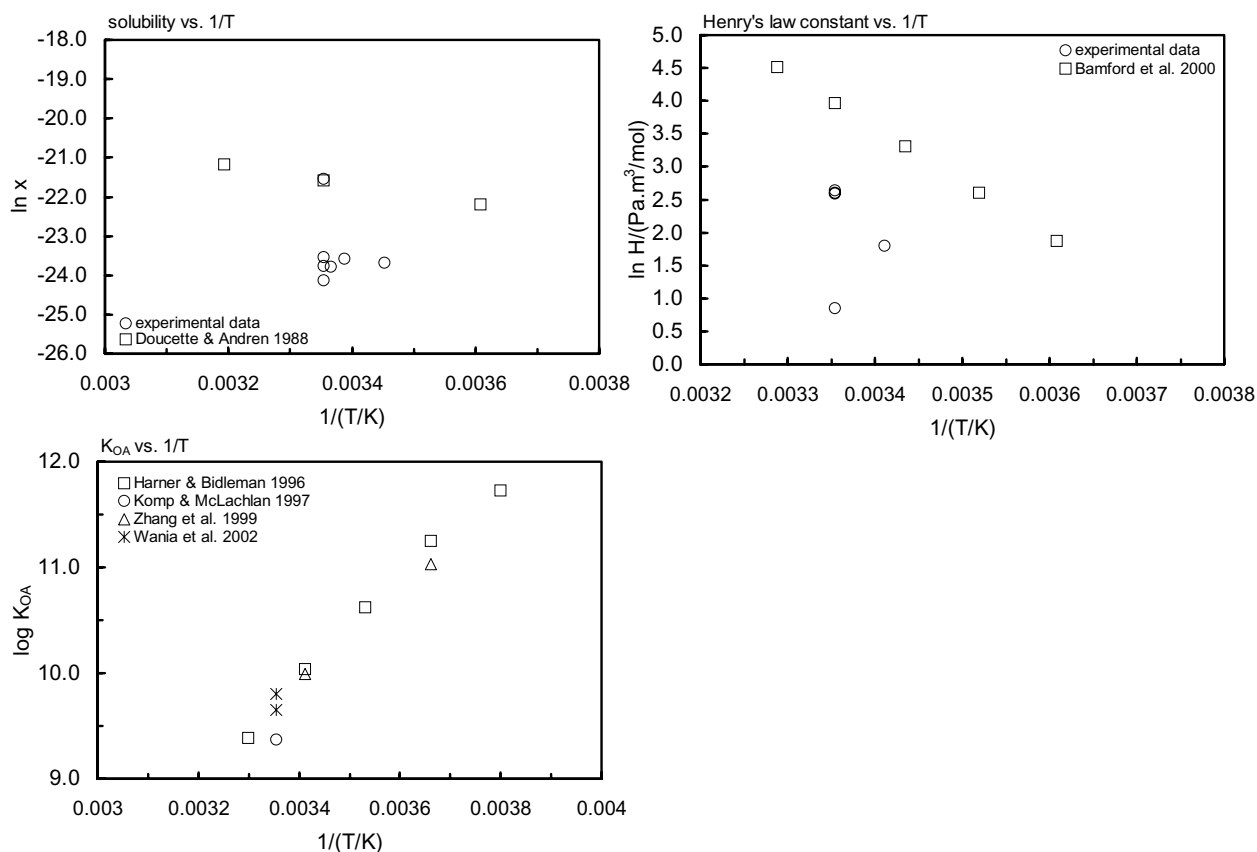
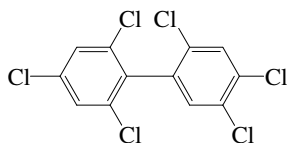


FIGURE 7.1.1.153.1 Logarithm of mole fraction solubility, Henry's law constant and K_{OA} versus reciprocal temperature for 2,2',4,4',5,5'-hexachlorobiphenyl (PCB-153).

7.1.1.154 2,2',4,4',5,6'-Hexachlorobiphenyl (PCB-154)



Common Name: 2,2',4,4',5,6'-Hexachlorobiphenyl

Synonym: PCB-154, 2,2',4,4',5,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',4,4',5,6'-hexachlorobiphenyl

CAS Registry No: 60145-22-4

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

oil (Erickson 1986)

117 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0106 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00173, 0.00137, 0.00293, 0.00213 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.71×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.86×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

0.00182 (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4681/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

58.46 (calculated-P/C, Burkhard 1984)

48.84 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

38.7 (calculated-QSPR, Dunnivant et al. 1992)

17.34, 29.16, 47.85, 76.7 \pm 2.2, 113.7 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 15.155 - 5556.89/(T/K)$; temp range $4-31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(46.2/kJ \cdot mol^{-1})/RT] + (0.126/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314\ J \cdot K^{-1} \cdot mol^{-1}$ and temp range: $4-31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

75.4 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 46 \pm 5\ kJ/mol$, $\Delta S_H = 0.13 \pm 0.02\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.87 (calculated-TSA, Burkhard 1984)

6.67, 6.81, 6.47, 6.64 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

6.76 (calculated-TSA, Hawker & Connell 1988a)

7.05, 7.03; 6.48, 6.43 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

- 6.65 (recommended, Sangster 1993)
6.89 (recommended, Hansch et al. 1995)
6.6326 (molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.91 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.66 (suspended particulate matter, Burkhard 1984)
5.064 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16-0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

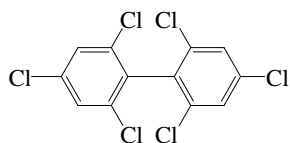
Ground water:

Sediment:

Soil:

Biota:

7.1.1.155 2,2',4,4',6,6'-Hexachlorobiphenyl (PCB-155)



Common Name: 2,2',4,4',6,6'-Hexachlorobiphenyl

Synonym: PCB-155, 2,2',4,4',6,6'-hexachloro-1,1'-biphenyl

Chemical Name: 2,2',4,4',6,6'-hexachlorobiphenyl

CAS Registry No: 33979-03-2

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

112.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.3482

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.5 (differential scanning calorimetry, Miller et al. 1984; Ruelle et al. 1993; Chickos et al. 1999)

20.30 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

45.19 (Miller et al. 1984)

45.25, 66.9 (exptl., calculated, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.139 (mp at $112.5^{\circ}C$)

0.131 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00090 (generator column-GC/ECD, Weil et al. 1974)

0.00041 (generator column-GC/ECD, Miller et al. 1984,1985)

0.0000528 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)

2.50×10^{-3} , 1.34×10^{-3} , 6.27×10^{-3} , 2.68×10^{-3} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0023 (generator column-GC/ECD, Dunnivant & Elzerman 1988)

0.00109 ($22^{\circ}C$, generator column-GC/ECD, Opperhuizen et al. 1988)

0.0033 (generator column-GC/ECD, Li et al. 1992; Li & Doucette 1993)

0.00284 (shake flask-GC/ECD, Li & Andren 1994)

$0.0028^* \pm 0.00013$ (generator column-GC/ECD, Shiu et al. 1997)

1.89×10^{-3} , 0.0050 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

$\ln x = -8.9206 - 4112.07/(T/K)$, temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.0142, 0.0138 (supercooled liquid S_L : derivation of literature-derived value LDV, final-adjusted value FAV, Li et al. 2003)

$\log [S_L/(mol\ m^{-3})] = -861/(T/K) - 1.52$ (supercooled liquid, linear regression of literature data, Li et al. 2003)

$\log [S_L/(mol\ m^{-3})] = -1268/(T/K) - 0.16$ (supercooled liquid, final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0016 (GC-RT, Westcott et al. 1981)

0.0122 (P_L calculated from P_s using fugacity ratio F, Westcott et al. 1981)

0.00173 (gas saturation, Westcott & Bidleman 1981)

0.00443 (supercooled liquid P_L , Burkhard 1984)

3.57×10^{-4} , 6.41×10^{-4} , 8.04×10^{-4} (calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985a)
 0.00443 (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)
 0.00159, 0.012(selected P_S , P_L , Shiu & Mackay 1986)
 4.76×10^{-4} (calculated-S \times HLC, Dunnivant & Elzerman 1988)
 3.54×10^{-4} (supercooled liquid P_L , calculated-mp, Dunnivant & Elzerman 1988)
 $\log(P_L/P_a) = -4303/(T/K) + 12.02$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)
 3.25×10^{-4} * (gas saturation-GC/ECD, measured range -10 to 30°C , Wania et al. 1994)
 $\log(P_S/P_a) = 14.84 - 5399/(T/K)$; temp range -10 to 30°C (gas saturation-GC, Wania et al. 1994)
 2.188×10^{-3} (20°C , supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)
 0.000285–0.0016; 0.00344–0.00443 (exptl. solid P_S range; exptl. liquid P_L range, Delle Site 1997)
 3.42×10^{-4} (supercooled P_L : calculated-MCI χ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)
 3.31×10^{-3} ; 3.47×10^{-3} (supercooled P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log P_L/P_a = -4697/(T/K) + 13.27$ (supercooled liquid, LDV linear regression of literature data, Li et al. 2003)
 $\log P_L/P_a = -4562/(T/K) + 12.85$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

11.65 (gas stripping-GC, Coates 1984)
 157.0 (calculated-P/C, Burkhard et al. 1985b)
 12.46 (calculated, Coates & Elzerman 1986)
 817.9 (calculated-P/C, Shiu & Mackay 1986)
 76.5 (gas stripping-GC, Dunnivant et al. 1988, Dunnivant & Elzerman 1988)
 60.8 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)
 85.25 (calculated-QSPR, Dunnivant et al. 1992)
 81.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 27 \pm 5 \text{ kJ/mol}$, $\Delta S_H = 0.06 \pm 0.02 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004
 75.86, 91.2 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
 $\log[H/(\text{Pa m}^3/\text{mol})] = -3294/(T/K) + 13.01$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.70 (shake flask-GC, Chiou et al. 1977)
 6.34 (shake flask-GC, Karickhoff et al. 1979)
 6.37 (HPLC- k' correlation, McDuffie 1981)
 7.12 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 6.88 (calculated-TSA, Burkhard 1984)
 7.55 (generator column-GC/ECD, Miller et al. 1984, 1985)
 6.39 (HPLC-RT/MS correlation, Burkhard et al. 1985c)
 6.01 (HPLC- k' correlation, Tomlinson & Hafkenscheid 1986)
 7.24 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
 6.54, 6.81, 6.24, 6.57 (RP-HPLC-RI correlations, Brodsky & Ballschmiter 1988)
 7.24 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
 7.287 ± 0.065 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 7.08, 7.03; 6.24, 6.22 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
 6.83 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 7.24 (shake flask-GC/ECD, Li & Doucette 1993)
 6.54 (recommended, Sangster 1993)
 7.29 (recommended, Hansch et al. 1995)
 7.36, 7.19 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

8.99* (generator column-GC/ECD; measured range -10 to $+20^\circ\text{C}$; Harner & Mackay 1995)
 $\log K_{OA} = -2.20 + 3954/(T/K)$; (temp range -10 to $+20^\circ\text{C}$, generator column-GC, Harner & Mackay 1995)

- 9.15 (20°C, generator column-GC, Harner & Bidleman 1996)
 $\log K_{OA} = -2.21 + 3954/(T/K)$; temp range -10 to +20°C (generator column-GC, Harner & Bidleman 1996)
 10.19, 9.13; 9.16 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
 9.24 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
 8.89, 9.14 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
 $\log K_{OA} = 4357/(T/K) - 5.47$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, log BCF at 25°C or as indicated:

- 1.02 (poultry, Garten & Trabalka 1983)
 2.79–3.68 highest value 3.68, not equilibrated (rainbow trout, 15°C, steady-state BCF of 7-d to 96-d laboratory study, Oliver & Niimi 1985)
 > 4.94; 3.68 (rainbow trout, laboratory data: kinetic BCF (k_1/k_2), steady-state BCF (C_F/C_W), Oliver & Niimi 1985)
 4.53 (worms, Oliver 1987c)
 3.68 (fish, Isnard & Lambert 1988)
 5.99, 7.29 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} :

- 6.08 (natural sediment, sorption isotherm by batch equilibrium technique-GC, Karickhoff et al. 1979)
 5.95, 7.28, 5.95 (calculated- K_{OW} , calculated- C_L , calculated- C_S , Karickhoff 1981)
 6.68 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 4.905 (calculated-MCI χ , marine humic substances with 5 mg/L of DOC, reported as association coefficient log K_h , Sabljic et al. 1989)
 6.08; 6.17 (soil, quoted lit.; calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_1 = 8.6-29.5 \text{ h}^{-1}$ in pond-sediment system, $k_1 = 22.9-14.6 \text{ h}^{-1}$ in river-water system, $k_1 = 29.6-39.8 \text{ h}^{-1}$ in river-sediment system, $k_1 = 26.7-47.0 \text{ h}^{-1}$ in sand-sediment system (*Chironomus tentans* larvae, Muir et al. 1983)
 $k_2 = 0.0029 \text{ h}^{-1}$ with $t_{1/2} = 241 \text{ h}$ in pond-sediment system, $k_2 = 0.0059 \text{ h}^{-1}$ with $t_{1/2} = 117 \text{ h}$ in river-water system, $k_2 = 0.0034 \text{ h}^{-1}$ with $t_{1/2} = 203 \text{ h}$ in river-sediment system, $k_2 = 0.0030 \text{ h}^{-1}$ with $t_{1/2} = 230 \text{ h}$ in sand-sediment system (*Chironomus tentans* larvae, Muir et al. 1983)
 $k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
 $k_1 = 60 \text{ d}^{-1}$; $k_2 > 0.0007 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985; Thomann 1989)
 $\log 1/k_2 = 3.1, 3.6 \text{ h}$ (fish, quoted, calculated- K_{OW} , Hawker & Connell 1988b)
 $1/k_2 = 141 \text{ d}$ (guppy, Gobas et al. 1989; quoted, Clark et al. 1990)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 117\text{--}241$ h in sediment-water systems (*Chironomus tentans* larvae, Muir et al. 1983)
 $t_{1/2} > 1000$ d in rainbow trout (Niimi & Oliver 1983; Oliver & Niimi 1985), and $t_{1/2} = 77$ d in its muscle (Niimi & Oliver 1983).

TABLE 7.1.1.155.1

Reported aqueous solubilities and octanol-air partition coefficients log of 2,2',4,4',6,6'-hexachlorobiphenyl (PCB-155) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1997		Wania et al. 1994		Harner & Mackay 1995	
generator column-GC/ECD		gas saturation-GC		generator column-GC	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K_{OA}
5	1.0×10^{-3}	-10	1.634×10^{-6}	-10	10.49
15	1.70×10^{-3}	0	1.185×10^{-5}	0	9.97
25	2.80×10^{-3}	10	8.039×10^{-5}	10	9.635
35	4.30×10^{-3}	20	3.250×10^{-4}	20	9.158
45	6.40×10^{-3}	30	7.739×10^{-4}	25	8.99
$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 34.2$ for 5–45°C		log (P/Pa) = A – B/(T/K) A 14.84 B 5399		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 63.9$ log $K_{OA} = A + B/RT$ A –2.2 B 3337.4	
		$\Delta H_{subl}/(\text{kJ mol}^{-1}) = 103.4$			

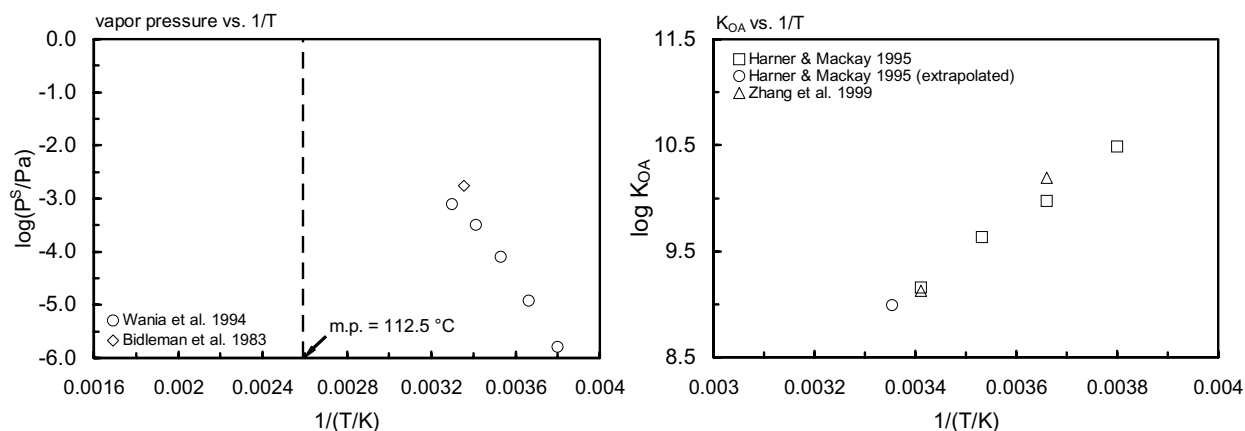
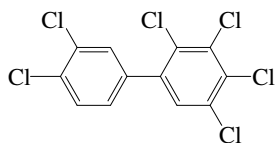


FIGURE 7.1.1.155.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 2,2',4,4',6,6'-hexachlorobiphenyl (PCB-155).

7.1.1.156 2,3,3',4,4',5-Hexachlorobiphenyl (PCB-156)



Common Name: 2,3,3',4,4',5-Hexachlorobiphenyl

Synonym: PCB-156, 2,3,3',4,4',5-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,4',5-hexachlorobiphenyl

CAS Registry No: 38380-08-4

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

127 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.100 (mp at $127^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00533 ($20^{\circ}C$, supercooled liquid S_L , Murphy et al. 1987)

0.00361, 0.00244, 0.00112, 0.00102 (RP-HPLC- k' correlation, different stationary and mobile phases Brodsky & Ballschmiter 1988)

0.000397 (generator column-GC/ECD, Hong & Qiao 1995)

0.0011 (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see Comment by van Noort 2004

0.000513, 0.000711, 0.00110, 0.00153 ($5, 15, 25, 35^{\circ}C$, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.000215 (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

7.34×10^{-4} (supercooled liquid P_L , GC-RT correlation, Burkhard et al. 1985a)

0.000809 (GC-RI correlation, Burkhard et al. 1985b)

0.00021, 0.00016 (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.26×10^{-4} , 1.62×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4949/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

88.14 (concn ratio-GC, Murphy & Mullin 1983)

17.53 (calculated-P/C, Burkhard et al. 1985)

2.23 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

8.97 (calculated-QSPR, Dunnivant et al. 1992)

1.50 (calculated-QSPR, Achman et al. 1993)

3.72 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

37.0 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 112 \pm 10$ kJ/mol, $\Delta S_H = 0.34 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.13, 7.26, 7.84, 7.53 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 7.14, 7.12; 7.16, 7.13 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
 6.70 (generator column-GC, Larsen et al. 1992)
 7.11 (recommended, Sangster 1993)
 7.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.07, 10.87; 10.87 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 10.36 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.88, 7.18 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.51 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.40 (as $\log K_h$, association coefficient with marine humic substance, calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.024 \text{ d}^{-1}$ with an elimination $t_{1/2} = 29 \text{ d}$ (earthworm, Belfroid et al. 1995)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 163 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 182 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

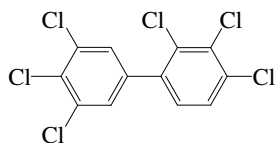
Biota: clearance $t_{1/2} = 50\text{--}100 \text{ d}$ in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);

reported biological half-lives for hexachlorobiphenyls: $t_{1/2} = 87$ to $> 850 \text{ d}$ for trout, $t_{1/2} = 77\text{--}91 \text{ d}$ for trout muscle; $t_{1/2} > 200 \text{ d}$ for carp; $t_{1/2} = 75\text{--}175 \text{ d}$ for guppy (Niimi 1987);

elimination $t_{1/2} = 29 \text{ d}$ from earthworm (Belfroid et al. 1995)

depuration $t_{1/2} = 163 \text{ d}$ for high-dose treatment, $t_{1/2} = 182 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.157 2,3,3',4,4',5'-Hexachlorobiphenyl (PCB-157)



Common Name: 2,3,3',4,4',5'-Hexachlorobiphenyl

Synonym: PCB-157, 2,3,3',4,4',5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,4',5'-hexachlorobiphenyl

CAS Registry No: 69782-90-7

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

141 (estimated-molecular properties, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0152 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00036 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.000119 (generator column-GC/ECD, Hong & Qiao 1995)

0.000296 (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see Comment by van Noort 2004

0.000084, 0.000139, 0.000296, 0.000540 ($5, 15, 25, 35^{\circ}C$, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.39×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

8.09×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

2.02×10^{-4} , 1.27×10^{-4} (supercooled liquid P_L , GC-RT correlation; different stationary phases, Foreman & Bidleman 1985)

1.17×10^{-4} , 1.58×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4994/(T/K) + 13.05$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.30 (calculated-P/C, Burkhard et al. 1985a)

58.76 (concn ratio-GC, Murphy & Mullin 1983)

6.69 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

8.56 (calculated-QSPR, Dunnivant et al. 1992)

1.50 (calculated-QSPR, Achman et al. 1993)

2.27 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

31.6 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 129 \pm 10$ kJ/mol, $\Delta S_H = 0.40 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.18 (calculated-TSA, Hawker & Connell 1988a)

7.26, 7.14; 7.19, 7.04 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.20 (quoted average values of Risby et al. 1990: GC-RV and HPLC- k' correlations, Sangster 1993)

- 7.60 (recommended, Hansch et al. 1995)
 6.9661 (calculated-molecular properties MNDO-AM1, Makino 1998)
 6.73; 6.90 (generator column-GC/ECD, calculated-QSPR, Yeh & Hong 2002)
 7.37, 6.97 (calculated-MCI χ , calculated-MNDO-AMI method, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.28, 11.07; 10.76 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
 10.57 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.51 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.40 (as $\log K_h$, association coefficient with marine humic substance, calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

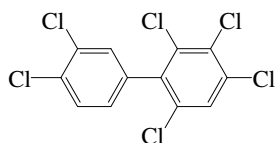
Ground water:

Sediment:

Soil:

Biota: clearance $t_{1/2} = 50-100 \text{ d}$ in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);
 reported biological half-lives for hexachlorobiphenyls: $t_{1/2} = 87$ to $> 850 \text{ d}$ for trout, $t_{1/2} = 77-91 \text{ d}$ for trout muscle; $t_{1/2} > 200 \text{ d}$ for carp; $t_{1/2} = 75-175 \text{ d}$ for guppy (Niimi 1987)

7.1.1.158 2,3,3',4,4',6-Hexachlorobiphenyl (PCB-158)



Common Name: 2,3,3',4,4',6-Hexachlorobiphenyl

Synonym: PCB-158, 2,3,3',4,4',6-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,4',6-hexachlorobiphenyl

CAS Registry No: 74472-42-7

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

107 (Kühne et al. 1995; Ruelle & Kesselring 1997; Ran et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.157 (mp at $107^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.0159 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00807 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00120 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00114 (TSA and mp, Abramowitz & Yalkowsky 1990)

0.00185 (calculated-group contribution method, Kühne et al. 1995)

0.00147, 0.00396 (molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

9.26×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.02×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

6.19×10^{-4} , 4.486×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

9.73×10^{-5} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

3.09×10^{-4} , 4.57×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4816/(T/K) + 12.94$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

20.97 (calculated-P/C, Burkhard 1984)

4.37 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

21.89 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

2.86 (calculated-QSPR, Achman et al. 1993)

16.74 (calculated-QSPR, Dunnivant et al. 1992)

9.64 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

49.9 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 80 \pm 7$ kJ/mol, $\Delta S_H = 0.24 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.69 (calculated-TSA, Burkhard 1984)
- 6.78 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
- 7.02 (calculated-TSA, Hawker & Connell 1988a)
- 7.10, 6.87; 6.84, 6.82 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)
- 6.78 (recommended, Sangster 1993)
- 7.25 (recommended, Hansch et al. 1995)
- 6.8874 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
- 7.69 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

- 9.51; 9.12 (generator column-GC.; K_{OW}/K_{AW} , Kömp & McLachlan 1997a)
- $K_{OA} = -5.17 + 4380/(T/K)$, temp range 10–43°C (Kömp & McLachlan 1997a)
- 10.28 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:Sorption Partition Coefficient, $\log K_{OC}$:

- 6.49 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 124 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 241 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

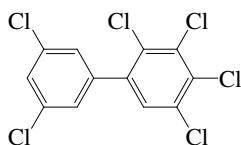
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 124 \text{ d}$ for high-dose treatment, $t_{1/2} = 241 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.159 2,3,3',4,5,5'-Hexachlorobiphenyl (PCB-159)



Common Name: 2,3,3',4,5,5'-Hexachlorobiphenyl

Synonym: PCB-159, 2,3,3',4,5,5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,5,5'-hexachlorobiphenyl

CAS Registry No: 39635-35-3

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

116 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0135 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

5.72×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

1.084×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00119 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

29.08 (calculated-P/C, Burkhard 1984)

31.41 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

2.027 (wetted wall column-GC/ECD, Brunner et al. 1990)

15.77 (calculated-QSPR, Dunnivant et al. 1992)

35.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 116 \pm 12\ kJ/mol$, $\Delta S_H = 0.35 \pm 0.04\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.76 (calculated-TSA, Burkhard 1984)

7.24 (calculated-TSA, Hawker & Connell 1988a)

7.09, 7.24; 7.02, 7.00 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.17, 7.01 (quoted average values of Risby et al. 1990, Sangster 1993)

7.43 (recommended, Hansch et al. 1995)

7.2038 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.37 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

6.56 (suspended particulate matter, Burkhard 1984)

5.381 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

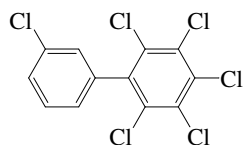
Ground water:

Sediment:

Soil:

Biota:

7.1.1.160 2,3,3',4,5,6-Hexachlorobiphenyl (PCB-160)



Common Name: 2,3,3',4,5,6-Hexachlorobiphenyl

Synonym: PCB-160, 2,3,3',4,5,6-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,5,6-hexachlorobiphenyl

CAS Registry No: 41411-62-5

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

99 (Burkhard et al. 1985b)

97–100 (Erickson 1986)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.188 (mp at $99^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0191 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00158 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$):

1.33×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00027 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

25.13 (calculated-P/C, Burkhard 1984)

25.74 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

2.027 (wetted wall column-GC/ECD, Brunner et al. 1990)

21.66 (calculated-QSPR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.62 (calculated-TSA, Burkhard 1984)

6.93 (calculated-TSA, Hawker & Connell 1988a)

6.88, 6.79; 6.89, 6.87 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.84, 6.88 (quoted average values of Risby et al. 1990, Sangster 1993)

7.30 (recommended, Hansch et al. 1995)

6.9006 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.42 (suspended particulate matter, Burkhard 1984)
5.259 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

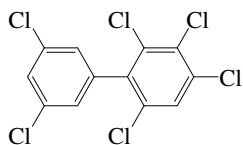
Ground water:

Sediment:

Soil:

Biota:

7.1.1.161 2,3,3',4,5',6-Hexachlorobiphenyl (PCB-161)



Common Name: 2,3,3',4,5',6-Hexachlorobiphenyl

Synonym: PCB-161, 2,3,3',4,5',6-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,5',6-hexachlorobiphenyl

CAS Registry No: 74472-43-8

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

84.0 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

1.37×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00150 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

34.96 (calculated-P/C, Burkhard 1984)

51.27 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

28.89 (calculated-QSPR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.76 (calculated-TSA, Burkhard 1984)

7.08 (calculated-TSA, Hawker & Connell 1988a)

7.16, 6.94; 6.69, 6.66 (multi-column HPLC-k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.05, 6.68 (quoted average values of Risby et al. 1990, Sangster 1993)

7.10 (recommended, Hansch et al. 1995)

7.0318 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.33 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.56 (suspended particulate matter, Burkhard 1984)
5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

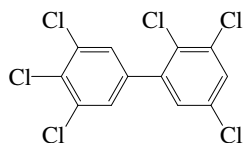
Ground water:

Sediment:

Soil:

Biota:

7.1.1.162 2,3,3',4',5,5'-Hexachlorobiphenyl (PCB-162)



Common Name: 2,3,3',4',5,5'-Hexachlorobiphenyl

Synonym: PCB-162, 2,3,3',4',5,5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4',5,5'-hexachlorobiphenyl

CAS Registry No: 39635-34-2

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

84.0 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0141 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00181 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

1.37×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00150 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

34.96 (calculated-P/C, Burkhard 1984)

51.27 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

28.89 (calculated-QSPR, Dunnivant et al. 1992)

35.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 116 \pm 12$ kJ/mol, $\Delta S_H = 0.35 \pm 0.04$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.76 (calculated-TSA, Burkhard 1984)

7.08 (calculated-TSA, Hawker & Connell 1988a)

7.16, 6.94; 6.69, 6.66 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.05, 6.68 (quoted average values of Risby et al. 1990, Sangster 1993)

7.10 (recommended, Hansch et al. 1995)

7.0318 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.42 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.56 (suspended particulate matter, Burkhard 1984)
5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

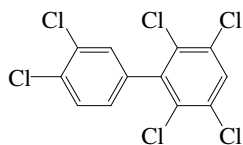
Ground water:

Sediment:

Soil:

Biota:

7.1.1.163 2,3,3',4',5,6-Hexachlorobiphenyl (PCB-163)



Common Name: 2,3,3',4',5,6-Hexachlorobiphenyl

Synonym: PCB-163, 2,3,3',4',5,6-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4',5,6-hexachlorobiphenyl

CAS Registry No: 74472-44-9

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

88.2 (Shiu & Mackay 1986)

122 (Ran et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F:

0.237 (assuming $\Delta S_{fus} = 56$ J/mol K, Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00531 (generator column-HPLC/UV, Huang 1983)

0.0053 (generator column-HPLC/UV, Billington et al. 1988)

0.0012 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

8.67×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

9.54×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

6.01×10^{-4} , 4.92×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.31×10^{-4} , 5.25×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4816/(T/K) + 12.93$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

18.54 (calculated-P/C, Burkhard 1984)

11.75 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

1.52 (wetted wall column-GC/ECD, Brunner et al. 1990)

12.73 (calculated-QSPR, Dunnivant et al. 1992)

9.37 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

49.5 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 81 \pm 7$ kJ/mol, $\Delta S_H = 0.24 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.78 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.08; 6.99; 6.84, 6.79 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.39 (generator column-GC, average, Larsen et al. 1992)

6.78 (recommended, Sangster 1993)

7.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

11.26, 10.16 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)

9.90 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.47 (suspended particulate matter, Burkhard 1984)

5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 170 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 198 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

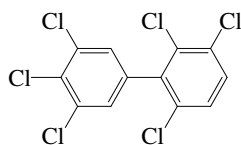
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 170 \text{ d}$ for high-dose treatment, $t_{1/2} = 198 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.164 2,3,3',4',5',6-Hexachlorobiphenyl (PCB-164)



Common Name: 2,3,3',4',5',6-Hexachlorobiphenyl

Synonym: PCB-164, 2,3,3',4',5',6-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4',5',6-hexachlorobiphenyl

CAS Registry No: 74472-45-0

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

96 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0161 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00194 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00144 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

4.478×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

4.97×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

10.04 (calculated-P/C, Burkhard 1984)

19.96 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

17.41 (calculated-QSPR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18\ kJ/mol$, $\Delta S_H = 0.23 \pm 0.03\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.69 (calculated-TSA, Burkhard 1984)

6.63 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.02 (calculated-TSA, Hawker & Connell 1988a)

7.22, 7.32; 6.79, 6.73 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

6.63 (recommended, Sangster 1993)

7.20 (recommended, Hansch et al. 1995)

6.6712 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.35 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.49 (suspended particulate matter, Burkhard 1984)
- 5.241 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

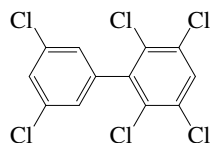
Ground water:

Sediment:

Soil:

Biota:

7.1.1.165 2,3,3',5,5',6-Hexachlorobiphenyl (PCB-165)



Common Name: 2,3,3',5,5',6-Hexachlorobiphenyl

Synonym: PCB-165, 2,3,3',5,5',6-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,3',5,5',6-hexachlorobiphenyl

CAS Registry No: 74472-46-1

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

101 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0150 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00114 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

1.292×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00140 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

30.9 (calculated-P/C, Burkhard 1984)

45.19 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

2.94 (wetted wall column-GC/ECD, Brunner et al. 1990)

27.91 (calculated-QSPR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.57, 7.37 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

6.72 (calculated-TSA, Burkhard 1984)

7.05 (calculated-TSA, Hawker & Connell 1988a)

7.17, 6.90; 6.70, 6.65 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.37, 6.68, 7.04 (quoted literature values, Sangster 1993)

7.37 (recommended, Hansch et al. 1995)

7.0191 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.88 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.52 (suspended particulate matter, Burkhard 1984)
5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

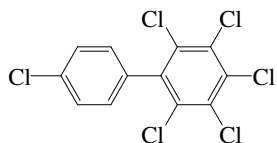
Ground water:

Sediment:

Soil:

Biota:

7.1.1.166 2,3,4,4',5,6-Hexachlorobiphenyl (PCB-166)



Common Name: 2,3,4,4',5,6-Hexachlorobiphenyl

Synonym: PCB-166, 2,3,4,4',5,6-hexachloro-1,1'-biphenyl

Chemical Name: 2,3,4,4',5,6-hexachlorobiphenyl

CAS Registry No: 41411-63-6

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

163.0 (Burkhard et al. 1985b)

160–165 (Erickson 1986)

145 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0443 (mp at $163^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0189 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

7.20×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

2.46×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$):

1.175×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

0.00140 (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

22.49 (calculated-P/C, Burkhard 1984)

17.43 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

18.65 (calculated-QSPR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18$ kJ/mol, $\Delta S_H = 0.23 \pm 0.06$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.62 (calculated-TSA, Burkhard 1984)

6.93 (calculated-TSA, Hawker & Connell 1988a)

7.13, 7.18; 6.90, 6.83 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.17, 6.87 (quoted average values of Risby et al. 1990, Sangster 1993)

7.31 (recommended, Hansch et al. 1995)

6.8501 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.08 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

6.42 (suspended particulate matter, Burkhard 1984)

5.259 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

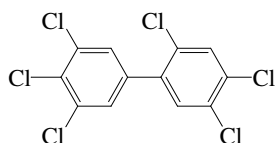
Ground water:

Sediment:

Soil:

Biota:

7.1.1.167 2,3',4,4',5,5'-Hexachlorobiphenyl (PCB-167)



Common Name: 2,3',4,4',5,5'-Hexachlorobiphenyl

Synonym: PCB-167, 2,3',4,4',5,5'-hexachloro-1,1'-biphenyl

Chemical Name: 2,3',4,4',5,5'-hexachlorobiphenyl

CAS Registry No: 52663-72-6

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

135 (calculated-molecular properties, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0128 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00223 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00036 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.000531 (generator column-GC/ECD, Hong & Qiao 1995)

0.000107 (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see Comment by van Noort 2004

0.000442, 0.000682, 0.00107, 0.00161 ($5, 15, 25, 35^{\circ}C$, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.88×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

2.12×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

2.80×10^{-4} , 2.39×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.34×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4994/(T/K) + 13.20$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.33 (calculated-P/C, Burkhard et al. 1985a)

12.46 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

20.55 (calculated-QSPR, Dunnivant et al. 1992)

4.47 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

39.28 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 106 \pm 8$ kJ/mol, $\Delta S_H = 0.32 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.29 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.24, 7.30; 7.00, 7.03 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.29 (recommended, Sangster 1993)

7.50 (recommended, Hansch et al. 1995)

6.82 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or indicated:

- 12.07, 10.77; 10.76 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 10.59 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.97, 7.27 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.58 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.381 (as $\log K_h$, association coefficient with marine humic substance, calculated-MCI χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29-60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_2 = 0.0263 \text{ d}^{-1}$ with an elimination $t_{1/2} = 26 \text{ d}$ (earthworm, Belfroid et al. 1995)
 $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 134 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 153 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water: photodegradation $t_{1/2} = 38 \text{ min}$ when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW Xenon lamp (De Felip et al. 1996)

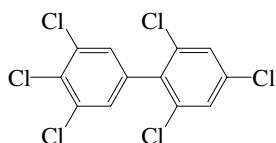
Ground water:

Sediment:

Soil:

Biota: clearance $t_{1/2} = 50-100 \text{ d}$ in guppy for hexachlorobiphenyl (Bruggeman et al. 1984);
 reported biological half-lives for hexachlorobiphenyls: $t_{1/2} = 87$ to $> 850 \text{ d}$ for trout, $t_{1/2} = 77-91 \text{ d}$ for trout muscle; $t_{1/2} > 200 \text{ d}$ for carp; $t_{1/2} = 75-175 \text{ d}$ for guppy (Niimi 1987);
 elimination $t_{1/2} = 26.4 \text{ d}$ from earthworm (Belfroid et al. 1995)
 depuration $t_{1/2} = 134 \text{ d}$ for high-dose treatment, $t_{1/2} = 153 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.168 2,3',4,4',5',6-Hexachlorobiphenyl (PCB-168)



Common Name: 2,3',4,4',5',6-Hexachlorobiphenyl

Synonym: PCB-168, 2,3',4,4',5',6-hexachloro-1,1'-biphenyl

Chemical Name: 2,3',4,4',5',6-hexachlorobiphenyl

CAS Registry No: 59291-65-5

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

110–111 (Erickson 1986)

133 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0134 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

5.72×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

9.76×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.87×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

5.40×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

6.88×10^{-4} , 6.24×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4816/(T/K) + 12.99$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

13.07 (calculated-P/C, Burkhard 1984)

46.91 (calculated-QSAR-MCI χ , Sabljic & Güsten 1989)

27.97 (calculated-QSAR, Dunnivant et al. 1992)

49.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 79 \pm 18\ kJ/mol$, $\Delta S_H = 0.23 \pm 0.06\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.76 (calculated-TSA, Burkhard 1984)

7.11 (calculated-TSA, Hawker & Connell 1988a)

7.23, 7.13; 6.76, 6.71 (multi-column HPLC- k' correlation; capillary GC-RV correlation, different stationary phases, Risby et al. 1990)

7.18, 6.74 (quoted average values from Risby et al. 1990, Sangster 1993)

7.17 (recommended, Hansch et al. 1995)

6.8539 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.39 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.56 (suspended particulate matter, Burkhard 1984)

5.222 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calc-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

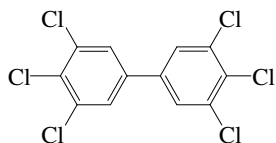
Ground water:

Sediment:

Soil:

Biota:

7.1.1.169 3,3',4,4',5,5'-Hexachlorobiphenyl (PCB-169)



Common Name: 3,3',4,4',5,5'-Hexachlorobiphenyl

Synonym: PCB-169, 3,3',4,4',5,5'-hexachloro-1,1'-biphenyl

Chemical Name: 3,3',4,4',5,5'-hexachlorobiphenyl

CAS Registry No: 32774-16-6

Molecular Formula: $C_{12}H_4Cl_6$

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

201–202.0 (Hutzinger et al. 1974)

201 (Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

310.0 (calculated-Le Bas method at normal boiling point)

237.4 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.0178 (calculated, Mackay et al. 1992; Passivirta et al. 1999)

0.0177 (Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.54×10^{-4} , 3.0×10^{-4} , 5.22×10^{-4} , 9.07×10^{-4} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.0000219; 0.000116 (generator column-GC, ECD; estimated, Hong & Qiao 1995)

$\log (S_L/(mol/L)) = -1.12 + 1403/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

0.000130 (generator column-GC/ECD, measured range 5 – $35^{\circ}C$, Huang & Hong 2002)—see Comment by van Noort 2004

0.000053, 0.000083, 0.000130, 0.000215 (5 , 15 , 25 , $35^{\circ}C$, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.08×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)

5.36×10^{-5} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

6.76×10^{-5} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log (P_L/Pa) = -5313/(T/K) + 13.64$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

1.03×10^{-4} , 1.82×10^{-6} (supercooled liquid P_L , solid P_S , Passivirta et al. 1999)

$\log (P_S/Pa) = 16.59 - 6715/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 13.64 - 5313/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1.57 (calculated-P/C, Burkhard et al. 1985b)

5.98 (calculated-QSPR-MCI χ , Sabljic & Güsten 1989)

6.60 (calculated-QSPR, Dunnivant et al. 1992)

0.85 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

23.4 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 162 \pm 20$ kJ/mol, $\Delta S_H = 0.51 \pm 0.07$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.42, 7.54, 7.62, 7.61 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 7.408 \pm 0.005 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 7.39, 7.55; 7.46, 7.42 (multi-column HPLC- k' correlation; capillary GC-RT correlation, different stationary phases, Risby et al. 1990)
 7.55 (recommended, Sangster 1993)
 7.41 (recommended, Hansch et al. 1995)
 7.01 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or indicated:

- 12.51, 11.32; 11.19 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 11.27 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 5.97; 7.50 (22°C, zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)
 5.97, 7.51 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.60 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for hexachlorobiphenyls, and the tropospheric lifetime $\tau(\text{calc}) = 29\text{--}60 \text{ d}$ at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_1 = 7200 \text{ d}^{-1}$; $k_2 = 0.00766 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 $k_1 = 2 \text{ (food lipid mg)/(g worm lipid-d)}$; $k_2 = 0.03 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)
 $k_2 = 0.0065 \text{ d}^{-1}$ with $t_{1/2} = 107 \text{ d}$ (newly contaminated oysters, Gardinali et al. 2004)
 $k_2 = 0.0082 \text{ d}^{-1}$ with $t_{1/2} = 85 \text{ d}$ (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995);
 $t_{1/2} = 6000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photodegradation $t_{1/2} = 548 \text{ min}$ when irradiated in a TiO_2 semiconductor aqueous suspension with a 1.5-kW high pressure Xenon lamp (De Felip et al. 1996);
 $t_{1/2} = 120000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Groundwater:

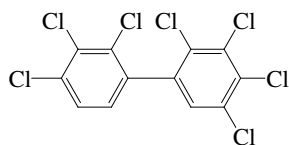
Sediment: $t_{1/2} = 165000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2} = 165000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2} = 24 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

Depuration $t_{1/2} = 107 \text{ d}$ for newly contaminated oysters, and $t_{1/2} = 85 \text{ d}$ for chronically contaminated oysters (Gardinali et al. 2004)

7.1.1.170 2,2',3,3',4,4',5-Heptachlorobiphenyl (PCB-170)



Common Name: 2,2',3,3',4,4',5-Heptachlorobiphenyl

Synonym: PCB-170, 2,2',3,3',4,4',5-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4',5-heptachlorobiphenyl

CAS Registry No: 35065-30-6

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

135 (Hutzinger et al. 1974; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0833 (mp at $135^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00767 (supercooled liquid S_L , Burkhard et al. 1985b)

0.00347 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.000504 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.000395 (calculated-TSA, Abramowitz & Yalkowsky 1990)

0.00052 (calculated-MCI χ , Patil 1991)

0.000130 (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

8.37×10^{-5} (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

3.37×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)

3.72×10^{-4} (supercooled liquid, GC-RI correlation, Burkhard et al. 1985b)

8.37×10^{-5} , 8.11×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.32×10^{-5} ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

5.13×10^{-5} , 7.76×10^{-5} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5139/(T/K) + 13.07$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19.25 (calculated-P/C, Burkhard 1985b)

1.52 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

0.912 (wetted-wall column-GC, Brunner et al. 1990)

8.85 (calculated-QSPR, Dunnivant et al. 1992)

0.128, 0.760, 4.139, $20.84^* \pm 0.80$, 78.50 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 61.342 - 19725.76/(T/K)$; temp range 4 – $31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(164.0/kJ\cdot mol^{-1})/RT] + (0.510/kJ\cdot mol^{-1}\cdot K^{-1})/R$; where $R = 8.314\ J\cdot K^{-1}\cdot mol^{-1}$ and temp range: 4 – $31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

19.4 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 164 \pm 9\ kJ/mol$, $\Delta S_H = 0.51 \pm 0.03\ kJ/mol\cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.05 (calculated-TSA, Burkhard 1984)
- 7.08 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
- 7.27 (calculated-TSA, Hawker & Connell 1988a)
- 7.03 (calculated-MCI χ , Patil 1991)
- 7.30 (calculated-TSA, Murray & Andren 1992)
- 6.83 (generator column-GC, Larsen et al. 1992)
- 6.96 (recommended, Sangster 1993)
- 7.10 (estimated, Girvin & Scott 1997)
- 7.0639 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 11.42 (10°C, estimated, Thomas et al. 1998)
- 12.34, 11.07; 11.02 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 10.69 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 2.43–4.76 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 3.75–4.61 (Various marine species, mean lipid-normalized BCF, Hope et al. 1999)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.85 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 5.63, 5.48, 5.42, 4.99 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
- 5.632, 5.675 (marine humic substances of 5 mg/L DOC, quoted; calculated-MCI χ , reported as association coefficient $\log K_h$, Sabljic et al. 1989)
- 6.10 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 6.60 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 164 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 180 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

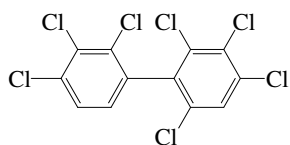
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 164 \text{ d}$ for high-dose treatment, $t_{1/2} = 180 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.171 2,2',3,3',4,4',6-Heptachlorobiphenyl (PCB-171)



Common Name: 2,2',3,3',4,4',6-Heptachlorobiphenyl

Synonym: PCB-171, 2,2',3,3',4,4',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4',6-heptachlorobiphenyl

CAS Registry No: 52663-71-5

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

117.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

250.3 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.29 (Miller et al. 1984; Ruelle et al. 1993)

22.80 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

51.04 (Miller et al. 1984; Shiu & Mackay 1986)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.124 (mp at $117.5^{\circ}C$)

0.109 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00624 (shake flask-GC/ECD, Dexter & Pavlou 1978)

0.00217 (generator column-GC/ECD, Miller et al. 1984,1985)

0.00412 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

9.81×10^{-6} (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)

0.00102, 0.000687, 0.000521 (RP-HPLC-k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.87×10^{-4} , 2.98×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Bidleman 1984)

5.71×10^{-4} (GC-RI correlation, Burkhard et al. 1985a)

4.69×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

2.57×10^{-4} , 3.17×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.73×10^{-5} , 2.50×10^{-4} (selected, solid P_S ; supercooled liquid P_L , Shiu & Mackay 1986)

1.26×10^{-4} , 2.09×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5008/(T/K) + 13.07$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

9.77×10^{-5} ($20^{\circ}C$, supercooled liquid P_L from Falconer & Bidleman 1994, Harner & Bidleman 1996)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

29.79 (calculated-P/C, Burkhard et al. 1985b)

5.40 (calculated-P/C, Shiu & Mackay 1986)

17.49 (calculated-QSPR, Dunnivant et al. 1992)

1.50 (calculated-QSPR, Achman et al. 1993)

59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K
 (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.14 (calculated-TSA, Burkhard 1984)
 6.68 (generator column-GC/ECD, Miller et al. 1984,1985)
 7.85 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
 7.04, 7.06 (RP-HPLC- k' correlation, different mobile phases, Brodsky & Ballschmiter 1988)
 7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
 6.99 (recommended, Sangster 1993)
 6.68 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

9.50 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
 10.51 (20°C, generator column-GC, measured range -10 to 30°C, Harner & Bidleman 1996)
 12.31, 11.78, 11.14, 10.51, 9.96 (-10, 0, 10, 20, 30°C, generator column-GC, Harner & Mackay 1995)
 $\log K_{OA} = -5.71 + 4757/(T/K)$; (temp range -10 to 30°C, Harner & Bidleman 1996)
 11.76, 10.51; 10.50 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 10.76 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.94 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.516 (marine humic substances of 5 mg/L DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.004$ d⁻¹ with $t_{1/2} = 156$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d⁻¹ with $t_{1/2} = 182$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

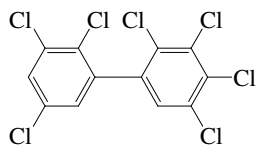
Sediment:

Soil:

Biota: $t_{1/2} = 260$ d in worms at 8°C (Oliver 1987c).

depuration $t_{1/2} = 156$ d for high-dose treatment, $t_{1/2} = 182$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.172 2,2',3,3',4,5,5'-Heptachlorobiphenyl (PCB-172)



Common Name: 2,2',3,3',4,5,5'-Heptachlorobiphenyl

Synonym: PCB-172, 2,2',3,3',4,5,5'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5,5'-heptachlorobiphenyl

CAS Registry No: 52663-74-8

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

113 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00688 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00430 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

3.14×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

4.98×10^{-4} (calculated-TSA and mp., Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.55×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

6.14×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

1.41×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -5109/(T/K) + 12.28$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

31.82 (calculated-P/C, Burkhard 1984)

1.317 (wetted wall column-GC/ECD, Brunner et al. 1990)

12.07 (calculated-QSPR, Dunnivant et al. 1992)

28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13 kJ/mol$, $\Delta S_H = 0.46 \pm 0.04 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.10 (calculated-TSA, Burkhard 1984)

7.21 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.85 (generator column-GC, Larsen et al. 1992)

7.33 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.03 (recommended, Sangster 1993)

7.2349 (molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

11.84, 10.67 (0, $20^{\circ}C$, multi-column GC- k' correlation, Zhang et al. 1999)

10.50 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.89 (suspended particulate matter, Burkhard 1984)
- 5.71, 5.44, 5.38, 4.97 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h , Lara & Ernst 1989)
- 5.711; 5.66 (marine humic substances with 5 mg/L DOC, reported as association coefficient log K_h , observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 165 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 179 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

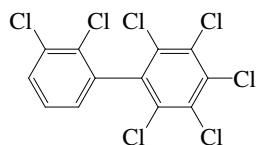
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 165 \text{ d}$ for high-dose treatment, $t_{1/2} = 179 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.173 2,2',3,3',4,5,6-Heptachlorobiphenyl (PCB-173)



Common Name: 2,2',3,3',4,5,6-Heptachlorobiphenyl

Synonym: PCB-173, 2,2',3,3',4,5,6-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5,6-heptachlorobiphenyl

CAS Registry No: 68194-16-1

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

145 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00731 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00416 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

6.265×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

5.55×10^{-5} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

6.14×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

29.89 (calculated-P/C, Burkhard 1984)

1.42 (wetted wall column-GC/ECD, Brunner et al. 1990)

18.48 (calculated-QSPR, Dunnivant et al. 1992)

59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9\ kJ/mol$, $\Delta S_H = 0.31 \pm 0.03\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.07 (calculated-TSA, Burkhard 1984)

7.02 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.30 (calculated-TSA, Murray & Andren 1992)

6.9556 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

11.79, 10.60 (0, $20^{\circ}C$, multi-column GC- k' correlation, Zhang et al. 1999)

10.48 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.87 (suspended particulate matter, Burkhard 1984)
- 5.532 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.40 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 2$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.03$ d⁻¹ (earthworm, Wågman et al. 2001)

$k_2 = 0.004$ d⁻¹ with $t_{1/2} = 162$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d⁻¹ with $t_{1/2} = 186$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

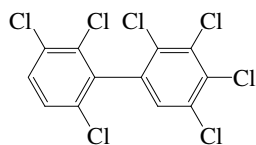
Sediment:

Soil:

Biota: elimination $t_{1/2} = 20$ d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2} = 162$ d for high-dose treatment, $t_{1/2} = 186$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.174 2,2',3,3',4,5,6'-Heptachlorobiphenyl (PCB-174)



Common Name: 2,2',3,3',4,5,6'-Heptachlorobiphenyl

Synonym: PCB-174, 2,2',3,3',4,5,6'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5,6'-heptachlorobiphenyl

CAS Registry No: 38411-25-5

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

130.6 (Burkhard 1985b)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (KJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.092 (mp at $130.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00625 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00525 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.001016 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.687×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

3.191×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.206×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.19×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

1.80×10^{-4} , 2.43×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

6.69×10^{-5} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

2.75×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4962/(T/K) + 12.90$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

93.53 (calculated-P/C, Burkhard 1984)

4.96 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

1.419 (wetted wall column-GC/ECD, Brunner et al. 1990;)

17.13 (calculated-QSPR, Dunnivant et al. 1992)

4.91 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

49.6 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 113 \pm 11$ kJ/mol, $\Delta S_H = 0.35 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.14 (calculated-TSA, Burkhard 1984)

6.85 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

- 6.85 (recommended, Sangster 1993)
7.10 (estimated, Girvin & Scott 1997)
6.9132 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 11.67, 10.51; 10.64 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
10.38 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Biota Sediment Accumulation Factor, BSAF:

- 89 (trout in Lake Ontario, Niimi 1996)
0.29, 2.8, 1.4 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.94 (suspended particulate matter, Burkhard 1984)
5.52 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)
5.82 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.60 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1979)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 160 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 194 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

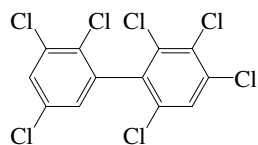
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 160 \text{ d}$ for high-dose treatment, $t_{1/2} = 194 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.175 2,2',3,3',4,5',6-Heptachlorobiphenyl (PCB-175)



Common Name: 2,2',3,3',4,5',6-Heptachlorobiphenyl

Synonym: PCB-175, 2,2',3,3',4,5',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5',6-heptachlorobiphenyl

CAS Registry No: 40186-70-7

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

133 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00557 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00894 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00104 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

4.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.00×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

7.72×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

3.98×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4962/(T/K) + 12.22$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

49.55 (calculated-P/C, Burkhard 1984)

22.63 (calculated-QSPR, Dunnivant et al. 1992)

2.069 (calculated-QSPR, Achman et al. 1993)

59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9\ kJ/mol$, $\Delta S_H = 0.31 \pm 0.03\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.19 (calculated-TSA, Burkhard 1984)

6.92 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988a)

7.17 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)

6.92 (recommended, Sangster 1993)

7.10 (estimated, Girvin & Scott 1997)

7.0957 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

11.35, 10.17 (0, $20^{\circ}C$, multi-column GC- k' correlation, Zhang et al. 1999)

10.83 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Biota Sediment Accumulation Factor, BSAF:

144 (trout in Lake Ontario, Niimi 1996)

Sorption Partition Coefficient, log K_{OC} :

6.99 (suspended particulate matter, Burkhard 1984)

5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

6.60 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 154 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 169 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

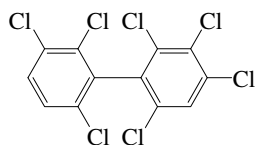
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 154 \text{ d}$ for high-dose treatment, $t_{1/2} = 169 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.176 2,2',3,3',4,6,6'-Heptachlorobiphenyl (PCB-176)



Common Name: 2,2',3,3',4,6,6'-Heptachlorobiphenyl

Synonym: PCB-176, 2,2',3,3',4,6,6'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,6,6'-heptachlorobiphenyl

CAS Registry No: 52663-65-7

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

101 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00601 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00585 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00280 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00314 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.52×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.66×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

5.31×10^{-4} , 8.83×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.35×10^{-5} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 11.50 - 5080/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

4.17×10^{-4} , 7.24×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4579/(T/K) + 12.07$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

100 (calculated-P/C, Burkhard 1984)

9.12 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

30.11 (calculated-QSPR, Dunnivant et al. 1992)

3.13 (calculated-QSPR, Achman et al. 1993)

107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.16 (calculated-TSA, Burkhard 1984)

6.55 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.76 (generator column-GC, Larsen et al. 1992)

6.65 (recommended, Sangster 1993)

6.6653 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 11.22, 10.06; 10.13 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
10.64 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.96 (suspended particulate matter, Burkhard 1984)
5.358 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 184 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 153 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

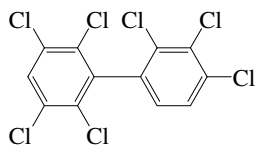
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 184 \text{ d}$ for high-dose treatment, $t_{1/2} = 153 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.177 2,2',3,3',4,5',6'-Heptachlorobiphenyl (PCB-177)



Common Name: 2,2',3,3',4,5',6'-Heptachlorobiphenyl

Synonym: PCB-177, 2,2',3,3',4,5',6'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5',6'-heptachlorobiphenyl

CAS Registry No: 52663-70-4

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

145 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00656 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00482 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00150 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

4.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.40×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

4.88×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

2.50×10^{-4} , 3.38×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

4.15×10^{-5} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

1.38×10^{-4} , 2.51×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4962/(T/K) + 13.04$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

26.45 (calculated-P/C, Burkhard 1984)

3.34 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

15.55 (calculated-QSPR, Dunnivant et al. 1992)

2.069 (calculated-QSPR, Achman et al. 1993)

5.12 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

50.6 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 112 \pm 11$ kJ/mol, $\Delta S_H = 0.34 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.12 (calculated-TSA, Burkhard 1984)

6.73 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.76 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.73 (recommended, Sangster 1993)

- 7.10 (estimated, Girvin & Scott 1997)
6.9207 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 11.74, 10.58 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
10.63 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.92 (suspended particulate matter, Burkhard 1984)
5.54, 5.39, 5.35, 4.90 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
5.359; 5.52 (marine humic substances with 5 mg/L of DOC, reported as association coefficient $\log K_h$, observed; calculated-molecular connectivity indices, Sabljic et al. 1989)
5.82 (Ispra soil, shake flask-GC, Paya-Perez et al. 1991)
6.60 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 147 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 186 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

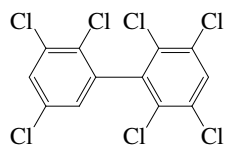
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 147 \text{ d}$ for high-dose treatment, $t_{1/2} = 186 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.178 2,2',3,3',5,5',6-Heptachlorobiphenyl (PCB-178)



Common Name: 2,2',3,3',5,5',6-Heptachlorobiphenyl

Synonym: PCB-178, 2,2',3,3',5,5',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',5,5',6-heptachlorobiphenyl

CAS Registry No: 52663-67-9

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

125 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00588 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00884 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.001016 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.000627 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.57×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

7.24×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

1.47×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P/mmHg) = 11.70 - 5220/(T/K)$ (GC-RT correlation, Tateya et al. 1988)

4.57×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4962/(T/K) + 13.28$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

44.08 (calculated-P/C, Burkhard 1984)

6.586 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

2.33 (wetted wall column-GC/ECD, Brunner et al. 1990)

21.61 (calculated-QSPR, Dunnivant et al. 1992)

11.2 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

71.4 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 90 \pm 10\ kJ/mol$, $\Delta S_H = 0.27 \pm 0.03\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.17 (calculated-TSA, Burkhard 1984)

6.85 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.14 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.85 (recommended, Sangster 1993)

7.0564 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

11.28, 10.12 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)

10.33 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.97 (suspended particulate matter, Burkhard 1984)

5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 156 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 166 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

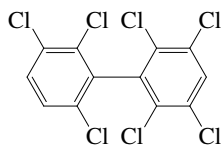
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 156 \text{ d}$ for high-dose treatment, $t_{1/2} = 166 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.179 2,2',3,3',5,6,6'-Heptachlorobiphenyl (PCB-179)



Common Name: 2,2',3,3',5,6,6'-Heptachlorobiphenyl

Synonym: PCB-179, 2,2',3,3',5,6,6'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',5,6,6'-heptachlorobiphenyl

CAS Registry No: 52663-64-6

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

99 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00632 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00454 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.0039 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.42×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.55×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

5.15×10^{-4} , 1.004×10^{-3} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

5.01×10^{-4} , 8.71×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4579/(T/K) + 12.07$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

88.96 (calculated-P/C, Burkhard 1984)

2.432 (wetted wall column-GC/ECD, Brunner et al. 1990)

27.91 (calculated-QSPR, Dunnivant et al. 1992)

37.3 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 144 \pm 7$ kJ/mol, $\Delta S_H = 0.45 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.77, 8.13 (RP-HPLC- k' correlation: uncorrected, with ortho correction, Rapaport & Eisenreich 1984)

7.14 (calculated-TSA, Burkhard 1984)

6.41 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.73 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.41 (recommended, Sangster 1993)

6.6366 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

11.26, 10.10 (0, 20°C, multi-column k' correlation, Zhang et al. 1999)

10.34 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.94 (suspended particulate matter, Burkhard 1984)

5.358 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 171 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 198 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

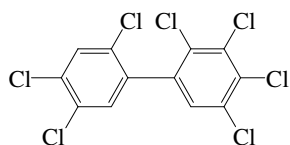
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 171 \text{ d}$ for high-dose treatment, $t_{1/2} = 198 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.180 2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB-180)



Common Name: 2,2',3,4,4',5,5'-Heptachlorobiphenyl

Synonym: PCB-180, 2,2',3,4,4',5,5'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',5,5'-heptachlorobiphenyl

CAS Registry No: 35065-29-3

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

109–110 (Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$): 240–280 (20mm Hg)

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

250.3 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.144 (calculated-Mackay et al. 1992; Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

0.00656 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

0.00385 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.00031 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00063 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.00053 (calculated-MCI χ , Patil 1991)

2.45×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

$\log S_L$ (mol/L) = $-1.676 + 1132/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

3.17×10^{-3} ; 5.22×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)

$\log S_L/(mol\ m^{-3}) = -1356/(T/K) - 0.33$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

8.10×10^{-5} (Verlag Chemie 1983)

1.30×10^{-4} , 1.29×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Bidleman 1984)

8.07×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)

5.06×10^{-4} (supercooled liquid P_L , calculated-GC-RI correlation, Burkhard 1985b)

1.21×10^{-4} , 1.43×10^{-4} (supercooled liquid. P_L , GC-RT correlation, different stationary phases Foreman & Bidleman 1985)

3.14×10^{-5} ($20^{\circ}C$, supercooled liquid, calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

8.13×10^{-5} , 1.20×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log (P_L/Pa) = -5042/(T/K) + 13.03$ (GC-RT correlation, Falconer & Bidleman 1994)

1.45×10^{-4} , 2.09×10^{-5} (supercooled liquid P_L , solid P_S , Passivirta et al. 1999)

$\log (P_S/Pa) = 15.98 - 6173/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 13.03 - 5042/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.32×10^{-4} ; 1.072×10^{-4} (supercooled P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log P_L/Pa = -4809/(T/K) + 12.16$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m³/mol at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 30.40 (calculated-P/C, Burkhard et al. 1985b)
- 3.24 (20°C, calculated-P/C, Murphy et al. 1987)
- 1.013 (wetted-wall column-GC/ECD, Brunner et al. 1990)
- 10.88 (calculated-QSPR, Dunnivant et al. 1992)
- 7.10 (estimated, Girvin & Scott 1997)
- $\log H/(\text{Pa m}^3/\text{mol}) = 14.71 - 3910/(T/K)$ (Passivirta et al. 1999)
- 37.0* \pm 0.20 (gas stripping-GC, measured range 4–31°C, Bamford et al. 2000)
- $K_{AW} = \exp[-(143.6/\text{kJ}\cdot\text{mol}^{-1})/RT] + (0.447/\text{kJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})/R$; where $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and temp range: 4–31°C, (gas stripping-GC, Bamford et al. 2000)
- 37.3 (exptl. data, Bamford et al. 2002)—see Comment by Goss et al. 2004
- $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 144 \pm 7 \text{ kJ/mol}$, $\Delta S_H = 0.45 \pm 0.03 \text{ kJ/mol}\cdot\text{K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004
- 5.89, 8.51 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)
- $\log H/(\text{Pa m}^3/\text{mol}) = -3453/(T/K) + 12.49$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.12 (calculated-TSA, Burkhard 1984)
- 6.70 (calculated-chlorine substituents, Oliver 1987a)
- 7.21 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)
- 7.36 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 7.02 (calculated-MCI χ , Patil 1991)
- 7.40 (calculated-TSA, Murray & Andren 1992)
- 6.56 (average, generator column-GC, Larsen et al. 1992)
- 6.89 (recommended, Sangster 1993)
- 7.2506 (calculated-molecular properties MNDO-AM1, Makino 1998)
- 7.20 (calculated, Passivirta et al. 1999)
- 7.29, 7.16 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

- 10.75* (20°C, generator column-GC, measured range –10 to 30°C, Harner & Bidleman 1996)
- $\log K_{OA} = -4.70 + 4535/(T/K)$; (temp range –10 to 30°C, Harner & Bidleman 1996)
- 9.88; 9.72 (fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
- $\log K_{OA} = -3.31 + 3930/(T/K)$; (fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
- 11.22 (10°C, estimated, Thomas et al. 1998)
- 9.88 (quoted, Kömp & McLachlan 1997b; Kaupp & McLachlan 1999)
- 11.94, 10.72; 10.86 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 10.85 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)
- 10.12, 10.16 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)
- $\log K_{OA} = 4975/(T/K) - 6.55$ (LDV linear regression of literature data, Li et al. 2003)
- $\log K_{OA} = 4845/(T/K) - 6.09$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$:

- 2.99–5.68 (various marine species, mean dry wt. BCF, Hope et al. 1998)
- 4.22–6.41 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)
- 4.45, 6.45 (*Daphnia magna*, 21-d exposure: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 6.06, 7.36 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$ at 25°C or as indicated:

- 6.92 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 6.2–7.4, 6.9; 7.30 (suspended sediments, range; average, algae > 50 μm , Oliver 1987a)
- 6.51 (Lake Michigan water column, Swackhamer & Armstrong 1987)

- 5.73, 5.54, 5.50, 5.09 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
- 5.73; 5.66 (marine humic substances at 5 mg/L DOC, quoted; calculated-MCI χ , reported as $\log K_h$, Sabljic et al. 1989)
- 6.36, 6.23, 6.10 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
- 5.78 (Ispra soil, shake flask-GC/ECD, Paya-Perez et al. 1991)
- 6.60 (colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 6.60 (soil, calculated- K_{ow} , Girvin & Scott 1997)
- 6.53–7.76; 5.80–7.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
- 5.42; 6.56, 7.42, 6.83 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
- 6.31–6.98 (field contaminated sediment, initial-final values for 2–1461 d contact time, gas-purge technique-GC/ECD, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.049 \text{ h}^{-1}$; $k_1 = 0.008 \text{ h}^{-1}$ (mayfly-sediment model II, Gobas et al. 1989)

$k_2 = 0.0246 \text{ d}^{-1}$ with an elimination $t_{1/2} = 282 \text{ d}$ (earthworm, Belfroid et al. 1995)

$k_1 = 0.00348 \text{ h}^{-1}$; $k_2 = 0.111 \text{ h}^{-1}$ (blood plasma of ring doves, Drouillard & Norstrom 2000)

$k_1(\text{calc}) = 2$ (food lipid mg)/(g worm lipid-d); $k_2(\text{calc}) = 0.03 \text{ d}^{-1}$ (earthworm, Wågman et al. 2001)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 162 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 186 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

$k_2 = 0.021 \text{ d}^{-1}$ with $t_{1/2} = 33.0 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004)

Half-Lives in the Environment:

Air: $t_{1/2} = 12000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 240000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent, $t_{1/2} = 25 \text{ yr}$ (Geyer et al. 2000)

$t_{1/2} = 330000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2} = 333000 \text{ h}$ at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2} = 28.3 \text{ d}$ from earthworm (Belfroid et al. 1995);

elimination $t_{1/2} = 22 \text{ d}$ in earthworm given contaminated food (predicted, Wågman et al. 2001)

depuration $t_{1/2} = 162 \text{ d}$ for high-dose treatment, $t_{1/2} = 186 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

depuration $t_{1/2} = 33.0 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004)

TABLE 7.1.1.180.1

Reported Henry's law constants and octanol-air partition coefficients of 2,2',3,4,4',5,5'-heptachlorobiphenyl (PCB-180) at various temperatures and temperature dependence equations

Henry's law constant		log K _{OA}	
Bamford et al. 2000		Harner & Bidleman 1996	
gas stripping-GC/MS		generator column-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
4	0.425	-10	12.46
11	2.025	0	12.00
18	8.96	10	11.38
25	37.0	20	10.75
31	118.5	30	10.23

$\ln K_{AW} = -\Delta H/RT + \Delta S/R$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 86.83$	
A	53.7647	$\log K_{OA} = A + B/T$	
B	17272	A	-4.695
enthalpy, entropy change:		B	4535
$\Delta H/(\text{kJ}\cdot\text{mol}^{-1}) = 143.6 \pm 7.4$			
$\Delta S/(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) = 447 \pm 26$			

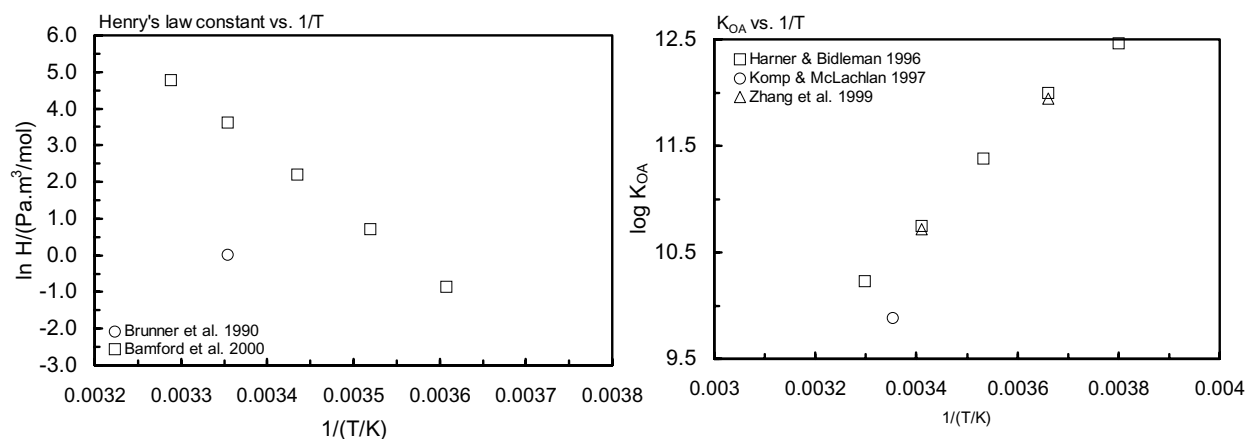
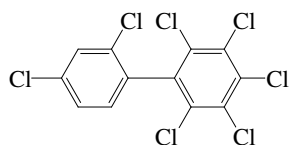


FIGURE 7.1.1.180.1 Logarithm of Henry's law constant and K_{OA} versus reciprocal temperature for 2,2',3,4,4',5,5'-heptachlorobiphenyl (PCB-180).

7.1.1.181 2,2',3,4,4',5,6-Heptachlorobiphenyl (PCB-181)



Common Name: 2,2',3,4,4',5,6-Heptachlorobiphenyl

Synonym: PCB-181, 2,2',3,4,4',5,6-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',5,6-heptachlorobiphenyl

CAS Registry No: 74472-47-2

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

140 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00625 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

4.44×10^{-4} , 5.21×10^{-4} , 2.30×10^{-4} , 4.54×10^{-4} (RP-HPLC- k' correlation, different stationary and mobile phases Brodsky & Ballschmiter 1988)

3.95×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.44×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

7.11×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

2.92×10^{-4} , 4.206×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.54×10^{-4} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P_L/Pa) = -4962/(T/K) + 13.11$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

40.83 (calculated-P/C, Burkhard 1984)

23.31 (calculated-QSPR, Dunnivant et al. 1992)

59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.14 (calculated-TSA, Burkhard 1984)

7.11, 7.12, 7.19, 7.11 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.13 (recommended, Sangster 1993)

7.0558 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.61 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log K_B$ or $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

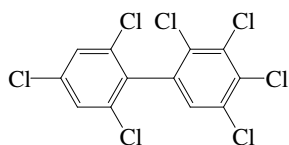
6.94 (suspended particulate matter, Burkhard 1984)

5.516 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constant and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.182 2,2',3,4,4',5,6'-Heptachlorobiphenyl (PCB-182)



Common Name: 2,2',3,4,4',5,6'-Heptachlorobiphenyl

Synonym: PCB-182, 2,2',3,4,4',5,6'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',5,6'-heptachlorobiphenyl

CAS Registry No: 60145-23-5

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

152 (Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.0567 (mp at $152^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.34×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

8.26×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

3.95×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

1.36×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.31×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.43×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

3.66×10^{-4} , 3.56×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.14×10^{-4} , 3.72×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4962/(T/K) + 13.11$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

97.07 (calculated-P/C, Burkhard 1984)

26.04 (calculated-QSPR, Dunnivant et al. 1992)

2.07 (calculated-QSPR, Achman et al. 1993)

8.71 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

63.8 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 97 \pm 10\ kJ/mol$, $\Delta S_H = 0.30 \pm 0.04\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.22 (calculated-TSA, Burkhard 1984)

6.92 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.92 (recommended, Sangster 1993)

7.0964 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.42 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

7.02 (suspended particulate matter, Burkhard 1984)

5.501 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calc-molecular connectivity indices, Sabljic et al. 1989)

6.10 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 159 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 182 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

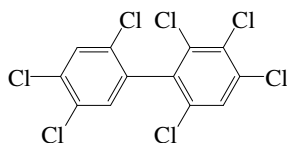
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 159 \text{ d}$ for high-dose treatment, $t_{1/2} = 182 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.183 2,2',3,4,4',5',6-Heptachlorobiphenyl (PCB-183)



Common Name: 2,2',3,4,4',5',6-Heptachlorobiphenyl

Synonym: PCB-183, 2,2',3,4,4',5',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',5',6-heptachlorobiphenyl

CAS Registry No: 52663-69-1

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

152 (estimated, Abramowitz & Yalkowsky 1990)

83 (Kühne et al. 1995; Ruelle & Kesselring 1997; Ran et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

250.3 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.270 (mp at $83^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00534 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00490 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

3.14×10^{-4} , 4.98×10^{-4} , 6.27×10^{-4} , 5.09×10^{-4} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

3.14×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

0.000641 (calculated-group contribution method, Kühne et al. 1995)

9.27×10^{-4} , 2.49×10^{-3} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.77×10^{-3} (calculated-mp and K_{OW} , Ran et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.38×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

7.05×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

3.57×10^{-4} , 5.09×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

8.61×10^{-5} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

2.0×10^{-4} , 3.24×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4962/(T/K) + 13.19$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

47.32 (calculated-P/C, Burkhard 1984)

6.89 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

20.40 (calculated-QSPR, Dunnivant et al. 1992)

2.069 (calculated-QSPR, Achman et al. 1993)

0.326, 0.954 (0, $15^{\circ}C$, from modified two-film exchange model, Hornbuckle et al. 1994)

8.02 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

61.5 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 100 \pm 10$ kJ/mol, $\Delta S_H = 0.30 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 7.22 (calculated-TSA, Burkhard 1984)
- 7.02, 7.13, 6.96, 7.07 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
- 7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 6.78 (generator column-GC, Larsen et al. 1992)
- 6.92 (recommended, Sangster 1993)
- 7.0868 (calculated-molecular properties MNDO-AM1 method, Makino 1998)
- 8.27 (calculated-CLOGP ver. 4, Ran et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.80 (10°C, estimated, Thomas et al. 1998)
- 11.44, 10.26; 10.35 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
- 10.83 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.84, 7.37 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor, BSAF:

- 220 (trout in Lake Ontario, Niimi 1996)
- 0.52, 4.2, 0.84 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, $\log K_{oc}$:

- 7.02 (suspended particulate matter, Burkhard 1984)
- 5.53, 5.40, 5.35, 4.92 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
- 5.53; 5.50 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, observed; calculated-molecular connectivity indices, Sabljic et al. 1989)
- 6.36, 6.25, 6.09 (North Sea sediments, field measurement-GC/ECD, Lara & Ernst 1990)
- 5.82 (Ispra soil, batch equilibrium-GC/ECD, Paya-Perez et al. 1991)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 165 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.003 \text{ d}^{-1}$ with $t_{1/2} = 206 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

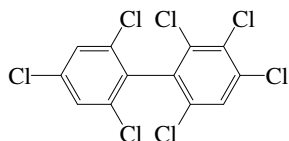
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 165 \text{ d}$ for high-dose treatment, $t_{1/2} = 206 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.184 2,2',3,4,4',6,6'-Heptachlorobiphenyl (PCB-184)



Common Name: 2,2',3,4,4',6,6'-Heptachlorobiphenyl

Synonym: PCB-184, 2,2',3,4,4',6,6'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',6,6'-heptachlorobiphenyl

CAS Registry No: 74472-48-3

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

108 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00514 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00198 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$):

1.65×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.80×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

126.7 (calculated-P/C, Burkhard 1984)

46.42 (calculated-QSPR, Dunnivant et al. 1992)

3.94 (calculated-QSPR, Achman et al. 1993)

107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5\ kJ/mol$, $\Delta S_H = 0.18 \pm 0.02\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.23 (calculated-TSA, Burkhard 1984)

6.85 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.76 (generator column-GC, Larsen et al. 1992)

6.65 (recommended, Sangster 1993)

6.8203 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.73 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

7.03 (suspended particulate matter, Burkhard 1984)

5.342 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 2$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.03$ d⁻¹ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air:

Surface water:

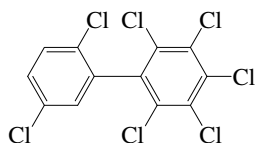
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 20$ d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.185 2,2',3,4,5,5',6-Heptachlorobiphenyl (PCB-185)



Common Name: 2,2',3,4,5,5',6-Heptachlorobiphenyl

Synonym: PCB-185, 2,2',3,4,5,5',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,5,5',6-heptachlorobiphenyl

CAS Registry No: 52712-05-7

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

149 (Bruggeman et al. 1982; Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.3702

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

250.3 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0607 (mp at $149^{\circ}C$)

0.0595 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00047 (generator column-GC/ECD, Weil et al. 1974)

0.00546 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

5.71×10^{-4} , 8.26×10^{-4} , 6.27×10^{-4} , 6.56×10^{-4} (RP- HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.75×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)

7.28×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

3.21×10^{-4} , 4.78×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.70×10^{-4} , 2.95×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4962/(T/K) + 13.15$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

46.0 (calculated-P/C, Burkhard et al. 1985b)

1.62 (wetted-wall column-GC, Brunner et al. 1990)

21.71 (calculated-QSPR, Dunnivant et al. 1992)

2.67 (calculated-QSPR, Achman et al. 1993)

59.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 101 \pm 9$ kJ/mol, $\Delta S_H = 0.31 \pm 0.03$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.93 (TLC-RT correlation, Bruggeman et al. 1982)

7.01, 6.98, 6.96, 7.00 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.11 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.99 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.58 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

4.36 (*Picea omorika*, Reischl et al. 1989 from Reischl 1988)
 5.93; 7.46 (22°C, zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)
 5.93, 7.47 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

5.95 (Koch 1983)
 6.94 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.52 (marine humic substances of 5 mg/L DOC, calculated-MCI χ , reported as $\log K_h$, Sabljic et al. 1989)
 5.33 (calculated- K_{OW} , Bahnick & Doucette 1988)
 6.43 (calculated after Karickhoff et al. 1979, Capel & Eisenreich 1990)
 5.28 (calculated after Schwarzenbach & Westall 1981, Capel & Eisenreich 1990)
 6.29, 6.08, 6.13 (North Sea sediments, field measurement-GC/ECD, Lara & Ernst 1990)
 5.80 (calculated-MCI, Park & Lee 1993)
 6.50 (soil, calculated- K_{OW} , Girvin & Scott 1997)
 6.40 (soil, calculated-universal solvation model; Winglet et al. 2000)

Sorption Partition Coefficient, $\log K_{OM}$:

5.95, 5.31 (selected, calculated-molecular connectivity indices χ , Sabljic 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 5810 \text{ d}^{-1}$; $k_2 = 0.00677 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 156 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 184 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

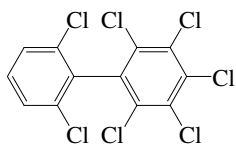
Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 48 \text{ d}$ in *Picea omorika* (Reischl et al. 1989 from Reischl 1988).
 depuration $t_{1/2} = 156 \text{ d}$ for high-dose treatment, $t_{1/2} = 184 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.186 2,2',3,4,5,6,6'-Heptachlorobiphenyl (PCB-186)



Common Name: 2,2',3,4,5,6,6'-Heptachlorobiphenyl

Synonym: PCB-186

Chemical Name: 2,2',3,4,5,6,6'-heptachlorobiphenyl

CAS Registry No: 74472-49-4

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

142 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00672 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00157 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.35×10^{-3} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.47×10^{-3} (GC-RI correlation, Burkhard et al. 1985b)

4.68×10^{-4} , 7.55×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -4579/(T/K) + 12.03$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

79.13 (calculated-P/C, Burkhard 1984)

37.3 (calculated-QSPR, Dunnivant et al. 1992)

107.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.11 (calculated-TSA, Burkhard 1984)

6.69 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.7069 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.36 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.91 (suspended particulate matter, Burkhard 1984)

5.383 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air:

Surface water:

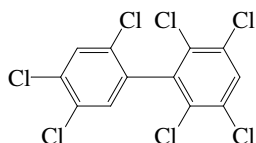
Ground water:

Sediment:

Soil:

Biota:

7.1.1.187 2,2',3,4',5,5',6-Heptachlorobiphenyl (PCB-187)



Common Name: 2,2',3,4',5,5',6-Heptachlorobiphenyl

Synonym: PCB-187, 2,2',3,4',5,5',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',5,5',6-heptachlorobiphenyl

CAS Registry No: 52663-68-0

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

149.0 (Mackay et al. 1980; Burkhard et al. 1985a)

147 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

417 (calculated, Mackay et al. 1982; Shiu & Mackay 1986)

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

250.3 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0607 (mp at $149^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.70×10^{-4} (generator column-GC/ECD, Weil et al. 1974)

0.00451 ($20^{\circ}C$, supercooled liquid S_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

0.0826 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.05×10^{-4} (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)

3.92×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)

5.98×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

3.47×10^{-4} , 5.74×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

9.42×10^{-5} ($20^{\circ}C$, supercooled liquid P_L , calculated-mole fraction of Aroclor mixtures, Murphy et al. 1987)

2.14×10^{-4} , 3.72×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -4977/(T/K) + 12.96$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

42.15 (calculated-P/C, Burkhard et al. 1985b)

8.41 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

20.55 (calculated-QSPR, Dunnivant et al. 1992)

2.07 (calculated-QSPR, Achman et al. 1993)

3.304, 8.72, 23.84, 82.20 ± 2.2 , 136.7 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 35.242 - 11582.87/(T/K)$; temp range 4 – $31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(96.3/kJ \cdot mol^{-1})/RT] + (0.293/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314 J \cdot K^{-1} \cdot mol^{-1}$ and temp range: 4 – $31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

65.9 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 96 \pm 7$ kJ/mol, $\Delta S_H = 0.29 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.19	(calculated-TSA, Burkhard 1984)
6.92	(RP-HPLC-RI correlation, Brodsky & Ballschmiter 1988)
7.17	(calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
7.40	(calculated-TSA, Murray & Andren 1992)
6.76	(generator column-GC, Larsen et al. 1992)
6.84	(recommended, Sangster 1993)
7.10	(estimated, Girvin & Scott 1997)
7.0464	(calculated-molar properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

9.87; 9.25	(fugacity meter/generator column-GC; calculated, Kömp & McLachlan 1997a)
$\log K_{OA} = -5.20 + 4490/(T/K)$	(fugacity meter, temp range 10–43°C, Kömp & McLachlan 1997a)
10.85	(10°C, estimated, Thomas et al. 1998)
11.36, 10.22	(0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
10.54	(calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

3.51–5.48	(various marine species, mean dry wt. BCF, Hope et al. 1998)
4.94–6.05	(various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Biota Sediment Accumulation Factor, BSAF:

244	(trout in Lake Ontario, Niimi 1996)
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Sorption Partition Coefficient, $\log K_{OC}$:

6.99	(suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
5.51, 5.40, 5.33, 4.90	(marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
5.51; 5.50	(marine humic substances of 5 mg/L DOC, quoted; calculated-MCI χ , reported as $\log K_h$, Sabljic et al. 1989)
6.60	(colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
6.60	(soil, calculated- K_{OW} , Girvin & Scott 1997)
6.40; 6.00	(soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 131 \text{ d}$ and $k_2 = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 71 \text{ d}$ for food concn of 22 ng/g and 125 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 159 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
- $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 190 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

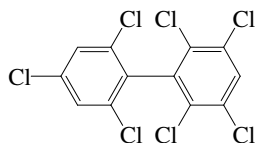
Sediment:

Soil:

Biota: depuration $t_{1/2} = 71\text{--}131$ d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 159$ d for high-dose treatment, $t_{1/2} = 190$ d for high-dose + enzyme CYP1A-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.188 2,2',3,4',5,6,6'-Heptachlorobiphenyl (PCB-188)



Common Name: 2,2',3,4',5,6,6'-Heptachlorobiphenyl

Synonym: PCB-188, 2,2',3,4',5,6,6'-heptachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4',5,6,6'-heptachlorobiphenyl

CAS Registry No: 74487-85-7

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

130 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.00538 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

0.00451 ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

0.00128 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00125 (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.55×10^{-3} (S_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

9.55×10^{-4} , 1.69×10^{-3} , 2.96×10^{-5} (P_L supercooled liquid values: calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

8.51×10^{-4} , 1.50×10^{-3} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

9.42×10^{-5} ($20^{\circ}C$, supercooled liquid, Murphy et al. 1987)

$\log(P_L/Pa) = -4579/(T/K) + 13.29$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

113.5 (calculated-P/C, Burkhard 1984)

8.41 ($20^{\circ}C$, calculated-P/C, Murphy et al. 1987)

44.95 (calculated-QSPR, Dunnivant et al. 1992)

15.77, 31.39, 60.5, 113.1 ± 4.0 , 188.6 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 21.891 - 7457.3/(T/K)$; temp range $4-31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(62.0/kJ \cdot mol^{-1})/RT] + (0.182/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314 J \cdot K^{-1} \cdot mol^{-1}$ and temp range: $4-31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

107.9 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 62 \pm 5$ kJ/mol, $\Delta S_H = 0.18 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.21 (calculated-TSA, Burkhard 1984)

6.78 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

- 6.82 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
6.78 (recommended, Sangster 1993)
6.7947 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 10.22 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.01 (suspended particulate matter, Burkhard 1984)
5.342 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$$k_1 = 2 \text{ (food lipid mg)/(g worm lipid-d)}; k_2 = 0.03 \text{ d}^{-1} \text{ (earthworm, Wågman et al. 2001)}$$

Half-Lives in the Environment:

Air:

Surface water:

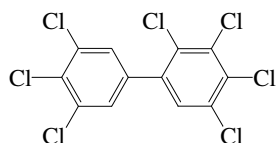
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 21 \text{ d}$ in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.189 2,3,3',4,4',5,5'-Heptachlorobiphenyl (PCB-189)



Common Name: 2,3,3',4,4',5,5'-Heptachlorobiphenyl

Synonym: PCB-189, 2,3,3',4,4',5,5'-heptachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,4',5,5'-heptachlorobiphenyl

CAS Registry No: 39635-31-9

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

170 (Burkhard et al. 1985b)

163 (Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0378 (mp at $170^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0063 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

7.53×10^{-5} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.26×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

1.30×10^{-4} ; 4.47×10^{-5} (generator column-GC/ECD, estimated, Hong & Qiao 1995)

4.05×10^{-4} (calculated-mp and K_{ow} , Ran et al. 2002)

0.000063 (generator column-GC/ECD, measured range $5-35^{\circ}C$, Huang & Hong 2002)—see Comment by van Noort 2004

0.000029, 0.000044, 0.000063, 0.000136 ($5, 15, 25, 35^{\circ}C$, generator column-GC/ECD, Huang & Hong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.44×10^{-4} (P_L supercooled liquid GC-RT correlation, Burkhard et al. 1985a)

5.95×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)

4.77×10^{-5} , 3.30×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.69×10^{-5} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -5300/(T/K) + 13.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

9.18 (calculated-P/C, Burkhard et al. 1985a)

6.74 (calculated-QSPR, Dunnivant et al. 1992)

0.903 (calculated-QSPR, Achman et al. 1993)

28.8 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.14 (calculated-TSA, Burkhard 1984)

7.72 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.71 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

- 6.75 (generator column-GC, Larsen et al. 1992)
- 7.24 (recommended, Sangster 1993)
- 7.15 (generator column-GC/ECD, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.81, 11.54; 11.45 (0, 20°C, multi-column GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
- 11.15 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 6.41, 7.71 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.94 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
- 5.817 (as $\log K_h$, association coefficient with marine humic substance, calculated- χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.011 \text{ d}^{-1}$ with $t_{1/2} = 64 \text{ d}$ and $k_2 = 0.012 \text{ d}^{-1}$ with $t_{1/2} = 58 \text{ d}$ for food concn of 19 ng/g and 138 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 176 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 171 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

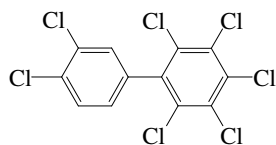
Sediment:

Soil:

Biota: reported biological $t_{1/2} > 200 \text{ d}$ for heptachlorobiphenyls in carp (Niimi 1987)

Depuration $t_{1/2} = 58\text{--}64 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 176 \text{ d}$ for high-dose treatment, $t_{1/2} = 171 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.190 2,3,3',4,4',5,6-Heptachlorobiphenyl (PCB-190)

Common Name: 2,3,3',4,4',5,6-Heptachlorobiphenyl

Synonym: PCB-190, 2,3,3',4,4',5,6-heptachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,4',5,6-heptachlorobiphenyl

CAS Registry No: 41411-64-7

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

117.0 (Burkhard et al. 1985b)

116 (Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.125 (mp at $117^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00767 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

4.98×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

1.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

2.20×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.96×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

2.70×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)

1.09×10^{-4} , 1.47×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

5.13×10^{-5} , 7.08×10^{-5} (supercooled liquid P_L : GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5109/(T/K) + 13.17$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

10.06 (calculated-P/C, Burkhard 1984)

11.37 (calculated-QSPR, Dunnivant et al. 1992)

28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13 kJ/mol$, $\Delta S_H = 0.46 \pm 0.04 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.05 (calculated-TSA, Burkhard 1984)

7.08 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.46 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.08 (recommended, Sangster 1993)

7.2887 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

12.09, 10.87 (0, $20^{\circ}C$, multi-column GC- k' correlation, Zhang et al. 1999)

10.90 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

- 6.84 (suspended particulate matter, Burkhard 1984)
- 5.675 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 2$ (food lipid (mg)/(g worm lipid-d); $k_2 = 0.03$ d⁻¹ (earthworm, Wågman et al. 2001)

$k_2 = 0.004$ d⁻¹ with $t_{1/2} = 160$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004$ d⁻¹ with $t_{1/2} = 184$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

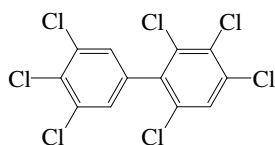
Sediment:

Soil:

Biota: elimination $t_{1/2} = 25$ d in earthworm given contaminated food (Wågman et al. 2001)

depuration $t_{1/2} = 160$ d for high-dose treatment, $t_{1/2} = 184$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.191 2,3,3',4,4',5',6-Heptachlorobiphenyl (PCB-191)



Common Name: 2,3,3',4,4',5',6-Heptachlorobiphenyl

Synonym: PCB-191, 2,3,3',4,4',5',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,4',5',6-heptachlorobiphenyl

CAS Registry No: 74472-50-7

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

126 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.60×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

3.14×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

1.98×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.89×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

9.55×10^{-4} , 2.04×10^{-4} , 5.68×10^{-6} (supercooled liquid P_L , calculated- MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

1.05×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -5109/(T/K) + 13.15$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

17.33 (calculated-P/C, Burkhard 1984)

13.48 (calculated-QSAR, Dunnivant et al. 1992)

1.367 (calculated-QSPR, Achman et al. 1993)

28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.12 (calculated-TSA, Burkhard 1984)

7.21 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.55 (calculated-TSA, Hawker & Connell 1988; quoted, Hansch et al. 1995)

7.21 (recommended, Sangster 1993)

7.3254 (calculated-molecular properties MNDO-AMI method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

12.07, 10.91; 10.93 (0, $20^{\circ}C$, multi-column GC- k' correlation; calculated at $20^{\circ}C$, Zhang et al. 1999)

11.10 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

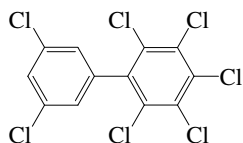
6.92 (suspended particulate matter, Burkhard 1984)

5.659 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.192 2,3,3',4,5,5',6-Heptachlorobiphenyl (PCB-192)



Common Name: 2,3,3',4,5,5',6-Heptachlorobiphenyl

Synonym: PCB-192, 2,3,3',4,5,5',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,5,5',6-heptachlorobiphenyl

CAS Registry No: 74472-51-8

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

142 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.92×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

3.14×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

1.57×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.89×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

9.55×10^{-4} , 3.23×10^{-4} , 2.96×10^{-5} (P_L , calculated-MW, GC-RI correlation, calculated-MCI χ , Burkhard et al. 1985b)

1.75×10^{-4} , 2.49×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

9.12×10^{-5} , 1.41×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5109/(T/K) + 13.38$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

16.52 (calculated-P/C, Burkhard 1984)

19.40 (calculated-QSPR, Dunnivant et al. 1992)

1.37 (calculated-QSPR, Achman et al. 1993)

28.8 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 149 \pm 13\ kJ/mol$, $\Delta S_H = 0.46 \pm 0.04\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.09 (calculated-TSA, Burkhard 1984)

7.21 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.52 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.21 (recommended, Sangster 1993)

7.409 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.81 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

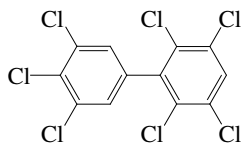
6.89 (suspended particulate matter, Burkhard 1984)

5.659 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.193 2,3,3',4',5,5',6-Heptachlorobiphenyl (PCB-193)



Common Name: 2,3,3',4',5,5',6-Heptachlorobiphenyl

Synonym: PCB-193, 2,3,3',4',5,5',6-heptachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4',5,5',6-heptachlorobiphenyl

CAS Registry No: 69782-91-8

Molecular Formula: $C_{12}H_3Cl_7$

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

154 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

330.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.96×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

3.14×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

1.25×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.70×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.91×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

1.37×10^{-4} , 8.79×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

7.59×10^{-5} , 1.20×10^{-4} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5109/(T/K) + 13.27$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

9.70 (calculated-P/C, Burkhard 1984)

13.61 (calculated-QSPR, Dunnivant et al. 1992)

1.37 (calculated-QSPR, Achman et al. 1993)

1.93 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

32.9 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 140 \pm 13\ kJ/mol$, $\Delta S_H = 0.43 \pm 0.05\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.09 (calculated-TSA, Burkhard 1984)

7.21 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.52 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.21 (recommended, Sangster 1993)

7.409 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 11.99, 10.82; 10.02 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
- 10.93 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.89 (suspended particulate matter, Burkhard 1984)
- 5.659 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 5$ (food lipid mg)/(g worm lipid-d); $k_2 = 0.03$ d⁻¹ (earthworm, Wågman et al. 2001)

Half-Lives in the Environment:

Air:

Surface water:

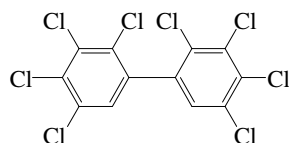
Ground water:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 21$ d in earthworm given contaminated food (Wågman et al. 2001)

7.1.1.194 2,2',3,3',4,4',5,5'-Octachlorobiphenyl (PCB-194)



Common Name: 2,2',3,3',4,4',5,5'-Octachlorobiphenyl

Synonym: PCB-194, 2,2',3,3',4,4',5,5'-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4',5,5'-octachlorobiphenyl

CAS Registry No: 35694-08-7

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

159–160 (Binns & Suschitzky 1971)

156 (Kühne et al. 1995; Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3): 1.507 (at $22^{\circ}C$)

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

263.2 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.0484 (mp at $159^{\circ}C$)

0.0474 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0072 (shake flask-GC/ECD, Wallnöfer et al. 1973)

0.000272 (generator column-GC/ECD, Weil et al. 1974)

8.58×10^{-5} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

0.00124 ($22^{\circ}C$, generator column-GC/ECD, Opperhuizen et al. 1988)

3.79×10^{-3} ; 2.40×10^{-3} (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Li et al. 2003)

$\log S_L/(mol\ m^{-3}) = -1533/(T/K) - 0.11$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.03×10^{-5} (GC-RI correlation, Burkhard et al. 1985a)

3.86×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

2.07×10^{-5} , 1.79×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.29×10^{-5} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log (P_L/Pa) = -5402/(T/K) + 13.43$ (GC-RT correlation, Falconer & Bidleman 1994)

2.04×10^{-5} ; 2.45×10^{-5} (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log P_L/Pa = -5099/(T/K) + 12.49$ (supercooled liquid, FAV final adjusted eq., Li et al. 2003)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

47.52 (calculated-P/C, Burkhard et al. 1985b; quoted, Eisenreich 1987)

10.13 (wetted-wall column-GC, Brunner et al. 1990)

6.79 (calculated-QSPR, Dunnivant et al. 1992)

1.01 (calculated-QSPR, Achman et al. 1993)

0.34 ($11^{\circ}C$, gas stripping-GC/ECD, Bamford et al. 2002)

10.9 (from $11^{\circ}C$ exptl. data and compensation point, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 169 \pm 6$ kJ/mol, $\Delta S_H = 0.52 \pm 0.02$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

6.76, 4.37 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

$\log [H/(\text{Pa m}^3/\text{mol})] = -3566/(T/K) + 12.60$ (FAV final adjusted eq., Li et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.68 (RP-TLC-RT correlation, Bruggeman et al. 1982)

9.35 (HPLC-RT correlation, Shaw & Connell 1982)

7.62 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.67 (generator column-GC, Hawker & Connell 1988a)

6.94 (generator column-GC, Larsen et al. 1992)

7.65 (recommended, Sangster 1993)

7.67, 7.80, 9.35 (quoted lit. values, Hansch et al. 1995)

7.67, 7.76 (LDV literature-derived value, FAV final adjusted value, Li et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

10.50 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)

12.83, 11.59; 11.71 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)

11.17 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

11.31, 11.13 (LDV literature derived value, FAV final adjusted value, Li et al. 2003)

$\log K_{OA} = 4906/(T/K) - 5.33$ (FAV final adjusted eq., Li et al. 2003)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

5.81 (guppy, 3.5% lipid, Bruggeman et al. 1984; quoted, Gobas et al. 1987)

4.35 (guppy, Gobas et al. 1987; quoted, Banerjee & Baughman 1991)

4.18 (worms, Oliver 1987c)

4.35 (guppy, calculated- C_B/C_W or k_1/k_2 , Connell & Hawker 1988; Hawker 1990)

4.81 (guppy, estimated, Banerjee & Baughman 1991)

5.81; 7.34 (22°C, zebrafish: $\log BCF_W$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)

5.81, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

7.27 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

6.5–7.1, 6.8; 7.80 (suspended sediment, average; algae > 50 μm , Oliver 1987a)

5.94, 5.72, 5.68, 5.36 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)

5.943, 6.016 (marine humic substances or 5 mg/L DOC, quoted; calculated-MCI χ , reported as $\log K_h$, Sabljic et al. 1989)

6.41, 6.20, 6.06 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

6.96 (soil, calculated-Characteristic Root Index CRI model, Saçan & Balcioglu 1996)

7.30 (soil, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 > 0.0007$ d⁻¹ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)

$k_1 = 150$ d⁻¹; $k_2 = 0.007$ d⁻¹ (guppy, Bruggeman et al. 1984)

$k_1 = 1000$ d⁻¹ (guppy, Opperhuizen 1986)

$\log k_1 = 2.18 \text{ d}^{-1}$; $\log 1/k_2 = 2.15 \text{ d}$ (fish, quoted, Connell & Hawker 1988)

$k_1 = 5640 \text{ d}^{-1}$; $k_2 = 0.00865 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 158 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 174 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

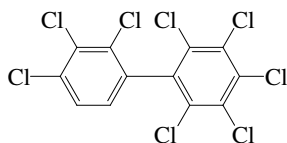
Biota: $t_{1/2} > 1000 \text{ d}$ in rainbow trout and $t_{1/2} = 78 \text{ d}$ in its muscle (Niimi & Oliver 1983);

$t_{1/2} = 100 \text{ d}$ in guppy (Bruggeman et al. 1984);

$t_{1/2} = 220 \text{ d}$ in worms at 8°C (Oliver 1987c).

depuration $t_{1/2} = 158 \text{ d}$ for high-dose treatment, $t_{1/2} = 174 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.195 2,2',3,3',4,4',5,6-Octachlorobiphenyl (PCB-195)



Common Name: 2,2',3,3',4,4',5,6-Octachlorobiphenyl

Synonym: PCB-195, 2,2',3,3',4,4',5,6-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4',5,6-Octachlorobiphenyl

CAS Registry No: 52663-78-2

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

176 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00334 (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

2.204×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

9.92×10^{-5} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.12×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

4.53×10^{-5} , 7.46×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.19×10^{-5} , 3.63×10^{-5} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5244/(T/K) + 13.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

12.77 (calculated-P/C, Burkhard 1984)

1.115 (wetted-wall column-GC/ECD, Brunner et al. 1990)

12.01 (calculated-QSPR, Dunnivant et al. 1992)

14.13 ± 0.78 (gas stripping-GC/ECD, measured range $4-31^{\circ}C$, Bamford et al. 2000)

0.079, 0.485, 2.724, 14.13, 54.5 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$\ln K_{AW} = 62.305 - 20086.6/(T/K)$; temp range $4-31^{\circ}C$ (gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(167.0/kJ \cdot mol^{-1})/RT] + (0.518/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314 J \cdot K^{-1} \cdot mol^{-1}$ and temp range: $4-31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

15.1 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13 kJ/mol$, $\Delta S_H = 0.52 \pm 0.05 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.49 (calculated-TSA, Burkhard 1984)

7.35 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.56 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

- 6.95 (generator column-GC, Larsen et al. 1992)
7.15 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 11.13, 10.04; 10.02 (0, 20°C, GC-k' correlation; calculated at 20°C, Zhang et al. 1999)
11.26 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.92; 7.45 (zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.29 (suspended particulate matter, Burkhard 1984)
5.78, 5.59, 5.55, 5.32 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
5.78; 5.87 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, observed; calculated-MCI χ , Sabljic et al. 1989)
6.42, 6.26, 6.14 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_1 = 5930 \text{ d}^{-1}$; $k_2 = 0.00711 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 $k_2 = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 67 \text{ d}$ and $k_2 = 0.011 \text{ d}^{-1}$ with $t_{1/2} = 61 \text{ d}$ for food concn of 24 ng/g and 126 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
 $k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 143 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 158 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

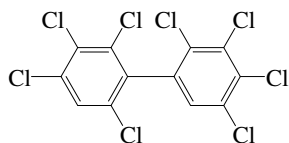
Sediment:

Soil:

Biota: depuration $t_{1/2} = 61\text{--}67 \text{ d}$ in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 143 \text{ d}$ for high-dose treatment, $t_{1/2} = 158 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.196 2,2',3,3',4,4',5,6'-Octachlorobiphenyl (PCB-196)



Common Name: 2,2',3,3',4,4',5,6'-Octachlorobiphenyl

Synonym: PCB-196, 2,2',3,3',4,4',5,6'-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4',5,6'-Octachlorobiphenyl

CAS Registry No: 42740-50-1

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

170 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.91×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

1.63×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.87×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

5.40×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

6.11×10^{-5} , 8.41×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.47×10^{-5} , 5.89×10^{-5} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5244/(T/K) + 13.37$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

71.94 (calculated-P/C, Burkhard 1984)

1.013 (wetted wall column-GC/ECD, Brunner et al. 1990)

13.23 (calculated-QSPR, Dunnivant et al. 1992)

0.990 (calculated-QSPR, Achman et al. 1993)

15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13\ kJ/mol$, $\Delta S_H = 0.52 \pm 0.05\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.57 (calculated-TSA, Burkhard 1984)

7.43 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.65 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.43 (recommended, Sangster 1993)

7.70 (estimated, Girvin & Scott 1997)

7.4190 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

12.27, 11.03; 11.19 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
11.40 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

7.37 (suspended particulate matter, Burkhard 1984)
5.857 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)
7.30 (soil-organic carbon, calculated- K_{OW} , Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 156 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 168 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

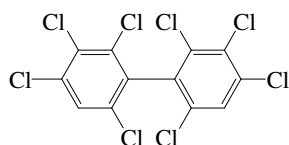
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 156 \text{ d}$ for high-dose treatment, $t_{1/2} = 168 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.197 2,2',3,3',4,4',6,6'-Octachlorobiphenyl (PCB-197)



Common Name: 2,2',3,3',4,4',6,6'-Octachlorobiphenyl

Synonym: PCB-197, 2,2',3,3',4,4',6,6'-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4',6,6'-Octachlorobiphenyl

CAS Registry No: 33091-17-7

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

132 (Brodsky & Ballschmiter 1988)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0892 (mp at $132^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.81×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

3.41×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

1.71×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

1.03×10^{-4} (calculated-QSPR, Dunnivant et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

6.79×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

5.93×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)

1.90×10^{-4} , 1.22×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

9.12×10^{-5} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4581/(T/K) + 12.52$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

94.03 (calculated-P/C, Burkhard 1984)

25.69 (calculated-QSPR, Dunnivant et al. 1992)

97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.59 (calculated-TSA, Burkhard 1984)

7.21 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.30 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.21 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

11.74, 10.52; 10.68 (0, $20^{\circ}C$, multi-column GC- k' correlation; calculated at $20^{\circ}C$, Zhang et al. 1999)

11.30 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

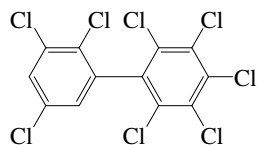
7.39 (suspended particulate matter, Burkhard 1984)

5.699 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.198 2,2',3,3',4,5,5',6-Octachlorobiphenyl (PCB-198)



Common Name: 2,2',3,3',4,5,5',6-Octachlorobiphenyl

Synonym: PCB-198, 2,2',3,3',4,5,5',6-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5,5',6-Octachlorobiphenyl

CAS Registry No: 68194-17-2

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

162 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.03×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

1.63×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

8.58×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

1.48×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

3.44×10^{-4} , 1.67×10^{-4} , 5.68×10^{-6} (GC-RI correlation, Burkhard et al. 1985b)

6.85×10^{-5} , 1.224×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

5.01×10^{-5} , 7.08×10^{-5} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5244/(T/K) + 13.42$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

20.97 (calculated-P/C, Burkhard 1984)

1.419 (wetted wall column-GC/ECD, Brunner et al. 1990)

15.62 (calculated-QSPR, Dunnivant et al. 1992)

15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13 kJ/mol$, $\Delta S_H = 0.52 \pm 0.05 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.55 (calculated-TSA, Burkhard 1984)

7.43 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.62 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.43 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

12.32, 11.05; 10.02 (0, $20^{\circ}C$, multi-column GC- k' correlation; calculated at $20^{\circ}C$, Zhang et al. 1999)

11.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.35 (suspended particulate matter, Burkhard 1984)
5.91, 5.63, 5.56, 5.23 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
5.91; 5.86 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, observed; calculated-MCI $^1\chi$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 158 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 185 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

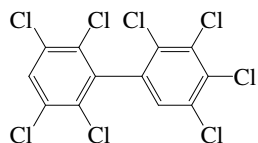
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 158 \text{ d}$ for high-dose treatment, $t_{1/2} = 185 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.199 2,2',3,3',4,5,5',6'-Octachlorobiphenyl (PCB-199)



Common Name: 2,2',3,3',4,5,5',6'-Octachlorobiphenyl

Synonym: PCB-199, 2,2',3,3',4,5,5',6'-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5,5',6'-Octachlorobiphenyl

CAS Registry No: 52663-75-9

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

170 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.23×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

3.41×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

5.41×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.20×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

3.57×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

9.35×10^{-5} , 1.67×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.05×10^{-4} , 2.04×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, reported as the revised order PCB-200-2,2',3,3',4,5,6,6'- Fischer et al. 1992)

$\log(P_L/Pa) = -5244/(T/K) + 13.36$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

42.66 (calculated-P/C, Burkhard 1984)

1.013 (wetted wall column-GC/ECD, Brunner et al. 1990)

23.0 (calculated-QSPR, Dunnivant et al. 1992)

15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.51 (calculated-TSA, Burkhard 1984)

7.21 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.20 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.21 (recommended, Sangster 1993)

7.28 (quoted lit., Maruya & Lee 1998-reported as revised order PCB-200: 2,2',3,3',4,5,6,6'-PCB)

7.21 (revised previously quoted value; Maruya & Lee 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

12.28, 11.05; 10.02 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)

11.01 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Biota Sediment Accumulation Factor, BSAF:

96 (trout in Lake Ontario, Niimi 1996)

0.26, 7.1, 1.1 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

7.31 (suspended particulate matter, Burkhard 1984)

5.94, 5.72, 5.68, 5.36 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)

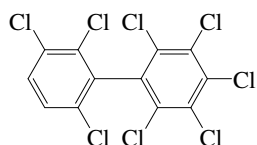
5.711 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

6.44, 6.18, 6.02 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.200 2,2',3,3',4,5,6,6'-Octachlorobiphenyl (PCB-200)



Common Name: 2,2',3,3',4,5,6,6'-Octachlorobiphenyl

Synonym: PCB-200, 2,2',3,3',4',5,6,6'-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5,6,6'-Octachlorobiphenyl

CAS Registry No: 52663-73-7

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

130 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.93×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

4.105×10^{-4} , 1.79×10^{-4} , 1.08×10^{-4} , 2.01×10^{-4} (RP-HPLC- k' correlation, different and mobile stationary phases, Brodsky & Ballschmiter 1988)

4.30×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.56×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

6.37×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

1.75×10^{-4} , 3.32×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.89×10^{-5} , 5.89×10^{-5} (supercooled liquid P_L , GC-RI correlation, different stationary phases, reported in revised order as PCB-201-2,2',3,3',4,5',6,6'-, Fischer et al. 1992)

$\log(P_L/Pa) = -4851/(T/K) + 12.24$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

2.34×10^{-5} (P_L , calculated-MCI $^3\chi$ and Characteristic Root Index CRI, Saçan & Balcioglu 1998)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

66.98 (calculated-P/C, Burkhard 1984)

1.50 (calculated-QSPR, Achman et al. 1993)

24.36 (calculated-QSPR, Dunnivant et al. 1992)

97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.57 (calculated-TSA, Burkhard 1984)

7.16, 7.54, 7.16, 7.36; 7.35 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.35 (recommended, Sangster 1993)

7.27 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

- 8.16; 7.27–7.30 (calculated-Characteristic Root Index CRI; min.-max. range, Saçan & Inel 1995)
7.63; 7.28 (previously quoted; revised value, Maruya & Lee 2000)
7.32 (calculated-QSPR, Yeh & Hong 2002- reported as PCB-201 for 2,2',3,3',4,5,6,6'-octachlorobiphenyl)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.05, 10.82 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)
11.05 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

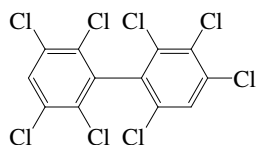
Sorption Partition Coefficient, $\log K_{OC}$:

- 7.36 (suspended particulate matter, Burkhard 1984)
5.50, 5.72, 5.68, 5.36 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
5.68; 5.70 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, observed; calculated-MCI χ , Sabljic et al. 1989)
7.05 (soil, calculated-Characteristic Root Index CRI, Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.201 2,2',3,3',4,5',6,6'-Octachlorobiphenyl (PCB-201)



Common Name: 2,2',3,3',4,5',6,6'-Octachlorobiphenyl

Synonym: PCB-201, 2,2',3,3',4,5',6,6'-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5',6,6'-Octachlorobiphenyl

CAS Registry No: 40186-71-8

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

162 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.06×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

2.204×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

8.58×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.56×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

5.06×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

5.94×10^{-5} , 1.0×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.41×10^{-4} (supercooled liquid P_L : GC-RI correlation, different stationary phases, reported as revised order PCB-199, 2,2',3,3',4,5',6,6'-octachlorobiphenyl, Fischer et al. 1992)

$\log(P_L/Pa) = -4581/(T/K) + 12.51$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

64.54 (calculated-P/C, Burkhard 1984)

1.72 (wetted wall column-GC/ECD, Brunner et al. 1990)

13.23 (calculated-QSPR, Dunnivant et al. 1992)

0.990 (calculated-QSPR, Achman et al. 1993)

0.156, 0.457 (0, $15^{\circ}C$, from modified two-film exchange model, Hornbuckle et al. 1994)

95.8 ± 4.4 (gas stripping-GC/ECD, measured range $4-31^{\circ}C$, Bamford et al. 2000)

1.069, 5.14, 22.98, 95.8, 308 (4, 11, 18, 25, $31^{\circ}C$, gas stripping-GC, Bamford et al. 2000)

$K_{AW} = \exp[-(144.5/kJ \cdot mol^{-1})/RT] + (0.458/kJ \cdot mol^{-1} \cdot K^{-1})/R$; where $R = 8.314 J \cdot K^{-1} \cdot mol^{-1}$ and temp range: $4-31^{\circ}C$, (gas stripping-GC, Bamford et al. 2000)

97.5 (exptl. data, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7 kJ/mol$, $\Delta S_H = 0.46 \pm 0.03 kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.54 (calculated-TSA, Burkhard 1984)

7.35 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

- 7.21 (generator column-GC, Hawker & Connell 1988)
- 7.62 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)
- 7.80 (calculated-TSA, Murray & Andren 1992)
- 7.31 (recommended, Sangster 1993)
- 7.70 (estimated, Girvin & Scott 1997)
- 7.21 (quoted lit., Maruya & Lee 1998, reported as the revised order PCB-199, 2,2',3,3',4',5,5',6-octachlorobiphenyl)
- 7.62 (revised previously quoted value, Maruya & Lee 2000)
- 7.21; 7.32 (quoted exptl.-generator column method; calculated-QSPR, Yeh & Hong 2002, reported as PCB-201 for 2,2',3,3',4,5,6,6'-octachlorobiphenyl-should be PCB-200 in B&Z/IUPAC numbering system for 2,2',3,3',4,5,5',6-octachlorobiphenyl)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.22, 10.98 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
- 11.30 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 5.88; 7.41 (zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.34 (suspended particulate matter, Burkhard 1984)
- 5.913; 5.857 (marine humic substances with 5 mg/L DOC, reported as association coefficient $\log K_h$, observed; calculated-MCI χ , Sabljic et al. 1989)
- 6.60 (average, colloids and micro-particulates in precipitation events, GC/ECD, Murray & Andren 1992)
- 7.30 (soil, estimated- $\log K_{OW}$, Girvin & Scott 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 5950 \text{ d}^{-1}$; $k_2 = 0.00776 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 153 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 172 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

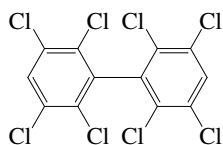
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 153 \text{ d}$ for high-dose treatment, $t_{1/2} = 172 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.202 2,2',3,3',5,5',6,6'-Octachlorobiphenyl (PCB-202)



Common Name: 2,2',3,3',5,5',6,6'-Octachlorobiphenyl

Synonym: PCB-202, 2,2',3,3',5,5',6,6'-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',5,5',6,6'-Octachlorobiphenyl

CAS Registry No: 2136-99-4

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

161 (Van Roosmalen 1934; Burkhard et al. 1985a; Erickson 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.507

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

263.2 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.80 (Miller et al. 1984; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

52.72 (Miller et al. 1984; Shiu & Mackay 1986; selected, Hinckley et al. 1990)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0463 (mp at $161^{\circ}C$)

0.0443 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.80×10^{-4} (generator column-GC/ECD, Weil et al. 1974;)

3.93×10^{-4} (generator column-GC/ECD, Miller et al. 1984,1985)

1.47×10^{-4} * (generator column-GC/ECD, measured range 20 – $50^{\circ}C$, Dickhut et al. 1986)

1.14×10^{-4} , 1.47×10^{-4} , 2.12×10^{-4} , 4.66×10^{-4} (4. 20, 25, $32^{\circ}C$, generator column-GC/ECD, Dickhut et al. 1986)

$\ln x = -6098/(T/K) - 5.333$, temp range 4 – $32^{\circ}C$, $\Delta H_{ss} = 50.7$ kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)

$\log x = -2652/(T/K) - 2.308$, $\Delta H_{ss} = 50.6$ kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or

$S/(mol/L) = 6.91 \times 10^{-11} \exp(0.064 \cdot t/^{\circ}C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)

2.53×10^{-4} , 5.93×10^{-4} , 6.51×10^{-4} , 2.36×10^{-4} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

$\ln x = -5.34 - 6100/(T/K)$, temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.90×10^{-5} * (extrapolated gas saturation-GC, measured range 29 – $61.2^{\circ}C$, Burkhard et al. 1984)

$\log (P/Pa) = 13.262 - 5307.3/(T/K)$; temp range 29 – $61.2^{\circ}C$ (gas saturation data, Clapeyron eq., Burkhard et al. 1984)

2.89×10^{-5} , 6.43×10^{-4} (solid P_s , P_L calculated from P_s using fugacity ratio F, Burkhard et al. 1985a)

5.40×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

1.70×10^{-4} , 3.91×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

6.59×10^{-4} , 5.26×10^{-4} (supercooled P_L , converted from literature P_s with different ΔS_{fus} values, Hinckley et al. 1990)

2.22×10^{-4} (P_{GC} by GC-RT correlation with p,p' -DDT as reference standard, Hinckley et al. 1990)

$\log P_L/Pa = 12.99 - 4851/(T/K)$ (GC-RT correlation, Hinckley et al. 1990)
 2.40×10^{-4} (supercooled liquid P_L : GC-RI correlation, Fischer et al. 1992)
 $\log (P_L/Pa) = -4851/(T/K) + 12.99$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)
 $(2.41 - 29.5) \times 10^{-6}$; $(1.73 - 5.40) \times 10^{-4}$ (literature solid P_s range; literature liquid P_L range, Delle Site 1997)
 $\log (P/Pa) = 13.282 - 5307.3/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry's Law Constant ($Pa\ m^3/mol$ at 25°C):

75.79 (calculated-P/C, Burkhard et al. 1985b)
 38.08 (calculated-P/C, Shiu & Mackay 1986)
 1.82 (wetted-wall column-GC, Brunner et al. 1990)
 22.63 (calculated-QSPR, Dunnivant et al. 1992)
 1.50 (calculated-QSPR, Achman et al. 1993)
 97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7\ kJ/mol$, $\Delta S_H = 0.46 \pm 0.03\ kJ/mol\cdot K$
 (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

9.77 (Hansch & Leo 1979)
 8.42 (TLC-RT correlation, Bruggeman et al. 1982)
 7.11 (generator column-GC/ECD, Miller et al. 1984, 1985)
 7.14 (generator column-HPLC, Woodburn et al. 1984)
 7.12 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
 7.01, 7.35, 6.98, 7.31 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 7.21 (generator column-GC, Hawker & Connell 1988a)
 7.67 (HPLC-RT correlation, Hawker & Connell 1988)
 7.729 ± 0.031 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 7.54 (HPLC- k' correlation, Noegrohati & Hammers 1992)
 7.15 (recommended, Sangster 1993)
 7.73 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

11.57, 10.38 (0, 20°C, multi-column GC- k' correlation; calculated at 20°C, Zhang et al. 1999)
 10.77 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

5.82; 7.35 (22°C, zebrafish: $\log BCF_w$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)
 5.82, 7.35 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

7.34 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 5.61, 5.46, 5.41, 4.99 (marine humic substances, in concentrations of 5, 10, 20, 40 mg/L DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
 5.610, 5.699 (marine humic substances with 5 mg/L of DOC, reported as association coefficient $\log K_h$, observed; calculated-MCI χ , Sabljic et al. 1989)
 6.36, 6.13, 6.01 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)
 7.04 (soil, calculated-Characteristic Root Index [CRI], Saçan & Balcioglu 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 5070 \text{ d}^{-1}$; $k_2 = 0.0077 \text{ d}^{-1}$ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)

$k_2 = 0.006 \text{ d}^{-1}$ with $t_{1/2} = 119 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 145 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 110 \text{ d}$ for high-dose treatment, $t_{1/2} = 145 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

TABLE 7.1.1.202.1

Reported aqueous solubilities and vapor pressures of 2,2',3,3',5,5',6,6'-octachlorobiphenyl (PCB-202) at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure	
Dickhut et al. 1986		Burkhard et al. 1984	
generator column-GC/ECD		gas saturation-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	P/Pa
20	1.29×10^{-4}	29.0	4.95×10^{-5}
25	1.29×10^{-4}	39.9	2.24×10^{-4}
32	2.15×10^{-4}	50.0	5.83×10^{-4}
50	7.73×10^{-4}	61.2	2.65×10^{-3}
		25.0	2.90×10^{-5}
$\ln x = A - B/(T/K)$		$\log (P/\text{Pa}) = A - B/(T/K)$	
A	-5.333	A	13.262
B	6098.15	B	5307.3
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 50.7 \pm 3.8$ for 25–50°C		temp range 29–61.2°C	
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 101.7$	

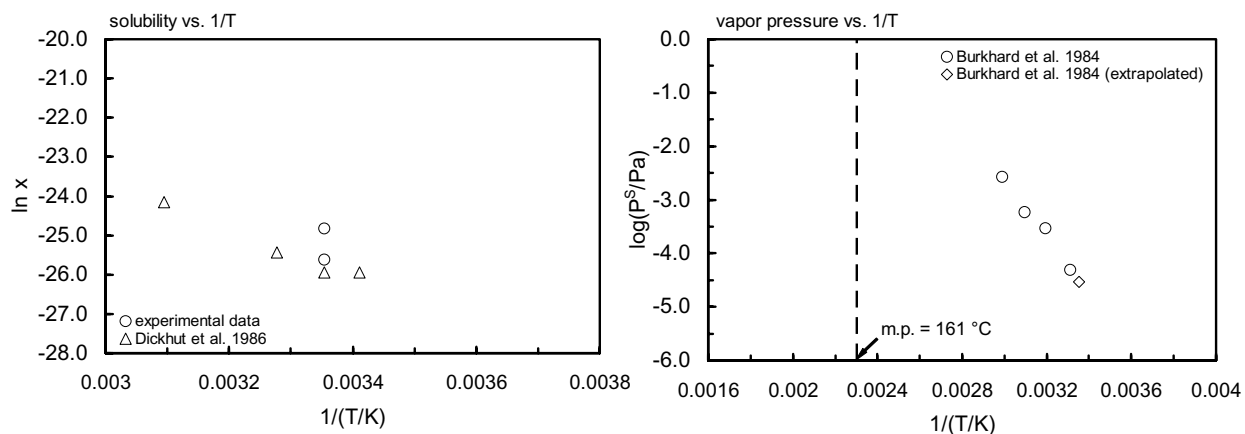
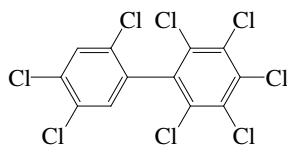


FIGURE 7.1.1.202.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,2',3,3',5,5',6,6'-octachlorobiphenyl (PCB-202).

7.1.1.203 2,2',3,4,4',5,5',6-Octachlorobiphenyl (PCB-203)



Common Name: 2,2',3,4,4',5,5',6-Octachlorobiphenyl

Synonym: PCB-203, 2,2',3,4,4',5,5',6-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',5,5',6-Octachlorobiphenyl

CAS Registry No: 52663-76-0

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

170 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.91×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

1.36×10^{-4} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

6.81×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence):

1.35×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

1.52×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

9.29×10^{-5} , 1.047×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

3.47×10^{-5} , 5.62×10^{-5} (supercooled liquid P_L , GC-RI correlation, different stationary phases, Fischer et al. 1992)

$\log(P_L/Pa) = -5244/(T/K) + 13.39$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.252 (calculated-P/C, Burkhard 1984)

14.21 (calculated-QSPR, Dunnivant et al. 1992)

0.990 (calculated-QSPR, Achman et al. 1993)

15.1 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.57 (calculated-TSA, Burkhard 1984)

7.49 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

7.65 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

6.93 (generator column-GC, Larsen et al. 1992)

7.21 (recommended, Sangster 1993)

7.4825 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated :

12.36, 11.10 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)

11.24 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

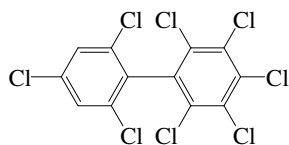
7.37 (suspended particulate matter, Burkhard 1984)

5.857 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.204 2,2',3,4,4',5,6,6'-Octachlorobiphenyl (PCB-204)



Common Name: 2,2',3,4,4',5,6,6'-Octachlorobiphenyl

Synonym: PCB-204, 2,2',3,4,4',5,6,6'-octachloro-1,1'-biphenyl

Chemical Name: 2,2',3,4,4',5,6,6'-Octachlorobiphenyl

CAS Registry No: 74472-52-9

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

132 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.81×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

1.49×10^{-4} , 9.85×10^{-5} , 1.83×10^{-4} , 1.49×10^{-4} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

4.30×10^{-4} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.49×10^{-4} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

3.88×10^{-4} (GC-RI correlation, Burkhard et al. 1985b)

1.54×10^{-4} , 2.76×10^{-4} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

1.38×10^{-4} (supercooled liquid P_L , GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -4851/(T/K) + 12.46$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

53.3 (calculated-P/C, Burkhard 1984)

34.89 (calculated-QSAR, Dunnivant et al. 1992)

97.5 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol-K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.59 (calculated-TSA, Burkhard 1984)

7.46, 7.63, 7.37, 7.45 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.30 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.48 (recommended, Sangster 1993)

7.2632 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$:

11.15 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

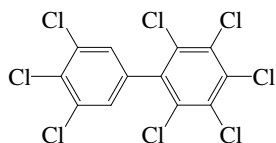
7.39 (suspended particulate matter, Burkhard 1984)

5.699 (marine humic substances 5 mg/L of DOC, reported as association coefficient log K_h , calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

7.1.1.205 2,3,3',4,4',5,5',6-Octachlorobiphenyl (PCB-205)



Common Name: 2,3,3',4,4',5,5',6-Octachlorobiphenyl

Synonym: PCB-205, 2,3,3',4,4',5,5',6-octachloro-1,1'-biphenyl

Chemical Name: 2,3,3',4,4',5,5',6-Octachlorobiphenyl

CAS Registry No: 74472-53-0

Molecular Formula: $C_{12}H_2Cl_8$

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

150 (estimated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

351.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.50×10^{-3} (S_L supercooled liquid, calculated-TSA, Burkhard et al. 1985a)

8.58×10^{-5} (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

3.41×10^{-5} (calculated-TSA and mp, Abramowitz & Yalkowsky 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.84×10^{-5} (P_L supercooled liquid, GC-RT correlation, Burkhard et al. 1985a)

4.40×10^{-5} (GC-RI correlation, Burkhard et al. 1985b)

2.49×10^{-5} , 2.91×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -5402/(T/K) + 13.51$ (GC-RT correlation, supercooled liquid, Falconer & Bidleman 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

4.70 (calculated-P/C, Burkhard 1984)

8.644 (calculated-QSPR, Dunnivant et al. 1992)

10.9 (predicted based on homolog group and ortho-Cl, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 169 \pm 6\ kJ/mol$, $\Delta S_H = 0.52 \pm 0.05\ kJ/mol \cdot K$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.47 (calculated-TSA, Burkhard 1984)

7.62 (RP-HPLC- k' correlation, Brodsky & Ballschmiter 1988)

8.00 (calculated-TSA, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.62 (recommended, Sangster 1993)

7.7326 (calculated-molecular properties MNDO-AM1 method, Makino 1998)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated:

12.86, 11.62 (0, $20^{\circ}C$, multi-column GC- k' correlation, Zhang et al. 1999)

11.34 (calculated-QSPR-quantum chemical descriptors by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.27 (suspended particulate matter, Burkhard 1984)
6.016 (marine humic substances with 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices, Sabljic et al. 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 166 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 168 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

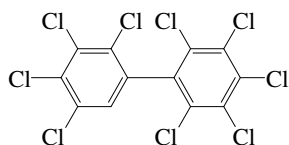
Ground water:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 166 \text{ d}$ for high-dose treatment, $t_{1/2} = 168 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.206 2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl (PCB-206)



Common Name: 2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl

Synonym: PCB-206, 2,2',3,3',4,4',5,5',6-nonachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4',5,5',6-nonachlorobiphenyl

CAS Registry No: 40186-72-9

Molecular Formula: $C_{12}HCl_9$

Molecular Weight: 464.213

Melting Point ($^{\circ}C$):

204.5–206.5 (Hutzinger et al. 1974)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.507

Molar Volume (cm^3/mol):

372.7 (calculated-Le Bas method at normal boiling point)

276.1 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.70 (Opperhuizen et al. 1988; Ruelle et al. 1993)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.016 (Mackay et al. 1980; Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.000112 (generator column-GC/ECD, Weil et al. 1974)

2.55×10^{-5} (generator column-GC/ECD, measured range 25 – $50^{\circ}C$, Dickhut et al. 1986)

2.55×10^{-5} , 5.117×10^{-5} , 6.59×10^{-5} , 1.32×10^{-4} (25 , 32 , 40 , $50^{\circ}C$, generator column-GC/ECD, Dickhut et al. 1986)

$\ln x = -5990/(T/K) - 7.427$, temp range 25 – $50^{\circ}C$, $\Delta H_{ss} = 49.8$ kJ/mol (generator column-GC/ECD, Dickhut et al. 1986)

$\log x = -2609/(T/K) - 3.222$, $\Delta H_{ss} = 50.0$ kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or

$S/(mol/L) = 1.27 \times 10^{-11} \exp(0.062 \cdot t/^{\circ}C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986)

0.00011 (selected, Shiu & Mackay 1986)

3.07×10^{-5} , 3.14×10^{-5} , 2.61×10^{-5} , 2.80×10^{-5} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.80×10^{-5} ($22^{\circ}C$, generator column-GC/ECD, Opperhuizen et al. 1988)

$\ln x = -7.4275 - 6004.5/(T/K)$, temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.88×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)

1.034×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

1.08×10^{-5} , 1.53×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log (P_L/Pa) = -5226/(T/K) + 13.57$ (supercooled liquid, GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

27.66 (calculated-P/C, Burkhard et al. 1985b)

8.845 (calculated-QSPR, Dunnivant et al. 1992)

0.474 (calculated-QSPR, Achman et al. 1993)

- 15.1 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 167 \pm 13$ kJ/mol, $\Delta S_H = 0.52 \pm 0.05$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 9.14 (RP-TLC- k' correlation, Bruggeman et al. 1982)
 7.94, 7.91, 7.98, 7.94 (RP- HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 7.07 (generator column-GC, Larsen et al. 1992)
 7.51 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 13.09, 11.79 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 11.81 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 5.71; 7.24 (zebrafish: $\log BCF_W$ wet wt basis; $\log BCF_L$ lipid wt basis, Fox et al. 1994)
 2.60–4.85 (various marine species, mean dry weight BCF, Hope et al. 1998)
 4.37–5.67 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.72 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
 6.15, 5.92, 5.83, 5.69 (marine humic substances, in concentrations of 5, 10, 20, 40 mg L⁻¹ DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)
 6.152; 6.133 (marine humic substances of 5 mg L⁻¹ DOC, quoted; calculated-MCI χ , reported as $\log K_h$, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_2 > 0.0007$ d⁻¹ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
 $k_1 = 4940$ d⁻¹; $k_2 = 0.00958$ d⁻¹ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 $k_2 = 0.016$ d⁻¹ with $t_{1/2} = 45$ d and $k_2 = 0.013$ d⁻¹ with $t_{1/2} = 53$ d for food concn of 20 ng/g and 141 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
 $k_2 = 0.005$ d⁻¹ with $t_{1/2} = 140$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 $k_2 = 0.005$ d⁻¹ with $t_{1/2} = 148$ d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

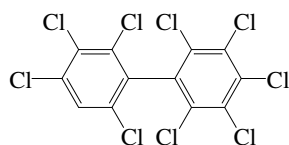
Soil:

Biota: $t_{1/2} > 1000$ d in rainbow trout, and $t_{1/2} = 84$ d in its muscle (Niimi & Oliver 1983)

Depuration $t_{1/2} = 45$ –53 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

depuration $t_{1/2} = 140$ d for high-dose treatment, $t_{1/2} = 148$ d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.207 2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl (PCB-207)



Common Name: 2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl

Synonym: PCB-207, 2,2',3,3',4,4',5,6,6'-nonachloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,4',5,6,6'-nonachlorobiphenyl

CAS Registry No: 52663-79-3

Molecular Formula: $C_{12}HCl_9$

Molecular Weight: 464.213

Melting Point ($^{\circ}C$):

161 (calculated, Abramowitz & Yalkowsky 1990)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

372.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00167 (supercooled liquid S_L , calculated-TSA, Burkhard et al. 1985b)

4.64×10^{-5} , 3.29×10^{-5} , 4.04×10^{-5} , 3.77×10^{-5} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

0.000058 (calculated-TSA, Abramowitz & Yalkowsky 1990)

2.10×10^{-5} (calculated-MCI χ , Patil 1991)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.47×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985a)

1.30×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

3.17×10^{-5} , 4.99×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

$\log(P_L/Pa) = -5127/(T/K) + 12.70$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

35.97 (calculated-P/C, Burkhard et al. 1985b)

17.13 (calculated-QSPR, Dunnivant et al. 1992)

0.717 (calculated-QSPR, Achman et al. 1993)

97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.94 (calculated-TSA, Burkhard 1984)

7.84, 7.97, 7.85, 7.86 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

7.52 (generator column-GC, Hawker & Connell 1988a; quoted, Hansch et al. 1995)

7.74 (calculated-TSA, Hawker & Connell 1988a)

7.80 (calculated-MCI χ , Patil 1991)

7.88 (recommended, Sangster 1993)

7.6190 (calculated-molecular properties MNDO-AM1, Makino 1998)

7.77 (calculated-QSPR, Yeh & Hong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

12.60, 11.26 (0, 20°C, multi-column GC-k' correlation, Zhang et al. 1999)

11.94 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

2.65–4.54 (various marine species, mean dry wt. BCF, Hope et al. 1998)

4.02–6.29 (various marine species, mean lipid-normalized BCF, Hope et al. 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

7.74 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)

5.98, 5.77, 5.67, 5.44 (marine humic substances, in concentrations of 5, 10, 20, 40 mg L⁻¹ DOC, reported as association coefficient $\log K_h$, Lara & Ernst 1989)

5.98, 5.97 (marine humic substances of 5 mg L⁻¹ DOC, quoted; calculated-MCI χ , reported as $\log K_h$, Sabljic et al. 1989)

6.39, 6.17, 6.19 (North Sea sediments, batch equilibrium, Lara & Ernst 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 162 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.004 \text{ d}^{-1}$ with $t_{1/2} = 155 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

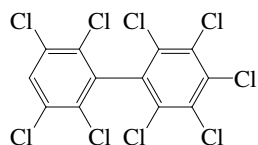
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 162 \text{ d}$ for high-dose treatment, $t_{1/2} = 155 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.208 2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl (PCB-208)



Common Name: 2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl

Synonym: PCB-208, 2,2',3,3',4,5,5',6,6'-nonochloro-1,1'-biphenyl

Chemical Name: 2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl

CAS Registry No: 52663-77-1

Molecular Formula: $C_{12}HCl_9$

Molecular Weight: 464.213

Melting Point ($^{\circ}C$):

180.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

372.7 (calculated-Le Bas method at normal boiling point)

276.1 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.60 (Ruelle et al. 1993; Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

49.45 (Shiu & Mackay 1986)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0298 (mp at $180.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.80×10^{-5} (generator column-GC/ECD, Miller et al. 1984,1985)

6.87×10^{-5} ; 4.64×10^{-5} , 6.87×10^{-5} , 3.95×10^{-5} , 4.97×10^{-5} (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

1.74×10^{-7} (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.78×10^{-6} (GC-RI correlation, Burkhard et al. 1985a)

1.22×10^{-4} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)

3.08×10^{-5} , 6.62×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)

2.19×10^{-5} (supercooled liquid P_L ; GC-RI correlation, Fischer et al. 1992)

$\log(P_L/Pa) = -5127/(T/K) + 12.68$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

32.53 (calculated-P/C, Burkhard et al. 1985b)

16.93 (calculated-QSPR, Dunnivant et al. 1992)

97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)

$\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7$ kJ/mol, $\Delta S_H = 0.46 \pm 0.04$ kJ/mol·K (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.92 (calculated-TSA, Burkhard 1984)

8.16 (generator column-GC/ECD, Miller et al. 1984,1985)

9.05 (calculated-UNIFAC activity coeff., Banerjee & Howard 1988)

7.72, 7.87, 7.69, 7.78 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)

8.18 (calculated-TSA, Hawker & Connell 1988a)

- 7.77 (recommended, Sangster 1993)
8.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.57, 11.26 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
11.71 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.72 (suspended particulate matter, calculated- K_{OW} , Burkhard 1984)
5.974 (marine humic substances 5 mg/L of DOC, reported as association coefficient $\log K_h$, calculated-molecular connectivity indices χ , Sabljic et al. 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 139 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)

$k_2 = 0.005 \text{ d}^{-1}$ with $t_{1/2} = 152 \text{ d}$ (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

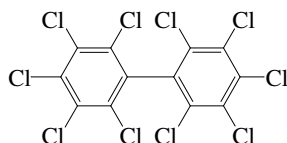
Groundwater:

Sediment:

Soil:

Biota: depuration $t_{1/2} = 139 \text{ d}$ for high-dose treatment, $t_{1/2} = 152 \text{ d}$ for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

7.1.1.209 2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl (PCB-209)



Common Name: 2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl

Synonym: PCB-209

Chemical Name: 2,2',3,3',4,4',5,5',6,6'-decachlorobiphenyl

CAS Registry No: 2051-24-3

Molecular Formula: $C_{12}Cl_{10}$

Molecular Weight: 498.658

Melting Point ($^{\circ}C$):

309 (Lide 2003)

Boiling Point ($^{\circ}C$):Density (g/cm^3 at $20^{\circ}C$): 1.507Molar Volume (cm^3/mol):

393.6 (calculated-Le Bas method at normal boiling point)

289.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.79 (differential scanning calorimetry, Miller et al. 1984; Ruelle & Kesselring 1997)

39.434 (Ruelle et al. 1993)

38.16 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

49.37 (Miller et al. 1984; Shiu & Mackay 1986; Hinckley et al. 1990)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.00164 (mp at $309^{\circ}C$)

0.0017 (Mackay et al. 1980; Shiu & Mackay 1986; Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.015 (shake flask-GC/ECD, Wallnöfer et al. 1973; Tulp & Hutzinger 1978)

 1.6×10^{-5} (generator column-GC/ECD, Weil et al. 1974) 7.43×10^{-6} (generator column-GC/ECD, Miller et al. 1984, 1985) 2.12×10^{-8} (calculated-UNIFAC activity coeff., converted from $\log \gamma$, Arbuckle 1986) 4.1×10^{-4} , 4.6×10^{-4} (exptl., calculated-UNIFAC, converted from $\log \gamma$, Burkhard et al. 1986) 6.48×10^{-7} * (generator column-GC/ECD, measured range 50 – $80^{\circ}C$, Dickhut et al. 1986) 6.48×10^{-7} , 8.38×10^{-6} , 1.76×10^{-5} , 4.95×10^{-5} (25 , 60 , 70 , $80^{\circ}C$, generator column-GC/ECD, Dickhut et al. 1986) $\ln x = -8010.6/(T/K) - 4.608$, temp range 50 – $80^{\circ}C$, $\Delta H_{ss} = 66.6$ kJ/mol (generator column-GC/ECD, Dickhut et al. 1986) $\log x = -3478/(T/K) - 2.001$, $\Delta H_{ss} = 66.6$ kJ/mol (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986); or $S/(mol/L) = 1.80 \times 10^{-13} \exp(0.077 \cdot t/^{\circ}C)$ (regression eq. given by Doucette & Andren 1988, based on exptl data of Dickhut et al. 1986) 7.37×10^{-6} , 8.67×10^{-6} , 7.04×10^{-6} , 9.07×10^{-6} (RP- HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988) 2.1×10^{-5} ($22^{\circ}C$, generator column-GC/ECD, Opperhuizen et al. 1988) $(7.9 \pm 0.38) \times 10^{-6}$ (generator column-SPME/GC, Paschke et al. 1998) $\ln x = -4.632 - 8001/(T/K)$, temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section): 1.4×10^{-5} (calculated-volatilization rate, Dobbs & Cull 1982) 4.0×10^{-5} (supercooled liquid P_L , Mackay et al. 1983)

5.30×10^{-8} * (extrapolated, gas saturation-GC, measured range 50.7–89.8°C, Burkhard et al. 1984)
 $\log (P/\text{Pa}) = 14.049 - 6358/(T/K)$; temp range 50.7–89.8°C (gas saturation, Burkhard et al. 1984)
 1.39×10^{-6} (supercooled liquid P_L , GC-RT correlation, Bidleman 1984)
 5.36×10^{-8} (GC-RI correlation, Burkhard et al. 1985a)
 2.75×10^{-5} (supercooled liquid P_L , GC-RI correlation, Burkhard et al. 1985b)
 5.58×10^{-6} , 1.32×10^{-5} (supercooled liquid P_L , GC-RT correlation, different stationary phases, Foreman & Bidleman 1985)
 5.00×10^{-8} ; 3.0×10^{-5} (selected, solid P_S ; supercooled liquid P_L , Shiu & Mackay 1986)
 9.44×10^{-6} (GC-RT correlation, Watanabe & Tatsukawa 1989)
 5.14×10^{-6} , 1.44×10^{-5} (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 1.303×10^{-5} (P_{GC} by GC-RT correlation with p,p' -DDT as reference standard, Hinckley et al. 1990)
 $\log (P_L/\text{Pa}) = 13.27 - 5402/(T/K)$ (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
 $\log (P_L/\text{Pa}) = -5402/(T/K) + 13.27$ (supercooled liquid P_L , GC-RT correlation, Falconer & Bidleman 1994)
 $2.89 \times 10^{-9} - 1.40 \times 10^{-5}$; $(5.58-27.5) \times 10^{-6}$ (literature P_S range; P_L range, Delle Site 1997)
 2.6×10^{-5} * (65°C, Knudsen effusion, measured range 65–85°C, Goodman 1997)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

100 (estimated, Mackay et al. 1983)
 12.46 (calculated-P/C, Burkhard et al. 1985b)
 20.84 (calculated-P/C, Shiu & Mackay 1986; Shiu et al. 1987)
 40.0 (calculated-QSPR, Dunnivant et al. 1992)
 97.5 (estimated based on homolog group and ortho chlorine number, Bamford et al. 2002)
 $\ln K_{AW} = -\Delta H_H/RT + \Delta S_H/R$; R is the ideal gas constant, $\Delta H_H = 145 \pm 7 \text{ kJ/mol}$, $\Delta S_H = 0.46 \pm 0.04 \text{ kJ/mol-K}$ (Bamford et al. 2002)—see Comment by Goss et al. 2004

Octanol/Water Partition Coefficient, $\log K_{OW}$:

11.19 (Hansch & Leo 1979)
 9.60 (TLC-RT correlation, Bruggeman et al. 1982; 1984)
 8.26 (generator column-GC/ECD, Miller et al. 1984, 1985)
 8.20 (generator column-HPLC, Woodburn et al. 1984)
 8.20 (shake flask/slow stirring-GC, Brooke et al. 1986)
 8.20 (generator column-GC/ECD, Doucette & Andren 1987, 1988)
 8.38, 8.37, 8.41, 8.28 (RP-HPLC- k' correlation, different stationary and mobile phases, Brodsky & Ballschmiter 1988)
 9.45, 11.2 (calculated-UNIFAC activity coeff., π const. or f const., Banerjee & Howard 1988)
 8.274 ± 0.001 (shake flask/slow stirring-GC/ECD, De Bruijn et al. 1989; De Bruijn & Hermens 1990)
 > 9.0 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
 8.24 (HPLC-retention indices correlation, Noegrohati & Hammers 1992)
 8.27 (recommended, Hansch et al. 1995)
 7.95 ± 0.68 (flask/slow stirring-SPME/GC, Paschke et al. 1998)
 7.59 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

13.36, 1.96 (0, 20°C, multi-column GC- k' correlation, Zhang et al. 1999)
 12.29 (calculated-QSPR-quantum chemical descriptor by PM3 Hamiltonian, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ at 25°C or as indicated:

5.48 (guppy, 3.5% extractable lipid, Bruggeman et al. 1984; quoted, Gobas et al. 1987)
 7.0 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
 1.48, 1.41 (human fat of lipid basis, calculated- K_{OW} , Geyer et al. 1987)
 1.38, 1.32 (human fat of wet wt. basis, calculated- K_{OW} , Geyer et al. 1987)
 4.02 (guppy, Gobas et al. 1987; quoted, Banerjee & Baughman 1991)
 4.02 (guppy, calculated- C_B/C_W or k_1/k_2 , Connell & Hawker 1988; Hawker 1990)

- 5.07 (guppy, estimated, Banerjee & Baughman 1991)
 5.44; 6.97 (22°C, zebrafish: log BCF_w wet wt basis; log BCF_L lipid wt basis, Fox et al. 1994)
 2.65–4.54 (various marine species, mean dry wt. BCF, Hope et al. 1998)
 > 5.44, > 6.97 (zebrafish: wet wt basis, lipid wt basis, Geyer et al. 2000)
 > 5.53, > 6.99 (guppy: wet wt basis, lipid wt basis, Geyer et al. 2000)
 6.95, 8.26 (fish 5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.32, 3.97 (human, steady-state not reached during whole life: wet wt basis, lipid wt basis, Geyer et al. 2000)

Biota Sediment Accumulation Factor, BSAF:

- 13 (trout in Lake Ontario, Niimi 1996)
 0.047, 0.42, 0.10 (grass shrimp, striped mullet, sea trout muscle, Maruya & Lee 1998)

Sorption Partition Coefficient, log K_{OC}:

- 8.09 (suspended particulate matter, calculated-K_{OW}, Burkhard 1984)
 6.19, 5.99, 5.83, 5.61 (marine humic substances, in concentrations. of 5, 10, 20, 40 mg/L DOC, reported as association coefficient log K_h, Lara & Ernst 1989)
 6.19, 6.17 (marine humic substances of 5 mg L⁻¹ DOC, quoted; calculated-MCI χ , reported as log K_h, Sabljic et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization/Evaporation: 8.5×10^{-7} g m⁻¹ h⁻¹ (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

- k₂ > 0.0007 d⁻¹ (rainbow trout, Niimi & Oliver 1983; quoted, Clark et al. 1990)
 k₁ = 40 d⁻¹; k₂ = 0.004 d⁻¹ (guppy, Bruggeman et al. 1984)
 k₁ = 600 d⁻¹ (guppy, Opperhuizen 1986)
 log k₁ = 1.60 d⁻¹; log 1/k₂ = 2.39 d (fish, quoted, Connell & Hawker 1988)
 k₁ = 3640 d⁻¹; k₂ = 0.0132 d⁻¹ (22°C, zebrafish, 30-d exposure, Fox et al. 1994)
 k₂ = 0.013 d⁻¹ with t_{1/2} = 52 d and k₂ = 0.013 d⁻¹ with t_{1/2} = 52 d for food concn of 62 ng/g and 688 ng/g, respectively, in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
 k₂ = 0.005 d⁻¹ with t_{1/2} = 127 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose treatment, Buckman et al. 2004)
 k₂ = 0.005 d⁻¹ with t_{1/2} = 149 d (8°C, juvenile rainbow trout, 30-d uptake followed by 160-d depuration expt.- high-dose + CYPIA-inducing compounds (hCYP) treatment, Buckman et al. 2004)

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

- Biota: t_{1/2} > 1000 d in rainbow trout, and t_{1/2} = 122 d its muscle (Niimi & Oliver 1983);
 t_{1/2} = 175 d in guppy (Bruggeman et al. 1984).
 Depuration t_{1/2} = 52 d in a 30-d dietary exposure followed by 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)
 depuration t_{1/2} = 127 d for high-dose treatment, t_{1/2} = 149 d for high-dose + enzyme CYPIA-inducing compounds (hCYP) treatment (8°C, juvenile rainbow trout, Buckman et al. 2004)

Reported aqueous solubilities and vapor pressures of decachlorobiphenyl at various temperatures and the reported empirical temperature dependence equations

Aqueous solubility		Vapor pressure			
Dickhut et al. 1986		Burkhard et al. 1984		Goodman 1997	
generator column-GC/ECD		gas saturation-GC/ECD		Knudsen effusion	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
25	6.48 × 10 ⁻⁷	50.7	2.69 × 10 ⁻⁶	65	2.6 × 10 ⁻⁵
60	8.38 × 10 ⁻⁶	64.9	1.68 × 10 ⁻⁵	70	5.1 × 10 ⁻⁵
70	1.76 × 10 ⁻⁵	72.3	4.00 × 10 ⁻⁵	75	8.1 × 10 ⁻⁵
80	4.95 × 10 ⁻⁵	80.5	1.43 × 10 ⁻⁴	80	1.10 × 10 ⁻⁴
		85.2	1.88 × 10 ⁻⁴	85	1.80 × 10 ⁻⁴
ln <i>x</i> = A – B/(T/K)		89.8	3.36 × 10 ⁻⁴	log (P/Pa) = A – B/(T/K)	
A	–4.608	25.0	5.30 × 10 ⁻⁸		
B	8010.6	log (P/Pa) = A – B/(T/K)			
enthalpy of solution:		P/Pa		A	9.91
ΔH _{sol} /(kJ mol ⁻¹) = 66.6 ± 4.9		A	14.049	B	4886
for 40–80°C		B	6358.0		
		temp range 50.7–89.8°C			
		ΔH _{subl} /(kJ mol ⁻¹) = 101.7			

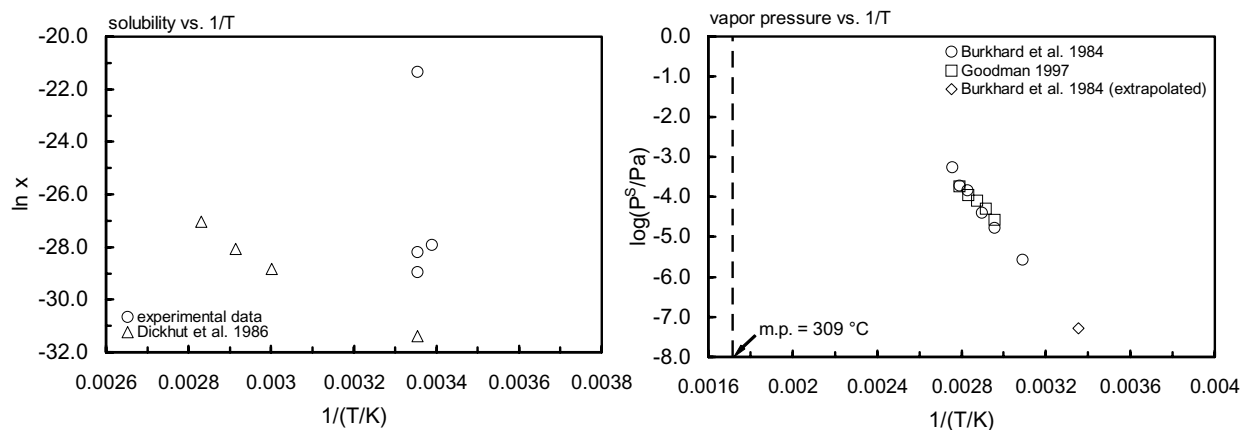


FIGURE 7.1.1.209.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,2',3,3',4,4',5,5',6,6'-decachlorobiphenyl (PCB-209).

7.1.2 ISOMER GROUPS

7.1.2.1 Monochlorobiphenyl

Common Name: Monochlorobiphenyl

Synonym: Dowtherm G

Chemical Name: monochlorobiphenyl

CAS Registry No: 27323-18-8

Molecular Formula: $C_{12}H_9Cl$

No. of Isomers: 3

Molecular Weight: 188.652

Melting Point ($^{\circ}C$):

25–77.9 (Shiu et al. 1987)

Boiling Point ($^{\circ}C$): 285

Chlorine Content: 18.79% (Hutzinger et al. 1974)

Density (g/cm^3): 1.1

Molar Volume (cm^3/mol):

205.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.30–1.0 (Mackay et al. 1983)

0.301–1.0 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.06–1.5 (selected, Mackay et al. 1983)

7.20 (selected, supercooled liq., Mackay et al. 1983a)

0.795–6.17, 4.08(exptl. range, calculated-UNIFAC, converted from $\log \gamma$, Burkhard et al. 1986)

1.2–5.5 (selected, Shiu et al. 1987)

2.5–6.73 (selected, supercooled liquid, Shiu et al. 1987)

1.2–9.5 (selected, Formica et al. 1988)

4.0 (selected, Metcalfe et al. 1988)

1.2–5.5 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

1.1–5.6 (selected, Mackay et al. 1983a)

2.30 (supercooled liquid P_L , Mackay et al. 1983a)

1.32 (selected, supercooled liq., Bopp 1983)

1.10 (average, liquid, Mackay 1986; Metcalfe et al. 1988)

0.271–2.04 (selected, solid, Shiu et al. 1987)

0.9–2.5 (selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

79.3 (calculated-P/C, Bopp 1983)

58–74 (calculated, Mackay et al. 1983a)

60.0 (selected, Mackay et al. 1983a,b)

42.56–75.55 (calculated, Shiu et al. 1987)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.66 (selected, Mackay et al. 1983b)

4.70 (selected, Mackay 1986; Metcalfe et al. 1988)

4.3–4.6 (selected, Shiu et al. 1987)

4.73 (calculated-no. Cl atoms, Formica et al. 1988)

4.50 (quoted, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

3.40 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC} :

Half-Lives in the Environment:

Air: atmospheric photodegradation, 0.62–1.4 d (Dilling et al. 1983); calculated tropospheric lifetime of 5–11 d due to calculated rate constant of gas-phase reaction with OH radicals for mono-chlorobiphenyls (Atkinson 1987); the tropospheric lifetime of 2.7–5.1 d based on the experimentally determined rate constant for gas-phase reaction with OH radicals for monochlorobiphenyls (Kwok et al. 1995).

Surface water: 1.4–4.9 d in Lake Michigan (Neely 1983); 2–3 d for river water (Bailey et al. 1983).

Groundwater:

Sediment:

Soil:

Biota:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 0.25 \text{ g/m}^2 \text{ h}$ (Mackay 1986; Metcalfe et al. 1988).

Photolysis: $t_{1/2} = 0.62\text{--}1.4 \text{ d}$ for photodegradation in the atmosphere (Dilling et al. 1983).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{exptl}) = (2.8 - 5.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = (3.1 - 4.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., and the tropospheric lifetime was calculated to be 5–11 d for monochlorobiphenyls (Atkinson 1987)

$k_{OH}(\text{exptl}) = (2.8 - 5.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{OH}(\text{calc}) = (3.2 - 4.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. for reaction with monochlorobiphenyls, the tropospheric lifetime was calculated to be 2.7–5.1 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of *Alcaligenes* and *Acinetobacter*, $7 \times 10^{-8} \text{ nmol cell}^{-1} \cdot \text{h}^{-1}$ (Furukawa et al. 1978; selected, NAS 1979); time for 50% biodegradation of an initial concentration of 1–100 $\mu\text{g/L}$ by river dieaway test is about 2–5 d (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

7.1.2.2 Dichlorobiphenyl

Common Name: Dichlorobiphenyl

Synonym:

Chemical Name: dichlorobiphenyl

CAS Registry No: 25512-42-9

Molecular Formula: $C_{12}H_8Cl_2$

No. of Isomers: 12

Molecular Weight: 223.098

Melting Point ($^{\circ}C$):

24.4–149 (Shiu & Mackay 1986; Shiu et al. 1987; quoted, Metcalfe et al. 1988)

Boiling Point ($^{\circ}C$):

312 (Shiu & Mackay 1986)

Chlorine Content: 31.77%

Density (g/cm^3 at $20^{\circ}C$): 1.30

Molar Volume (cm^3/mol):

226.4 (calculated-Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.06–1.5 (Mackay et al. 1983)

0.059–1.0 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.22 (quoted, Bopp 1983)

0.06–1.5, 2.20 (solid, supercooled liquid, Mackay et al. 1983a)

0.898–1.96, 1.60(exptl. range, calculated-UNIFAC, converted from log γ , Burkhard & Kuehl 1986)

1.6 (Mackay 1986; quoted, Metcalfe et al. 1988)

0.06–2.0, 1.02–2.26(selected, solid, supercooled liquid, Shiu et al. 1987)

0.06–2.0 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

0.223 (quoted, supercooled liquid, Bopp 1983)

0.60 (quoted, supercooled liquid, Mackay et al. 1983a)

0.03–0.36 (Mackay et al. 1983)

0.24 (average, liquid, Mackay 1986; Metcalfe et al. 1988)

0.0018–0.279, 0.008–0.60 (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

153.6 (calculated-P/C, Bopp 1983)

60.0 (Mackay et al. 1983a,b)

97.0 (calculated-P/C, Mackay et al. 1983a)

17–92.2 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{ow} :

5.19 (Mackay et al. 1983a,b)

5.10 (Mackay 1986; Metcalfe et al. 1988)

4.9–5.3 (selected, Shiu et al. 1987)

5.13 (calculated-chlorine atoms, Formica et al. 1988)

5.10 (quoted mean value for isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

3.89 (biota, Mackay et al. 1983b)

3.80 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

4.10 (calculated-MCI χ , Koch 1983)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 0.065 \text{ g m}^{-2} \text{ h}^{-1}$ (selected, Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (1.4 - 2.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 8–17 d at room temp. (Atkinson 1987)

$k_{OH}(\text{exptl}) = (2.0 - 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, the tropospheric lifetime is calculated to be 3.4–7.2 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of *Alcaligenes* and *Acinetobacter*, $6 \times 10^{-8} \text{ nmol cell}^{-1} \cdot \text{h}^{-1}$ (Furukawa et al. 1978; quoted, NAS 1979);

$t_{1/2} \sim 2\text{--}3 \text{ d}$ for degradation, using river water dieaway test (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 8–17 d due to calculated rate constant of gas-phase reaction with OH radicals for dichlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 3.4–7.2 d based on the calculated rate constant for gas-phase reaction with OH radicals for dichlorobiphenyls (Kwok et al. 1995).

Surface water: $t_{1/2} = 2\text{--}3 \text{ d}$ (Bailey et al. 1983).

Groundwater:

Sediment:

Soil:

Biota:

7.1.2.3 Trichlorobiphenyl

Common Name: Trichlorobiphenyl

Synonym:

Chemical Name: trichlorobiphenyl

CAS Registry No: 25323-68-6

Molecular Formula: $C_{12}H_7Cl_3$

No. of Isomers: 24

Molecular Weight: 257.543

Melting Point ($^{\circ}C$):

28–87 (Shiu & Mackay 1986; Metcalfe et al. 1988)

Boiling Point ($^{\circ}C$):

337 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 41.4%

Density (g/cm^3):

Molar Volume (cm^3/mol):

247.3 (calculated-Le Bas method at normal boiling point Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.24–0.65 (Mackay et al. 1983)

0.244–0.651 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.05 (Neely 1980)

0.15–0.64, 0.67(solid, supercooled liquid, Mackay et al. 1983)

0.0654–1.09 (exptl. range, calculated-UNIFAC, converted from log γ , Burkhard & Kuehl 1986)

0.65 (quoted, Mackay 1986; Metcalfe et al. 1988)

0.015–0.40 (selected, Shiu et al. 1987)

0.015–0.40 (quoted, Formica et al. 1988)

0.015–0.40 (quoted range for individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

0.200 (Neely 1980)

0.0375 (supercooled liquid, Bopp 1983)

0.01–0.27, 0.20(solid, supercooled liquid, quoted, Mackay et al. 1983)

0.054 (average, liquid, Mackay 1986; Metcalfe et al. 1988)

0.0136–0.143, 0.003–0.022 (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

81.76 (calculated-P/C, Bopp 1983)

82–102 (calculated-P/C, Mackay et al. 1983)

77 (selected, Mackay et al. 1983)

24.3–92.2 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, log K_{ow} :

5.76 (Mackay et al. 1983)

5.50 (Mackay 1986; Metcalfe et al. 1988)

5.5–5.9 (selected, Shiu et al. 1987)

5.53 (calculated-chlorine atoms, Formica et al. 1988)

5.80 (quoted mean value of isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

4.20 (fish, Mackay 1986; Metcalfe et al. 1988)

4.70 (calculated-MCI χ , Koch 1983)

Sorption Partition Coefficient, $\log K_{OC}$:

Sorption Partition Coefficient, $\log K_p$:

- 3.34 (lake sediment, calculated, Formica et al. 1988)
- 3.50 (calculated-MCI χ , Koch 1983)

Environmental Fate Rate Constants, k , or Half Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 0.017 \text{ g m}^{-2} \text{ h}^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.7 - 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 14–30 d at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (1.0 - 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radicals for trichlorobiphenyls, the tropospheric lifetime is calculated to be 6.9–15 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: rate of degradation using species of *Alcaligenes* and *Acinetobacter*, $5 \times 10^{-8} \text{ nmol cell}^{-1} \cdot \text{h}^{-1}$ (Furukawa et al. 1978; quoted, NAS 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 14–30 d due to calculated rate constant of gas-phase reaction with OH radicals for trichlorobiphenyls (Atkinson 1987);
tropospheric lifetime of 6.9–17 d based on the calculated rate constant for gas-phase reaction with OH radicals for trichlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: estimated $t_{1/2} = 134 \text{ h}$ from fish in simulated ecosystem (Neely 1980).

7.1.2.4 Tetrachlorobiphenyl

Common Name: Tetrachlorobiphenyl

Synonym:

Chemical Name: tetrachlorobiphenyl

CAS Registry No: 26914-33-0

Molecular Formula: $C_{12}H_6Cl_4$

No. of Isomers: 42

Molecular Weight: 291.988

Melting Point ($^{\circ}C$):

47–180 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)

Boiling Point ($^{\circ}C$):

360 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 48.6%

Density (g/cm^3 at $20^{\circ}C$): 1.5

Molar Volume (cm^3/mol):

268.2 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.1–0.68 (Mackay et al. 1983)

0.029–0.606 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.05 (Neely 1980)

0.0008–0.17 (Mackay et al. 1983)

0.017 (McCall et al. 1983)

0.02–0.0955, 0.224 (exptl. range, calculated-UNIFAC, converted from $\log \gamma$, Burkhard & Kuehl 1986)

0.26 (quoted, Mackay 1986; Metcalfe et al. 1988)

0.0043–0.10 (selected, Shiu et al. 1987)

0.039–0.38 (selected, supercooled liquid, Shiu et al. 1987)

0.001–0.10 (Formica et al. 1988)

0.001–0.10 (quoted range for individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0653 (Neely 1980)

0.0064 (supercooled liquid, Bopp 1983)

0.003–0.104 (Mackay et al. 1983)

0.06 (supercooled liquid, Mackay et al. 1983)

0.0653 (McCall et al. 1983)

0.012 (Mackay 1986; Metcalfe et al. 1988)

5.9×10^{-5} – 5.4×10^{-3} (selected, Shiu et al. 1987)

0.002 (selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

34.69 (calculated-P/C, Bopp 1983)

75–94 (calculated-P/C, Mackay et al. 1983)

76.0 (Mackay et al. 1983)

1.72–47.59 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.35 (suggested, Mackay et al. 1983)

5.90 (Mackay 1986; Metcalfe et al. 1988)

5.6–6.5 (selected, Shiu et al. 1987)

- 5.93 (calculated-chlorine atoms, Formica et al. 1988)
 6.00 (quoted mean value for isomers, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

- 3.98 (pinfish, Branson et al. 1975; quoted, Waid 1986)
 3.95 (trout, Branson et al. 1975; quoted, NAS 1979)
 4.79 (McCall et al. 1983)
 4.60 (fish, Mackay 1986; Metcalfe et al. 1988)
 5.30 (calculated-MCI χ , Koch 1983)

Sorption Partition Coefficient, log K_{OC} :

- 4.51 (correlated, McCall et al. 1983)
 3.43–5.11 (correlated of literature values in high clay soils, Sklarew & Girvin 1987)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 4.2 \times 10^{-3} \text{ g m}^{-2} \text{ h}^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.4 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 25–60 d at room temp. (Atkinson 1987)

$k_{OH}(\text{calc}) = (0.36 - 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radicals for tetrachlorobiphenyls, the tropospheric lifetime is calculated to be 8.5–40 d (Kwok et al. 1995).

Hydrolysis:

Biodegradation: rate of degradation for both rings substituted with chlorine using species of *Alcaligenes* and *Acinetobacter*, $2.5 \times 10^{-8} \text{ nmol cell}^{-1} \text{ h}^{-1}$ (Furukawa et al. 1978; selected, NAS 1979);
 no degradation by river dieaway test after 98 d of incubation (Bailey et al. 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 25–60 d due to calculated rate constant of gas-phase reaction with OH radicals for tetrachlorobiphenyls (Atkinson 1987);
 tropospheric lifetime of 8.5–40 d based on the calculated rate constant for gas-phase reaction with OH radicals for tetrachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil: volatilization $t_{1/2} \sim 10 \text{ d}$ from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).

Biota: estimated $t_{1/2} = 139 \text{ h}$ from fish in simulated ecosystem (Neely 1980).

7.1.2.5 Pentachlorobiphenyl

Common Name: Pentachlorobiphenyl

Synonym:

Chemical Name: pentachlorobiphenyl

CAS Registry No: 25429-29-2

Molecular Formula: $C_{12}H_5Cl_5$

No. of Isomers: 46

Molecular Weight: 326.433

Melting Point ($^{\circ}C$):

−23.5–124 (Shiu et al. 1987)

76.5–124 (Shiu & Mackay 1986; Metcalfe et al. 1988)

Boiling Point ($^{\circ}C$):

381 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 54.4%

Density (g/cm^3 at $20^{\circ}C$): 1.50

Molar Volume (cm^3/mol):

289.1 (Le Bas method at normal boiling point, Shiu & Mackay 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.1–0.31 (Mackay et al. 1983)

0.105–0.311 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.01 (Neely 1980)

0.004–0.03 (Mackay et al. 1983)

0.072 (supercooled liquid, Mackay et al. 1983)

0.0338–0.0525, 0.0829 (experimental range, calculated-UNIFAC, converted from $\log \gamma$, Burkhard & Kuehl 1986)

0.099 (Mackay 1986; Metcalfe et al. 1988)

0.004–0.02 (selected, Shiu et al. 1987)

0.03–0.11 (selected, supercooled liquid, Shiu et al. 1987)

0.004–0.02 (Formica et al. 1988)

0.024 (selected average value of isomers, Mackay 1989)

0.004–0.02 (quoted range of individual congeners, Luthy et al. 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

0.01026 (Neely 1980)

0.00111 (supercooled liquid, Bopp 1983)

0.015 (supercooled liquid, Mackay et al. 1983)

0.004–0.03 (Mackay et al. 1983)

0.0026 (Mackay 1986; Metcalfe et al. 1988)

0.000304–0.0093 (selected, Shiu et al. 1987)

0.0023–0.051 (selected, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

68.0 (suggested, Mackay et al. 1983)

17.34 (calculated-P/C, Bopp 1983)

24.8–151.4 (selected, Shiu et al. 1987)

12.2 (calculated, Mackay 1989)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.85 (suggested, Mackay et al. 1983)

6.33 (calculated-chlorine atoms, Formica et al. 1988)

- 6.30 (Mackay 1986; Metcalfe et al. 1988)
 6.2–6.5 (selected, Shiu et al. 1987)
 6.60 (selected, Mackay 1989)
 6.40 (quoted mean value for isomers of a homolog group, Luthy et al. 1997)

Bioconcentration Factor, log BCF:

- 5.0 (fish, Mackay 1986; Metcalfe et al. 1988)
 5.30 (Mackay 1989)
 5.90 (calculated-MCI χ , Koch 1983)

Sorption Partition Coefficient, log K_{OC} :

- 6.21 (calculated, $0.41K_{OW}$, Mackay 1989)

Sorption Partition Coefficient, log K_p :

- 4.15 (lake sediment, calculated- K_{OW} , f_{OC} , Formica et al. 1988)
 4.51 (calculated-MCI χ , Koch 1983)

Environmental Fate Rate Constants, k, and Half Lives, $t_{1/2}$:

Volatilization /Evaporation: $k = 1.0 \times 10^{-3} \text{ g m}^{-2} \text{ h}^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.2 - 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., with a calculated tropospheric lifetime of 60–120 d (Atkinson 1987);

$k_{OH}(\text{calc}) = (0.3 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radicals for pentachlorobiphenyls, the tropospheric lifetime is calculated to be 16–48 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.62\text{--}1.4 \text{ d}$ for atmospheric photodegradation (Dilling et al. 1983);

calculated tropospheric lifetime of 60–120 d due to calculated rate constant of gas-phase reaction with OH radicals for pentachlorobiphenyls (Atkinson 1987);

tropospheric lifetime of 17–48 d based on the calculated rate constant for gas-phase reaction with OH radicals for pentachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil: volatilization $t_{1/2} = 25 \text{ d}$ from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).

Biota: estimated $t_{1/2} = 226 \text{ d}$ from fish in simulated ecosystem (Neely 1980).

7.1.2.6 Hexachlorobiphenyl

Common Name: Hexachlorobiphenyl

Synonym:

Chemical Name: hexachlorobiphenyl

CAS Registry No: 26601-64-9

Molecular Formula: $C_{12}H_4Cl_6$

No. of Isomers: 42

Molecular Weight: 360.878

Melting Point ($^{\circ}C$):

85–160 (Shiu et al. 1987)

77–150 (Shiu & Mackay 1986; Metcalfe et al. 1988)

Boiling Point ($^{\circ}C$):

400 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 62.77% (Hutzinger et al. 1974)

Density (g/cm^3 at $20^{\circ}C$): 1.60

Molar Volume (cm^3/mol):

310.0 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.06–0.25 (Mackay et al. 1983)

0.0582–0.256 (Shiu & Mackay 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0004–0.01, 0.021 (solid, supercooled liquid, Mackay et al. 1983)

0.00303–0.0504, 0.00297 (experimental range, calculated-UNIFAC, converted from $\log \gamma$, Burkhard & Kuehl 1986)

0.038 (Mackay 1986; Metcalfe et al. 1988)

0.0004–0.001, 0.0022–0.01 (solid, supercooled liquid, Shiu et al. 1987)

0.0004–0.005 (Formica et al. 1988)

0.0035 (Mackay & Paterson 1991)

0.0004–0.001 (quoted range, Luthy et al. 1997)

Vapor Pressure (Pa at $25^{\circ}C$):

0.000182 (supercooled liquid, Bopp 1983)

0.0016, 0.005 (solid, supercooled liquid, Mackay et al. 1983)

5.8×10^{-4} (Mackay 1986; Metcalfe et al. 1988)

2.0×10^{-5} – 1.59×10^{-3} , 7.0×10^{-4} – 0.012 (solid, supercooled liquid, Shiu et al. 1987)

0.0005 (selected, Mackay & Paterson 1991)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

86.0 (Mackay et al. 1983)

6.70 (calculated-P/C, Bopp 1983)

11.9–81.8 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.70–7.30 (selected, Shiu et al. 1987)

6.70 (selected, Mackay 1986; Metcalfe et al. 1988)

6.80 (selected, Mackay & Paterson 1991)

7.00 (quoted mean value for isomers of a homolog group, Luthy et al. 1997)

Bioconcentration Factor, $\log BCF$:

6.50 (calculated-MCI χ , Koch 1983)

5.39 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

4.57 (green alga, Mailhot 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

4.785–6.869 (correlated literature values in high clay soils, Sklarew & Girvin 1987)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $2.5 \times 10^{-4} \text{ g m}^{-2} \text{ h}^{-1}$ (Mackay 1986; Metcalf et al. 1988).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (0.16 - 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., the tropospheric lifetime is calculated to be 29–60 d (Kwok et al. 1995)

Hydrolysis:

Biodegradation: degradation rate constants estimated to be $1.5 \times 10^{-5} \text{ h}^{-1}$ in water, soil and sediment (Mackay & Patterson 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the tropospheric lifetime of 29–90 d based on the calculated rate constant for gas-phase reaction with OH radicals for hexachlorobiphenyls (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil: volatilization $t_{1/2} = 40 \text{ d}$ from an Ottawa sand (estimated, Haque et al. 1974; selected, Pal et al. 1980).

Biota:

7.1.2.7 Heptachlorobiphenyl

Common Name: Heptachlorobiphenyl

Synonym:

Chemical Name: heptachlorobiphenyl

CAS Registry No: 28655-71-2

Molecular Formula: $C_{12}H_3Cl_7$

No. of Isomers: 24

Molecular Weight: 395.323

Melting Point ($^{\circ}C$):

122.4–149 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)

Boiling Point ($^{\circ}C$):

417 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 62.77% (Hutzinger et al. 1974)

Density (g/cm^3 at $20^{\circ}C$): 1.70

Molar Volume (cm^3/mol):

330.9 (Le Bas method at normal boiling point, Shiu & Mackay 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.0596–0.109 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0005, 0.006 (solid, supercooled liquid, Mackay et al. 1983)

0.00816–0.0205, 0.011 (experimental range, calculated-UNIFAC, converted from $\log \gamma$, Burkhard & Kuehl 1986)

0.014 (Mackay 1986; Metcalfe et al. 1988)

0.00045–0.002, 0.0076–0.018 (solid, supercooled liquid, selected, Shiu et al. 1987)

0.00046–0.002 (Formica et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0015 (supercooled liquid, Mackay et al. 1983)

1.3×10^{-4} (Mackay 1986; Metcalfe et al. 1988)

2.73×10^{-5} , 2.5×10^{-4} (solid, supercooled liquid, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol):

100.0 (Mackay et al. 1983)

5.4 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.1 (Mackay 1986; Metcalfe et al. 1988)

6.7–7.0 (selected, Shiu et al. 1987)

Bioconcentration Factor, $\log BCF$:

7.10 (calculated-MCI χ , Koch 1983)

5.80 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 6.2 \times 10^{-5} g m^{-2} h^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

7.1.2.8 Octachlorobiphenyl

Common Name: Octachlorobiphenyl

Synonym:

Chemical Name: octachlorobiphenyl

CAS Registry No: 31472-83-0

Molecular Formula: $C_{12}H_2Cl_8$

No. of Isomers: 12

Molecular Weight: 429.768

Melting Point ($^{\circ}C$):

159–162 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)

Boiling Point ($^{\circ}C$):

432 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 65.98% (Hutzinger et al. 1974)

Density (g/cm^3 at $20^{\circ}C$): 1.7

Molar Volume (cm^3/mol):

351.8 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.0443–0.0474 (Shiu et al. 1987)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0002–0.007, 0.020 (solid, supercooled liquid, estimated, Mackay et al. 1983)

0.00345–0.006, 0.00378 (experimental range, calculated-UNIFAC, converted from $\log \gamma$, Burkhard & Kuehl 1986)

0.0055 (Mackay 1986; Metcalfe et al. 1988)

0.0002–0.0003, 0.004–0.0068 (solid, supercooled liquid, Shiu et al. 1987)

Vapor Pressure (Pa at $25^{\circ}C$):

2.8×10^{-5} (Mackay 1986; Metcalfe et al. 1988)

2.66×10^{-5} , 6.0×10^{-3} (solid, supercooled liquid, selected, Shiu et al. 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

100.0 (suggested, Mackay et al. 1983)

38.08 (calculated-P/C, Shiu et al. 1987)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.55 (Mackay et al. 1983)

7.50 (Mackay 1986; Metcalfe et al. 1988)

7.1 (selected, Shiu et al. 1987)

Bioconcentration Factor, $\log BCF$:

6.20 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 1.5 \times 10^{-5}\ g\ m^{-2}\cdot h^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Half-Lives in the Environment:

7.1.2.9 Nonachlorobiphenyl

Common Name: Nonachlorobiphenyl

Synonym:

Chemical Name: nonachlorobiphenyl

CAS Registry No: 53742-07-7

Molecular Formula: $C_{12}HCl_9$

No. of Isomers: 3

Molecular Weight: 464.213

Melting Point ($^{\circ}C$):

182.8–206 (Shiu & Mackay 1986; Shiu et al. 1987; Metcalfe et al. 1988)

Boiling Point ($^{\circ}C$):

445 (average, Shiu & Mackay 1986; Metcalfe et al. 1988)

Chlorine Content: 68.73% (Hutzinger et al. 1974)

Density (g/cm^3 at $20^{\circ}C$): 1.80

Molar Volume (cm^3/mol):

372.7 (Le Bas method at normal boiling point, Shiu & Mackay 1986; Shiu et al. 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

0.016 (Mackay et al. 1983)

0.0163–0.0276 (Shiu et al. 1987)

Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0001, 0.0007 (solid, supercooled liquid, Mackay et al. 1983)

0.000678–0.00148, 0.00145 (exptl. range, calculated-UNIFAC, converted from $\log \gamma$, Burkhard & Kuehl 1986)

0.002 (Mackay 1986; Metcalfe et al. 1988)

0.000018–0.00011, 0.00065–0.0068 (solid, supercooled liquid, selected, Shiu et al. 1987)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00015 (supercooled liquid, Mackay et al. 1983)

6.3×10^{-6} (Mackay 1986; Metcalfe et al. 1988)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

100.0 (estimated, Mackay et al. 1983)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

9.14 (Mackay et al. 1983)

7.9 (Mackay 1986; Metcalfe et al. 1988)

7.2–8.16 (selected, Shiu et al. 1987)

Bioconcentration Factor, $\log BCF$:

6.60 (fish, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 3.5 \times 10^{-6}\ g\ m^{-2}\ h^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Half-Lives in the Environment:

7.1.3 AROCLOR MIXTURES

7.1.3.1 Aroclor 1016

Common Name: Aroclor 1016

Synonym:

Chemical Name:

CAS Registry No: 12674-11-2

Molecular Formula:

Average Molecular Weight: 257

Physical state: mobile oil

Distillation Range (°C):

323–356 (NAS 1979; Brinkman & De Kock 1980)

Chlorine Content: 41%

Density (g/cm³):

1.37 (20°C, Brinkman & De Kock 1980)

1.36–1.37 (25°C, NAS 1979)

1.33 (Mills et al. 1982)

1.40 (25°C, Mackay 1986)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

0.22–0.25 (estimated, Tucker et al. 1975)

0.906 (23°C, shake flask-GC/ECD, Griffin et al. 1978; quoted, Lee et al. 1979)

0.42 (shake flask-GC/ECD, Paris et al. 1978; Callahan et al. 1979; Mackay et al. 1980; Mills et al. 1982)

0.906 (shake flask-GC/ECD, Lee et al. 1979)

0.049, 0.490 (shake flask, nephelometric, Hollifield 1979)

0.085 (Kenaga & Goring 1980)

0.34 (quoted, Pal et al. 1980)

0.906 (23°C, shake flask-GC/ECD, Griffin & Chian 1981; quoted, Sklarew & Girvin 1987)

0.40–0.91 (selected, Mackay et al. 1983)

0.84 (selected, Mackay 1986; Metcalfe et al. 1988)

0.332 (quoted, Chou & Griffin 1986)

Vapor Pressure (Pa at 25°C):

0.0533 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)

0.060 (quoted, Mackay et al. 1983)

0.200 (quoted, supercooled liquid, Mackay et al. 1983)

0.10 (selected, Mackay 1986; Metcalfe et al. 1988)

0.12, 0.121 (GC-RT correlation, Foreman & Bidleman 1985)

Henry's Law Constant (Pa m³/mol at 25°C):

1368 (calculated, Paris et al. 1978)

33.4 (calculated-P/C, Mabey et al. 1982)

77.0 (calculated, Mackay et al. 1983)

Octanol/Water Partition Coefficient, log K_{ow} :

> 5.58 (shake flask, Chiou et al. 1977; Callahan et al. 1979; Veith et al. 1979a; Kenaga & Goring 1980; Mabey et al. 1982; Mackay 1982)

4.38 (shake flask-GC, Paris et al. 1978; quoted, Callahan et al. 1979; Ryan et al. 1988)

5.88 (HPLC-RT correlation, Veith et al. 1979b; Garten & Trabalka 1983)

3.48 (Pal et al. 1980; Sklarew & Girvin 1987)

- 4.3–5.48 (quoted, Mills et al. 1982)
 4.40–5.80 (selected, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988)
 5.31 (quoted, Chou & Griffin 1986)

Bioconcentration Factor, log BCF:

- 3.80, 3.81, 3.74 (bacteria: Doe Run pond, Hickory Hills pond, USDA pond, Paris et al. 1978)
 4.18 (fish in Hudson River, Skea et al. 1979; quoted, Waid 1986)
 4.63 (fathead minnow, 32-d exposure, Veith et al. 1979b; Veith & Kosian 1983)
 4.69, 3.81 (fish, flowing water, static water, Kenaga & Goring 1980)
 4.69 (quoted, Bysshe 1982)
 4.70 (microorganism, calculated- K_{OW} , Mabey et al. 1982)
 4.63; 4.56 (fish, quoted; calculated- K_{OW} , Mackay 1982)
 0.15 (rodents, Garten & Trabalka 1983)
 4.63 (fish, Garten & Trabalka 1983)
 4.63 (fathead minnow, quoted, Zaroogian et al. 1985)
 4.24, 4.30 (oyster, quoted, Zaroogian et al. 1985)
 3.11–4.5 (fish, selected, Mackay 1986; Metcalfe et al. 1988)

Sorption Partition Coefficient, log K_{OC} :

- 5.19, 5.23, 4.96, 4.73 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
 5.26 (calculated- K_{OW} , Mabey et al. 1982)
 4.87 (calculated, Sklarew & Girvin 1987)
 4.25 (soil, calculated-S, Chou & Griffin 1986)
 5.03, 4.97 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization/Evaporation: volatilization $t_{1/2} = 9.9$ h (Paris et al. 1978, quoted Callahan et al. 1979);
 rate constant $k = 0.031$ g m⁻² h⁻¹ (Mackay 1986; Metcalfe et al. 1988).
 Photolysis:
 Hydrolysis: not environmentally significant (Mabey et al. 1982).
 Oxidation: calculated rate constant for singlet oxygen, $k \ll 360$ M⁻¹ h⁻¹ and $k \ll 1$ M⁻¹ h⁻¹ for RO₂ (peroxy radical) (Mabey et al. 1982).
 Biodegradation: 32.9% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972);
 33% degraded by activated sludge for 48-h exposure (Tucker et al. 1975; Versar Inc. 1979; quoted, Pal et al. 1980);
 rate constant $k = 0.2$ d⁻¹ by acclimated activated sludge with $t_{1/2} = 3.5$ d (Callahan et al. 1979).
 96% loss by degradation with Nocardia strain NCIB 10603 and 91% loss with NCIB 10643, both within 52 d; > 98% loss with NCIB 10603 and > 96% loss with NCIB 10643, both within 100 d (Baxter et al. 1975; quoted, Pal et al. 1980).
 Biotransformation: $k \sim 3 \times 10^{-9}$ to 3×10^{-12} mL cell⁻¹ h⁻¹, estimated for bacteria transformation in water (Mabey et al. 1982).
 Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

- Air:
 Surface water: $t_{1/2} = 9.9$ h in 1 m³ water of 1-m deep (Paris et al. 1978; selected, Callahan et al. 1979; Mills et al. 1982)
 Groundwater:
 Sediment:
 Soil: $t_{1/2} > 50$ d (Ryan et al. 1988).
 Sludge: estimated $t_{1/2} = 15$ d for the volatilization from activated sludge under aerobic conditions (Tucker et al. 1975; quoted, Pal et al. 1980).
 Biota: $t_{1/2} \sim 1.2$ yr in fish in Hudson River (Armstrong & Sloan 1985).

7.1.3.2 Aroclor 1221

Common Name: Aroclor 1221

Synonym:

Chemical Name:

CAS Registry No: 11104-28-2

Molecular Formula:

Average Molecular Weight: 192–200.7

Physical State: mobile oil

Distillation Range (°C):

275–320 (NAS 1979; Brinkman & De Kock 1980)

Chlorine Content: 20.5–21.5%

Density (g/cm³):

1.182–1.19 (25°C, NAS 1979)

1.18 (20°C, Brinkman & De Kock 1980)

1.15 (Callahan et al. 1979; Mills et al. 1982)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

5.00 (Zitko 1970, 1971)

3.5 (23°C, shake flask-GC/ECD, Griffin et al. 1978; quoted, Chou & Griffin 1986)

15.0 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Pal et al. 1980; Mills et al. 1982)

3.52 (shake flask-GC/ECD, Lee et al. 1979)

0.59 (shake flask-nephelometric, Hollifield 1979)

40.0 (calculated- K_{OW} , Mabey et al. 1982)

3.50–15.0 (selected, Mackay et al. 1983)

Vapor Pressure (Pa at 25°C):

0.893 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)

0.93 (Pal et al. 1980)

0.89 (quoted, Mackay et al. 1983)

Henry's Law Constant (Pa m³/mol):

0.750 (Hetling et al. 1978)

17.23 (calculated-P/C, Mabey et al. 1982)

60.0 (suggested value, Mackay et al. 1983)

23.10 (calculated, Burkhard et al. 1985b)

Octanol/Water Partition Coefficient, log K_{OW} :

2.8 (Monsanto Co. 1972; quoted, Callahan et al. 1979)

2.81 (Pal et al. 1980)

4.08 (Callahan et al. 1979; Mabey et al. 1982)

4.10–4.70 (quoted, Mackay et al. 1980)

2.78–4.0 (quoted, Mills et al. 1982)

4.09 (quoted, Chou & Griffin 1986)

4.09 (quoted, Ryan et al. 1988)

Bioconcentration Factor, log BCF:

3.34 (microorganism, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC} :

3.76 (sediment, calculated- K_{OW} , Mabey et al. 1982)

3.62 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $k \sim 1.74 \text{ mg cm}^{-2} \text{ h}^{-1}$ from liquid substrate at 100°C (Hutzinger et al. 1974; quoted, Pal et al. 1980).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ and $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: 80.6% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980); 81% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980); $k = 0.8 \text{ d}^{-1}$ and $t_{1/2} = 0.9 \text{ d}$ for biodegradation by acclimated activated sludge (Callahan et al. 1979).

Biotransformation: estimated $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ rate of transformation for bacteria in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil: $t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988).

Sludge: estimated $t_{1/2} = 12 \text{ d}$ of volatilization from activated sludge to be 12 d under aerobic conditions (Tucker et al. 1975; quoted, Pal et al. 1980).

Biota:

7.1.3.3 Aroclor 1232

Common Name: Aroclor 1232

Synonym:

Chemical Name:

CAS Registry No: 11141-16-5

Molecular Formula:

Average Molecular Weight: 221–232.2

Physical State: mobile oil

Distillation Range (°C):

270–325 (NAS 1979; Brinkman & De Kock 1980)

Chlorine Content: 32%

Density (g/cm³):

1.260 (20°C, Brinkman & De Kock 1980)

1.27–1.28 (25°C, NAS 1979)

1.24 (Callahan et al. 1979; Mills et al. 1982)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

1.45 (Monsanto Co. 1972; quoted, Callahan et al. 1979; Chou & Griffin 1986)

1.45 (quoted, Pal et al. 1980; Mackay et al. 1983)

407 (calculated- K_{OW} , Mabey et al. 1982)

Vapor Pressure (Pa at 25°C):

0.54 (Monsanto Co. 1972; Callahan et al. 1979; Mabey et al. 1982)

0.533 (quoted, Mills et al. 1982)

0.54 (quoted, Mackay et al. 1983)

Henry's Law Constant (Pa m³/mol):

60.0 (suggested, Mackay et al. 1980)

1.14 (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, log K_{OW} :

3.2 (Monsanto Co. 1972; Callahan et al. 1979; Mabey et al. 1982)

4.54 (Tulp & Hutzinger 1978; Callahan et al. 1979)

3.23 (quoted, Pal et al. 1980)

3.18–4.48 (quoted, Mills et al. 1982)

4.10–5.20 (quoted, Mackay et al. 1983)

4.62 (calculated-S, Chou & Griffin 1986)

4.54 (quoted, Ryan et al. 1988)

Bioconcentration Factor, log BCF:

2.54 (microorganism, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC} :

2.89 (sediment, calculated- K_{OW} , Mabey et al. 1982)

3.85 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ and $k \ll 1 \text{ M}^{-1} \cdot \text{h}^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: aerobic biodegradation $t_{1/2} = 61.4 \text{ d}$ without the addition of polymer chitin, $t_{1/2} = 33.4 \text{ d}$ with chitin and $t_{1/2} = 26.8 \text{ d}$ with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1}$, estimated rate of transformation for bacteria in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: aerobic biodegradation $t_{1/2} = 61.4 \text{ d}$ without the addition of polymer chitin, $t_{1/2} = 33.4 \text{ d}$ with chitin and $t_{1/2} = 26.8 \text{ d}$ with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Groundwater:

Sediment:

Soil: $t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988).

Biota:

7.1.3.4 Aroclor 1242

Common Name: Aroclor 1242

Synonym:

Chemical Name:

CAS Registry No: 534-692-19

Molecular Formula:

Average Molecular Weight: 261–266.5

Physical State: mobile oil

Distillation Range (°C):

325–366 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)

Chlorine Content: 42%

Density (g/cm³):

1.38 (Brinkman & De Kock 1980)

1.30–1.39 (quoted, NAS 1979)

1.35 (Callahan et al. 1979; Mills et al. 1982)

1.40 (quoted, Mackay 1986; Metcalfe et al. 1988)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.20 (Monsanto Co. 1972; quoted, Hutzinger et al. 1974; Tucker et al. 1975 Sawhney 1987)

0.20 (20°C, Nisbet & Sarofim 1972)

0.24 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Brinkman & De Kock 1980; Geyer et al. 1980; Pal et al. 1980; Erickson 1986)

0.045 (shake flask-GC, Lawrence & Tosine 1976)

0.085 (Branson 1977; Kenaga & Goring 1980)

0.703 (23°C, shake flask-GC/ECD, Griffin et al. 1978)

0.34 (shake flask-GC/ECD, Paris et al. 1978)

0.1329 (11.5°C, shake flask-GC/ECD, Dexter & Pavlou 1978)

0.23 (quoted, Callahan et al. 1979; Mabey et al. 1982)

0.23–0.703 (shake flask-GC, Lee et al. 1979)

0.10 (shake flask-nephelometric, Hollifield 1979)

0.703 (20°C, Griffin & Chian 1980; quoted, Sklarew & Girvin 1987)

0.25 (quoted, Eisenreich et al. 1981)

0.34–0.703 (selected, Westcott et al. 1981)

0.10–0.30 (selected, Mills et al. 1982)

0.75 (selected, Mackay 1986; Metcalfe et al. 1988)

0.277 (20°C, calculated from mole fraction, Murphy et al. 1987)

0.097; 0.085–0.34 (21°C, shake flask-GC/ECD; quoted lit. range, Luthy et al. 1997)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.0133 (20°C, Nisbet & Sarofim 1972)

0.12 (20°C, extrapolated, Monsanto 1972; NAS 1979)

$\log(P_L/\text{mmHg}) = 8.80 - 3500/(T/K)$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)

0.055 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983; Bidleman & Christensen 1979)

0.054 (Callahan et al. 1979; Westcott et al. 1981; Eisenreich et al. 1981; Richardson et al. 1983)

0.054 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)

0.040 (38°C, average, Wingender & Williams 1984)

0.076, 0.077 (GC-RT correlation, Foreman & Bidleman 1985)

0.077 (quoted, Mackay et al. 1986)

0.0517 (quoted, Eisenreich 1987)

- 0.091 (selected, Mackay 1986; Metcalfe et al. 1988)
 0.033 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

- 58.06 (calculated, Mackay & Leinonen 1975)
 768 (calculated, Paris et al. 1978)
 59.5 (Slinn et al. 1978)
 56.74 (calculated-P/C, Eisenreich et al. 1981)
 20.32–41.62 (Westcott et al. 1981)
 20.27–41.54 (calculated, Westcott et al. 1981)
 79.02 (batch stripping, Atlas et al. 1982; quoted, Eisenreich et al. 1983; Atlas & Giam 1986)
 34.69 (radiotracer-equilibration, Atlas et al. 1982; Atlas & Giam 1986)
 200.6 (calculated-P/C, Mabey et al. 1982)
 22.29 (direct concn. ratio-GC/ECD, Murphy et al. 1983)
 40.3 (16°C, calculated-P/C, Richardson et al. 1983)
 34.75 (calculated, Burkhard et al. 1985b)
 50.0 (calculated, Mackay et al. 1986)
 34.45 (calculated-P/C, Eisenreich 1987)
 23.0 (20°C, quoted, Murphy et al. 1987 from Burkhard et al. 1985b)
 28.31 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
 28.27 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 12.869 - 4339/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.11 (Callahan et al. 1979; Mabey et al. 1982; quoted, Ryan et al. 1988)
 5.58 (HPLC-RT correlation, Veith et al. 1979a; quoted, Kenaga & Goring 1980)
 0.703 (shake flask-GC/ECD, Lee et al. 1979)
 3.54 (Pal et al. 1980; quoted, Sklarew & Girvin 1987)
 4.0–5.6 (quoted, Mills et al. 1982)
 4.50–5.80 (quoted, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
 5.90 (Rapaport & Eisenreich 1984)
 5.74 (literature mean, Di Toro et al. 1985)
 5.29 (quoted, Chou & Griffin 1986)

Bioconcentration Factor, $\log BCF$:

- 3.92, 3.65, 3.46 (bacteria: Doe Run pond, Hickory Hills pond, USDA pond, Paris et al. 1978)
 0.08, –0.22 (adipose tissue of male, female Albino rats, Geyer et al. 1980)
 4.69, 3.81 (fish, flowing water, static water, Kenaga & Goring 1980)
 4.69 (quoted, Bysshe 1982)
 3.36 (microorganism, calculated- K_{OW} , Mabey et al. 1982)
 0.30, 0.13, –0.11, –0.50, –0.27 (rodent, poultry, sheep, small birds, swine, Garten & Trabalka 1983)
 3.20–4.51 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
 4.69, 5.99 (fish 5% lipid in flow-through system: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.13, 5.18, 4.89, 4.70 (bottom sediments of: Oconee River pH 6.5, USDA Pond pH 6.4, Doe Run Pond pH 6.1, Hickory Hill Pond pH 6.3, batch equilibration-GC, Steen et al. 1978)
 3.80 (sediment, calculated- K_{OW} , Mabey et al. 1982)
 4.17 (Lake Michigan sediment, 0.7–3.8% OC, Eadie et al. 1983)
 3.36 (calculated, Sklarew & Girvin 1987)
 4.09 (soil, calculated-S, Chou & Griffin 1986)
 4.30, 4.12, 4.64 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH 2.0 to > 10, average, Delle Site 2001)
 4.82, 4.74 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: $k = 0.23 \mu\text{g m}^{-2} \text{d}^{-1}$ with $t_{1/2} = 17 \text{ d}$ (Baker et al. 1986);
 $k = 0.029 \text{ g m}^{-2} \text{h}^{-1}$ (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, $k \ll 360 \text{ M}^{-1} \text{h}^{-1}$ and $k \ll 1 \text{ M}^{-1} \text{h}^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: 26.3% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972; quoted, Pal et al. 1980);
26% degraded by activated sludge for 48-h exposure (Versar Inc. 1979; quoted, Pal et al. 1980);
degraded by acclimated activated sludge with a first-order rate constant $k = 0.15 \text{ d}^{-1}$ and $t_{1/2} = 4.5 \text{ d}$ (Callahan et al. 1979).

88% loss by degradation with *Nocardia* strain NCIB 10603, 76% loss with NCIB 10643 both within 52 d; 95% loss with NCIB 10603 and 85% loss with NCIB 10643 both within 100 d (Baxter et al. 1975; quoted, Pal et al. 1980).

Biotransformation: estimated $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 12 \text{ h}$ (Paris et al. 1978); volatilization $t_{1/2} \sim 12 \text{ h}$ at 1 m depth in 1 m^3 of water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

Groundwater:

Sediment:

Soil: $t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988).

Biota:

7.1.3.5 Aroclor 1248

Common Name: Aroclor 1248

Synonym:

Chemical Name:

CAS Registry No: 12672-29-6

Molecular Formula:

Average Molecular Weight: 288–299.5

Physical State: mobile oil

Distillation Range (°C):

340–375 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)

Chlorine Content: 48%

Density (g/cm³):

1.44 (20°C, Brinkman & De Kock 1980)

1.40–1.41 (NAS 1979)

1.41 (Callahan et al. 1979)

1.40 (Mackay 1986; Mills et al. 1982; Metcalfe et al. 1988)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

0.10 (20°C, Nisbet & Sarofim 1972)

0.10 (Monsanto Co. 1972; selected, Hutzinger et al. 1974; Sawhney 1987)

0.043 (26°C, Hutzinger et al. 1974)

0.054 (Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983, 1986)

0.054 (NAS 1979; Callahan et al. 1979; Pal et al. 1980; Mabey et al. 1982; Mills et al. 1982; Chou & Griffin 1986)

0.060 (shake flask-nephelometry, Hollifield 1979)

0.052 (quoted, Brinkman & De Kock 1980; Erickson 1986)

0.32 (selected, Mackay 1986; Metcalfe et al. 1988)

0.056 (selected, Eisenreich 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.004 (20°C, Nisbet & Sarofim 1972)

0.066 (selected, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; quoted, Mills et al. 1982)

0.11 (20°C, extrapolated, Monsanto 1972; quoted, NAS 1979)

$\log(P_L/\text{mmHg}) = 8.40 - 3400/(T/K)$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)

0.017 (Branson 1977; Kenaga & Goring 1980)

0.066 (Callahan et al. 1979; Mabey et al. 1982; Mackay et al. 1983)

0.025, 0.024 (GC-RT correlation, Foreman & Bidleman 1985)

0.0085 (selected, Eisenreich 1987)

0.023 (selected, Mackay 1986; Metcalfe et al. 1988)

Henry's Law Constant (Pa m³/mol):

355.7 (calculated, Mackay & Leinonen 1975)

372 (Slinn et al. 1978)

364 (calculated-P/C, Mabey et al. 1982)

86.0 (calculated-P/C, Mackay et al. 1983)

44.58 (calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)

50.0 (calculated-P/C, Mackay et al. 1986)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

5.75 (Callahan et al. 1979; Kenaga & Goring 1980; Mabey et al. 1982; Chou & Griffin 1986)

- 6.11 (shake flask-GC, Chiou et al. 1977; quoted, Callahan et al. 1979)
- 6.11 (HPLC-RT correlation, Veith et al. 1979a,b; quoted, Mackay 1982; Garten & Trabalka 1983)
- 6.0 (quoted, Mills et al. 1982)
- 5.8–6.3 (quoted, Mackay et al. 1983, 1986; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
- 5.60 (quoted, Ryan et al. 1988)
- 6.10 (selected, Thomann 1989)

Bioconcentration Factor, log BCF:

- 4.42 (bluegill sunfish, Stalling & Meyer 1972)
- 4.75–4.79 (channel catfish, Mayer et al. 1977; quoted, Waid 1986)
- 5.08 (fathead minnow, DeFoe et al. 1978; quoted, Waid 1986)
- 4.85 (fathead minnow, 32-d exposure, Veith et al. 1979b)
- 4.86, 4.07 (fish, flowing water, static water, Kenaga & Goring 1980)
- 4.86 (quoted, Bysshe 1982)
- 3.86–4.42, 4.19 (mussel, range, average, Geyer et al. 1982)
- 4.86 (microorganism, calculated- K_{OW} , Mabey et al. 1982)
- 4.85, 4.79 (fish: quoted, calculated- K_{OW} , Mackay 1982)
- 4.85, 0.82, 0.72 (fish, poultry, rodents, Garten & Trabalka 1983)
- 4.5–5.0 (fish, selected, Mackay 1986; Metcalfe et al. 1988)
- 4.80, 6.08 (fathead minnow, male: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 5.08, 6.08 (fathead minnow, female: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} :

- 5.44 (sediment, calculated- K_{OW} , Mabey et al. 1982)
- 4.74 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization/Evaporation: $k = 8.3 \times 10^{-3} \text{ g m}^{-2} \cdot \text{h}^{-1}$ (Mackay 1986; Metcalfe et al. 1988).
- Photolysis: TiO_2 catalyzed photolytic process destroyed 80% of total PCBs in an aqueous solution and clay suspension after 4 h of radiation, and 50% destroyed in sediment suspension within 6 h (Zhang et al. 1993).
- Hydrolysis: not environmentally significant (Mabey et al. 1982).
- Oxidation: calculated rate constant for singlet oxygen, $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ and $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).
- Biodegradation: aerobic biodegradation $t_{1/2} = 77.6 \text{ d}$ without the addition of polymer chitin, $t_{1/2} = 38.6 \text{ d}$ with chitin and $t_{1/2} = 31.9 \text{ d}$ with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials collected from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).
- Biotransformation: estimated $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1}$ for bacteria transformation in water (Mabey et al. 1982).
- Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
 $\log k_2 = -1.92 \text{ d}^{-1}$ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air:

- Surface water: volatilization $t_{1/2} \sim 10 \text{ h}$ at 1 m depth in 1 m^3 water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982);
 TiO_2 catalyzed photolytic process destroyed 80% of total PCBs in an aqueous solution and clay suspension after 4 h of radiation, and 50% destroyed in sediment suspension within 6 h (Zhang et al. 1993).

Groundwater:

Sediment:

- Soil: $t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988).

Biota:

7.1.3.6 Aroclor 1254

Common Name: Aroclor 1254

Synonym:

Chemical Name:

CAS Registry No: 11097-69-1

Molecular Formula:

Average Molecular Weight: 327–328.4

Physical State: viscous liquid

Distillation Range (°C):

365–390 (NAS 1979; Brinkman & De Kock 1980; Mackay et al. 1986)

Chlorine Content: 54%

Density (g/cm³):

1.505 (Monsanto 1972)

1.49–1.50 (65°C, NAS 1979)

1.54 (20°C Brinkman & De Kock 1980)

1.50 (Mills et al. 1982; Mackay 1986; Metcalfe et al. 1988)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.30 (Zitko 1971)

0.043 (26°C, Nelson et al. 1972)

0.050 (20°C, Nisbet & Sarofim 1972)

0.040 (Monsanto 1972; selected, Hutzinger et al. 1974; Sawhney 1987)

0.012–0.07 (Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Geyer et al. 1980; Mackay et al. 1983, 1986)

0.056 (shake flask-GC, Haque et al. 1974; quoted, Haque et al. 1980)

0.0001 (20°C, shake flask-GC/ECD, Schoor 1975)

0.045 (shake flask-GC, Lawrence & Tosine 1976)

0.070 (23°C, shake flask-GC/ECD, Griffin et al. 1978)

0.0242 (11.5°C, shake flask-GC/ECD, Dexter & Pavlou 1978)

0.012 (Brinkman & De Kock 1980; Giam et al. 1980; Pal et al. 1980; Erickson 1986)

0.010 (Kenaga & Goring 1980)

0.031 (Callahan et al. 1979; Mabey et al. 1982)

0.070 (shake flask-GC/ECD, Lee et al. 1979)

0.057 (shake flask-nephelometry, Hollifield 1979)

0.070 (23°C, Griffin & Chian 1980; quoted, Sklarew & Girvin 1987)

0.0115 (quoted, Eisenreich et al. 1981)

0.045–0.07 (quoted literature range, Westcott et al. 1981)

0.010–0.06 (quoted literature range, Mills et al. 1982)

0.042 (quoted, Chou & Griffin 1986)

0.035 (quoted, Eisenreich 1987)

0.14 (selected, Mackay 1986; Metcalfe et al. 1988)

0.043 (20°C, calculated-mole fraction, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.00107 (ebulliometry, Burrows 1946)

0.00048 (20°C, Nisbet & Sarofim 1972)

0.0103 (Monsanto 1972; quoted, Callahan et al. 1979; Mabey et al. 1982; Mills et al. 1982)

$\log (P_{\text{L}}/\text{mmHg}) = 8.80 - 3700/(T/\text{K})$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)

0.0103 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Bidleman & Christensen 1979; Giam et al. 1980; Westcott et al. 1980)

0.024	(20°C, extrapolated, Monsanto 1974; quoted, NAS 1979)
0.0101	(quoted, Eisenreich et al. 1981)
0.004	(38°C, Average, Wingender & Williams 1984)
0.00435, 0.00424	(GC-RT correlation, Foreman & Bidleman 1985)
0.043	(selected, Mackay et al. 1986)
0.00263	(quoted, Eisenreich 1987)
6.7×10^{-3}	(selected, Mackay 1986; Metcalfe et al. 1988)
0.00294	(20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

279.7	(calculated, Mackay & Leinonen 1975)
0.0993	(Murphy & Rzeszutko 1977; quoted, Eisenreich et al. 1983)
273	(Slinn et al. 1978)
274	(calculated-P/C, Eisenreich et al. 1981)
0.007	(Eisenreich et al. 1981a)
0.0142	(Doskey & Andren 1981; quoted, Eisenreich et al. 1983)
47.57–74.08	(calculated-P/C, Westcott et al. 1981)
16.60	(radiotracer-equilibration, Atlas et al. 1982; Atlas & Giam 1986)
21.0	(direct concn. ratio-GC/ECD, Murphy et al. 1983)
28.67	(calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)
50.0	(calculated, Mackay et al. 1986)
18.24	(20°C, selected, Murphy et al. 1987 from Burkhard et al. 1985b)
19.25	(20°C, equilibrium concn. ratio, Murphy et al. 1987)
19.25	(20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
$\log K_{AW} = 11.880 - 4099/(T/K)$, (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)	

Octanol/Water Partition Coefficient, $\log K_{ow}$:—See discussion by Linkov et al. 2005.

6.03	(Hansch et al. 1973; Callahan et al. 1979; Mabey et al. 1982)
6.47	(GC-RT correlation, Veith et al. 1979b; Veith & Kosian 1983; quoted, Mackay 1982; Garten & Trabalka 1983; Zaroogian et al. 1985; Södergren 1987; Travis & Arms 1988)
6.72	(HPLC-RT correlation, Veith et al. 1979a)
4.08	(Pal et al. 1980; quoted, Sklarew & Girvin 1987)
6.0	(quoted, Mills et al. 1982)
6.79	(literature mean, Di Toro et al. 1985)
6.1–6.8	(selected, Mackay et al. 1983, 1986; Metcalfe et al. 1988)
7.17	(Rapaport & Eisenreich 1984)
6.11	(quoted, Chou & Griffin 1986)
6.50	(quoted, Thomann 1989)

Bioconcentration Factor, $\log BCF$:

4.57	(spot fish, Hansen et al. 1971; quoted, Waid 1986)
4.85	(bluegill sunfish, Stalling & Mayer 1972)
4.75–4.79	(channel catfish, Mayer et al. 1977; quoted, Waid 1986)
5.08, 5.57, 6.08	(Mysis, sculpins, pelagic fish, Veith et al. 1977)
5.00	(fathead minnow, 32-d exposure, Veith et al. 1979b; Veith & Kosian 1983)
5.0–5.22; 4.41; 4.57	(oyster; shrimp, estuarine fish, Hansen et al. 1976; NAS 1979)
0.79, 0.78	(adipose tissue of male, female Albino rats, Geyer et al. 1980)
4.66, 4.08	(fish, flowing water, static water, Kenaga & Goring 1980)
4.66	(quoted, Bysshe 1982)
5.12	(microorganism, calculated- K_{ow} , Mabey et al. 1982)
5.00, 5.15	(fish: quoted, calculated- K_{ow} , Mackay 1982)
4.57	(fish, estuarine, Hansen et al. 1976; NAS 1979)
0.53, 4.70, 0.77, 0.79, 0.18, 0.98, 0.03	(cow, fish, poultry, rodents, sheep, small birds, swine, Garten & Trabalka 1983)

- 5.69, 5.63; 6.11, 5.76 (live bacteria, dead bacteria; live algae, dead algae, Weber, Jr. et al. 1983)
 5.0 (fathead minnow, quoted, Zaroogian et al. 1985)
 4.80, 4.68 (oyster, quoted, Zaroogian et al. 1985)
 4.8–5.51 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
 5.52 (oyster, Södergren 1987)
 –1.28; –1.95; –1.77 (beef; milk; vegetable, reported as biotransfer factor $\log B_b$, $\log B_m$, $\log B_v$, Travis & Arms 1988)
 4.95, 6.65 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
 > 5.0, > 5.98 (fathead minnow, 32-d uptake: wet wt basis, lipid wt basis, Geyer et al. 2000)

Bioaccumulation Factor, $\log BAF$:

- 7.21 (field data, lake trout-L/kg(Ip), Thomann 1989)
 6.9, 6.51, 6.67, 6.8 (field data, large-mouth bass, L/kg(Ip), Thomann 1989)

Partition Coefficient, $\log K_p$ or $\log K_d$

- 3.21, 3.22, 4.42, 3.56 (clay: Montmorillonite, Kaolinite, natural Blue clay, stripped Blue clay, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
 4.38, 3.06, 4.73, 5.18, 4.55, 5.01, 4.50, 4.89, 4.05 (sediments: Saginaw River 1. natural, Saginaw River 1. stripped, Saginaw R. 2. natural, Saginaw River 2. NaOH ext., Saginaw River 2. benzene/MeOH ext., Saginaw River 2. stripped, Saginaw River 2. 12°C, Saginaw River 2. < 75 -m, Saignaw Bay, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
 5.06, 4.95, 5.07 (suspended solids: Huron River, Saginaw River1, Saginaw River 2, Weber, Jr. et al. 1983)

Sorption Partition Coefficient, $\log K_{oc}$:

- 6.0 (sediment/pore water 2.0% OC of pond, Halter & Johnson 1977; selected, Di Toro et al. 1985)
 5.72 (sediment, calculated- K_{ow} , Mabey et al. 1982)
 5.44 (sediment/pore water 0.7–3.8% OC-Lake Michigan, Eadie et al. 1983; selected, Di Toro et al. 1985)
 6.17, 6.16, 5.89 (clay: Montmorillonite 0.11% OC, natural Blue clay 1.82% OC, stripped Blue clay 0.47% OC, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
 5.84, 5.04, 6.31, 6.68, 6.29, 6.19, 6.34, 7.20 (sediments: Saginaw River 1. natural 3.45% OC, Saginaw River 1. stripped 1.05% OC, Saginaw R. 2. natural 2.61% OC, Saginaw River 2. NaOH ext. 1.98% OC, Saginaw River 2. benzene/MeOH ext. 1.84% OC, Saginaw River 2. stripped 0.67% OC, Saginaw River 2. < 75 μ m 3.51% OC, Saignaw Bay 0.07% OC, batch equilibrium-sorption isotherm, Weber, Jr. et al. 1983)
 6.10, 5.97, 6.15 (suspended solids: Huron River 9.25% OC, Saginaw River 1. 9.48% OC, Saginaw River 2. 8.30% OC, batch equilibrium, Weber, Jr. et al. 1983)
 6.65 (suspended solids/subsurface water, 56% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
 5.88 (sediment/pore water, 0.7% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
 5.61 (sediment/pore water, 1.7% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
 4.82 (sediment/pore water, 3.8% OC-Lake Michigan, sorption isotherm, Voice & Weber 1985)
 6.62 (calculated, Sklarew & Girvin 1987)
 4.81 (soil, calculated-S, Chou & Griffin 1986)
 6.02 (sediment: organic carbon OC \geq 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

- Volatilization/Evaporation: volatilization rate $k \sim 2 \times 10^{-6} \text{ g cm}^{-2} \text{ d}^{-1}$ at 26°C and $k = 8.6 \times 10^{-5} \text{ g cm}^{-2} \text{ d}^{-1}$ at 60°C (Haque et al. 1974);
 $k = 0.10 \text{ } \mu\text{g m}^{-2} \text{ d}^{-1}$ with $t_{1/2} = 28 \text{ d}$ (Baker et al. 1985);
 $k = 2.7 \times 10^{-3} \text{ g m}^{-2} \text{ h}^{-1}$ (Mackay 1986; Metcalfe et al. 1988).
 Photolysis:
 Hydrolysis: not environmentally significant.

Oxidation: calculated rate constant for singlet oxygen, $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ and, $k \ll 1 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 (peroxy radical) (Mabey et al. 1982).

Biodegradation: no reduction of concentration in the spilled transformer fluid contaminant of Aroclor was detected over a two-year period (Moein et al. 1976; quoted, Pal et al. 1980).

15.2% degraded by activated sludge in 47-h cycle (Monsanto Co. 1972);

19% degraded by activated sludge for 48-h exposure (Callahan et al. 1979);

biodegradation with a first-order $k = 0.1 \text{ d}^{-1}$ by acclimated activated sludge and $t_{1/2} = 7.0 \text{ d}$ (Callahan et al. 1979);

aerobic biodegradation $t_{1/2} = 81.9 \text{ d}$ without the addition of polymer chitin, $t_{1/2} = 36.4 \text{ d}$ with chitin and $t_{1/2} = 35.5 \text{ d}$ with chitin plus adapted microbes in flow microcosm systems with water and sedimentary materials from the field (Portier & Fujisaki 1988; quoted, Abramowicz 1990).

Biotransformation: estimated $k \sim 3 \times 10^{-9}$ to $3 \times 10^{-12} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1}$ for bacteria transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.023 \text{ d}^{-1}$ (0 to 1 d), $k_2 = 0.086 \text{ d}^{-1}$ (1 to 2 d), and $k_2 = 0.0899 \text{ d}^{-1}$ (2 to 6 d) with a biological $t_{1/2} = 5.5 \text{ d}$ (mosquito larvae, Gooch & Hamdy 1982; selected, Waid 1986)

$k_2 = 0.131 \text{ d}^{-1}$, 0.137 d^{-1} with biological $t_{1/2} = 4.7 \text{ d}$ (guppies, Gooch & Hamdy 1982; quoted, Waid 1986)

$k_2 = 0.102 \text{ d}^{-1}$ (first day), $k_2 = 0.057 \text{ d}^{-1}$ (thereafter) with a biological $t_{1/2} = 6.1 \text{ d}$ (cichlids, Gooch & Hamdy 1982; quoted, Waid 1986)

Half-Lives in the Environment:

Air:

Surface water: volatilization $t_{1/2} \sim 10 \text{ h}$ from 1 meter depth in 1 m^3 water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

Groundwater:

Sediment:

Soil: volatilization $t_{1/2} \sim 15 \text{ d}$ from an Ottawa sand (Haque et al. 1974; quoted, Pal et al. 1980);

$t_{1/2} > 50 \text{ d}$ in soil (Ryan et al. 1988).

Biota: $t_{1/2} < 12 \text{ d}$ in plant surface (Pal et al. 1980);

$t_{1/2} = 3.3 \text{ d}$ in guppies, and $t_{1/2} = 5.1 \text{ d}$ cichlids (Gooch & Hamdy 1982; quoted, Waid 1986).

7.1.3.7 Aroclor 1260

Common Name: Aroclor 1260

Synonym:

Chemical Name:

CAS Registry No: 11096-82-5

Molecular Formula:

Average Molecular Weight: 372–375.7

Physical State: sticky resin

Distillation Range (°C):

385–420 (NAS 1979; Brinkman & De Kock 1980)

Chlorine Content: 60%

Density (g/cm³):

1.62 (20°C, Brinkman & De Kock 1980)

1.55–1.56 (90°C, NAS 1979)

1.58 (Callahan et al. 1979; Mills et al. 1982)

1.60 (Mackay 1986; Metcalfe et al. 1988)

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

0.025 (Monsanto 1972)

0.025 (20°C, Nisbet & Sarofim 1972)

0.0027 (Mackay & Wolkoff 1973; quoted, Callahan et al. 1979; Geyer et al. 1980; Pal et al. 1980; Mabey et al. 1982; Mills et al. 1982; Richardson et al. 1983; Chou & Griffin 1986)

0.080 (shake flask-nephelometry, Hollifield 1979)

0.003 (quoted, Brinkman & De Kock 1980; Mackay et al. 1983; Eisenreich 1987)

0.0144 (20°C, calculated-mole fraction, Murphy et al. 1987)

Vapor Pressure (Pa at 25°C or indicated and reported temperature dependence equations):

2.67×10^{-5} (38°C, Nisbet & Sarofim 1972)

0.0054 (quoted, Mackay & Wolkoff 1973; Mackay & Leinonen 1975; Mackay et al. 1983)

0.012 (20°C, extrapolated, Monsanto 1972; NAS 1979)

$\log(P_L/\text{mmHg}) = 8.50 - 3700/(T/K)$ (temp range 150–300°C, from Monsanto 1972, NAS 1979)

0.0054 (Callahan et al. 1979; Mabey et al. 1982; Richardson et al. 1983)

0.0053 (Pal et al. 1980; Mills et al. 1982)

0.0004 (38°C, average, Wingender & Williams 1984)

0.00183, 0.00162 (GC-RT, Foreman & Bidleman 1985)

0.003 (quoted, Erickson 1986)

0.00064 (Mackay 1986; Metcalfe et al. 1988)

0.000284 (quoted, Eisenreich 1987)

0.000841 (20°C, calculated-mole fraction, Murphy et al. 1987)

Henry's Law Constant (Pa m³/mol):

722.4 (calculated, Mackay & Leinonen 1975)

718 (Slinn et al. 1978)

719 (quoted, Mills et al. 1982)

88.0 (suggested, Mackay et al. 1983)

72.24 (16°C, calculated-P/C, Richardson et al. 1983)

34.04 (calculated, Burkhard et al. 1985b; quoted, Eisenreich 1987)

21.27 (20°C, quoted, Murphy et al. 1987 from Burkhard et al. 1985b)

- 17.23 (20°C, equilibrium concn. ratio, Murphy et al. 1987)
 17.23 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 11.848 - 4104/(T/K)$ (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.14 (Chiou et al. 1977)
 6.11 (Chiou et al. 1977; Callahan et al. 1979; quoted, Ryan et al. 1988)
 7.15 (Callahan et al. 1979; Mabey et al. 1982)
 6.91 (GC-RT correlation, Veith et al. 1979a; Veith & Kosian 1983; quoted, Mackay 1982; Geyer et al. 1987)
 4.34 (Pal et al. 1980)
 > 6.0 (quoted, Mills et al. 1982)
 6.30–7.50 (quoted, Mackay et al. 1983; Mackay 1986; Metcalfe et al. 1988; Eisenreich 1987)
 6.61 (calculated-S, Chou & Griffin 1986)
 6.90 (quoted, Thomann 1989)

Bioconcentration Factor, $\log BCF$:

- 5.43 (fathead minnows, DeFoe et al. 1978; quoted, Waid 1986)
 5.29 (fathead minnow, 32-d exposure, Veith et al. 1979a; Veith & Kosian 1983)
 0.672 (adipose tissue of male albino rats, Geyer et al. 1980)
 5.29, 5.59 (fish: quoted, calculated- K_{OW} , Mackay 1982)
 6.11 (microorganism, calculated- K_{OW} , Mabey et al. 1982)
 5.0–6.20 (fish, quoted, Mackay 1986; Metcalfe et al. 1988)
 2.28–2.50 (human fat of lipid basis, calculated- K_{OW} , Geyer et al. 1987)
 2.11–2.36 (human fat of wet wt. basis, calculated- K_{OW} , Geyer et al. 1987)
 4.38 (*Rhabdosargus holubi*, De Kock & Lord 1988)
 4.80, 6.72 (oyster: wet wt basis, lipid wt basis, Geyer et al. 2000)
 5.22, 6.50 (fathead minnow, male, 250-d uptake: wet wt basis, lipid wt basis, Geyer et al. 2000)
 5.43, 6.53 (fathead minnow, female, 250-d uptake, wet wt basis, lipid wt basis, Geyer et al. 2000)
 2.24, 2.40 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.83 (sediment, calculated- K_{OW} , Mabey et al. 1982)
 5.54 (soil, calculated-S, Chou & Griffin 1986)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization/Evaporation: estimated evaporation rate from liquid surfaces at 100°C to be 0.009 mg/cm²·h (Hutzinger et al. 1974);
 $t_{1/2} \sim 7.53$ h of evaporation from water depth of 1 m (Mackay & Leinonen 1975)
 rate of evaporation $k = 2.9 \times 10^{-4}$ g m⁻²·h⁻¹ (Mackay 1986; Metcalfe et al. 1988).

Photolysis:

Hydrolysis: not environmentally significant (Mabey et al. 1982).

Oxidation: calculated rate constant for singlet oxygen, $k \ll 360$ M⁻¹·h⁻¹ and $k \ll 1$ M⁻¹·h⁻¹ for RO₂ (peroxy radical) (Mabey et al. 1982).

Biodegradation: no degradation over a 12-week period in natural water samples (Oloffs et al. 1972; quoted, Pal et al. 1980).

Biotransformation: $k \sim 3 \times 10^{-9}$ to 3×10^{-12} mL·cell⁻¹·h⁻¹, transformation for bacteria in water (Mabey et al. 1982)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 332$ d⁻¹; $k_2 = 0.014$ d⁻¹ (*Rhabdosargus holubi*, De Kock & Lord 1988)

$\log k_2 = -2.40$ d⁻¹ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air:

Surface water: volatilization $t_{1/2} \sim 10$ h at 1 m depth of 1 m³ of water (Mackay & Leinonen 1975; quoted, Pal et al. 1980; Mills et al. 1982).

River water: volatilization $t_{1/2} \sim 52$ d (Oloffs et al. 1972; selected, Pal et al. 1980).

Sediment:

Soil:

Biota: $t_{1/2} = 50$ d in *Rhabdosargus holubi* (De Kock & Lord 1988).

7.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 7.2.1

Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V _M (cm ³ /mol)
0	Biphenyl	92-52-4	154.207	68.93	256.1	0.371	184.6
1	2-	2051-60-7	188.652	34	274	0.816	205.5
2	3-	2051-61-8	188.652	16	284.5	1	205.5
3	4-	2051-62-9	188.652	78.8	292.9	0.297	205.5
4	2,2'-	13029-08-8	223.098	60.5		0.448	226.4
5	2,3-	16605-91-7	223.098	28		0.934	226.4
6	2,3'	25569-80-6	223.098				226.4
7	2,4-	33284-50-3	223.098	24.4		1	226.4
8	2,4'-	34883-43-7	223.098	43		0.666	226.4
9	2,5-	34883-39-1	223.098	22-23		1	226.4
10	2,6-	33146-45-1	223.098	35.5		0.789	226.4
11	3,3'-	2050-67-1	223.098	29	320	0.914	226.4
12	3,4-	2974-92-7	223.098	49	195-200	0.581	226.4
13	3,4'-	2974-90-5	223.098				226.4
14	3,5-	34883-41-5	223.098	31		0.873	226.4
15	4,4'-	2050-68-2	223.098	149.3	317	0.0603	226.4
16	2,2',3-	38444-78-9	257.543	28		0.934	247.3
17	2,2',4-	37680-66-3	257.543				247.3
18	2,2',5-	37680-65-2	257.543	44		0.651	247.3
19	2,2',6-	38444-73-4	257.543				247.3
20	2,3,3'-	38444-84-7	257.543				247.3
21	2,3,4-	55702-46-0	257.543	102		0.176	247.3
22	2,3,4'-	38444-85-8	257.543	73		0.338	247.3
23	2,3,5-	55720-44-0	257.543	41		0.697	247.3
24	2,3,6-	55702-45-9	257.543	49		0.581	247.3
25	2,3',4-	55712-37-3	257.543				247.3
26	2,3',5-	38444-81-4	257.543	40.5		0.705	247.3
27	2,3',6-	38444-76-7	257.543				247.3
28	2,4,4'-	7012-37-5	257.543	57		0.485	247.3
29	2,4,5-	15862-07-4	257.543	78.5		0.299	247.3

(Continued)

TABLE 7.2.1 (Continued)
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V _M (cm ³ /mol)
30	2,4,6-	35693-92-6	257.543	62.5		0.429	247.3
31	2,4',5-	16606-02-3	257.543	67		0.387	247.3
32	2,4',6-	38444-77-8	257.543				247.3
33	2,3',4'-	38444-86-9	257.543	60		0.454	247.3
34	2,3',5'-	37680-68-5	257.543	58		0.474	247.3
35	3,3',4-	37680-69-6	257.543	87		0.246	247.3
36	3,3',5-	38444-87-0	257.543				247.3
37	3,4,4'-	38444-90-5	257.543	87		0.246	247.3
38	3,4,5-	53555-66-1	257.543				247.3
39	3,4',5-	38444-88-1	257.543	88		0.241	247.3
40	2,2',3,3'-	38444-93-8	291.988	121		0.114	268.2
41	2,2',3,4-	52663-59-9	291.988				268.2
42	2,2',3,4'-	36559-22-5	291.988	69		0.370	268.2
43	2,2',3,5-	70362-46-8	291.988				268.2
44	2,2',3,5'-	41464-39-5	291.988	47		0.608	268.2
45	2,2',3,6-	70362-45-7	291.988				268.2
46	2,2',3,6'-	41464-47-5	291.988				268.2
47	2,2',4,4'-	2437-79-8	291.988	83		0.270	268.2
48	2,2',4,5-	70362-47-9	291.988	65.9		0.397	268.2
49	2,2',4, 5'-	41464-40-8	291.988	66.5		0.392	268.2
50	2,2',4,6-	62796-65-8	291.988				268.2
51	2,2',4,6'-	68194-04-7	291.988	66		0.396	268.2
52	2,2',5,5'-	35693-99-3	291.988	87		0.246	268.2
53	2,2',5,6'-	41464-41-9	291.988	104		0.168	268.2
54	2,2',6,6'-	15968-05-5	291.988	198		0.0201	268.2
55	2,3,3',4-	74338-24-2	291.988				268.2
56	2,3,3',4'-	41464-43-1	291.988				268.2
57	2,3,3',5-	70424-67-8	291.988				268.2
58	2,3,3',5'-	41464-49-7	291.988				268.2
59	2,3,3',6-	74472-33-6	291.988				268.2
60	2,3,4,4'-	33025-41-1	291.988	142		0.0711	268.2
61	2,3,4,5-	33284-53-6	291.988	92.2		0.219	268.2
62	2,3,4,6-	54230-23-7	291.988				268.2

63	2,3,4',5-	74472-34-7	291.988			268.2
64	2,3,4',6-	52663-58-8	291.988			268.2
65	2,3,5,6-	33284-54-7	291.988	79	0.295	268.2
66	2,3',4,4'-	32598-10-0	291.988	124	0.107	268.2
67	2,3',4,5-	73575-53-8	291.988			268.2
68	2,3',4,5'-	73575-52-7	291.988			268.2
69	2,3',4,6-	60233-24-1	291.988			268.2
70	2,3',4',5-	32598-11-1	291.988	104	0.168	268.2
71	2,3',4',6-	41464-46-4	291.988			268.2
72	2,4',5,5'-	41464-42-0	291.988			268.2
73	2,3',5',6-	74338-23-1	291.988			268.2
74	2,4,4',5-	32690-93-0	291.988	125	0.104	268.2
75	2,4,4',6-	32598-12-2	291.988			268.2
76	2,3',4',5'-	70362-48-0	291.988			268.2
77	3,3',4,4'-	32598-13-3	291.988	180	0.0301	268.2
78	3,3',4,5-	70362-49-1	291.988			268.2
79	3,3',4,5'-	41464-48-6	291.988			268.2
80	3,3',5,5'-	33284-52-5	291.988	164	0.0433	268.2
81	3,4,4',5-	70362-50-4	291.988			268.2
82	2,2',3,3',4-	52663-62-4	326.433			289.1
83	2,2',3,3',5-	60145-20-2	326.433	65	0.405	289.1
84	2,2',3,3',6-	52663-60-2	326.433			289.1
85	2,2',3,4,4'-	65510-45-4	326.433			289.1
86	2,2',3,4,5-	55312-69-1	326.433	100	0.184	289.1
87	2,2',3,4,5'-	38380-02-8	326.433	114	0.134	289.1
88	2,2',3,4,6-	55215-17-3	326.433	100	0.184	289.1
89	2,2',3,4,6'-	73575-57-2	326.433			289.1
90	2,2',3,4',5-	68194-07-0	326.433			289.1
91	2,2',3,4',6-	58194-05-8	326.433			289.1
92	2,2',3,5,5'-	52663-61-3	326.433			289.1
93	2,2',3,5,6-	73575-56-1	326.433			289.1
94	2,2',3,5,6'-	73575-55-0	326.433			289.1
95	2,2'3,5,6-	38379-99-6	326.433	100	0.184	289.1
96	2,2',3,6,6'-	73575-54-9	326.433			289.1
97	2,2',3,4',5'-	41464-51-1	326.433	82	0.276	289.1
98	2,2',3,4',6'-	60233-25-2	326.433			289.1
99	2,2',4,4',5-	38380-01-7	326.433			289.1

(Continued)

TABLE 7.2.1 (Continued)
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V _M (cm ³ /mol)
100	2,2',4,4',6-	39485-83-1	326.433				289.1
101	2,2',4,5,5'-	37680-73-2	326.433	78.5		0.299	289.1
102	2,2',4,5,6'-	68194-06-9	326.433				289.1
103	2,2',4,5',6-	60145-21-3	326.433				289.1
104	2,2',4,6,6'-	56558-16-8	326.433	85		0.258	289.1
105	2,3,3',4,4'-	32598-14-4	326.433	105		0.164	289.1
106	2,3,3',4,5-	70424-69-0	326.433				289.1
107	2,3,3',4',5-	70424-68-9	326.433				289.1
108	2,3,3',4,5'-	70362-41-3	326.433				289.1
109	2,3,3',4,6-	74472-35-8	326.433				289.1
110	2,3,3',4',6-	38380-03-9	326.433				289.1
111	2,3,3',5,5'-	39635-32-0	326.433				289.1
112	2,3,3',5,6-	74472-36-9	326.433				289.1
113	2,3,3',5',6-	68194-10-5	326.433				289.1
114	2,3,4,4',5-	74472-37-0	326.433	99		0.188	289.1
115	2,3,4,4',6-	74472-38-1	326.433				289.1
116	2,3,4,5,6-	18259-05-7	326.433	123.5		0.108	289.1
117	2,3,4',5,6-	68194-11-6	326.433				289.1
118	2,3',4,4',5-	31508-00-6	326.433	107		0.157	289.1
119	2,3',4,4',6-	56558-17-9	326.433				289.1
120	2,3',4,5,5'-	68194-12-7	326.433	77		0.309	289.1
121	2,3',4,5',6-	56558-18-0	326.433				289.1
122	2,3,3',4',5'-	76842-07-4	326.433				289.1
123	2,3',4,4',5'-	65510-44-3	326.433				289.1
124	2,3',4',5,5'-	70424-70-3	326.433				289.1
125	2,3',4',5',6-	74472-39-2	326.433				289.1
126	3,3',4,4',5-	57465-28-8	326.433	106		0.160	289.1
127	3,3',4,5,5'-	39635-33-1	326.433				289.1
128	2,2',3,3',4,4'-	38380-07-3	360.878	151		0.058	310.0
129	2,2',3,3',4,5-	55215-18-4	360.878	85		0.258	310.0
130	2,2',3,3',4,5'-	52663-66-8	360.878				310.0
131	2,2',3,3',4,6-	61798-70-7	360.878				310.0
132	2,2',3,3',4,6'-	38380-05-1	360.878				310.0

133	2,2',3,3',5,5'-	35694-04-3	360.878	129	0.0954	310.0
134	2,2',3,3',5,6-	52704-70-8	360.878	100	0.184	310.0
135	2,2',3,3',5,6'-	52744-13-5	360.878			310.0
136	2,2',3,3',6,6'-	38411-22-2	360.878	114.2	0.133	310.0
137	2,2',3,4,4',5-	35694-06-5	360.878	78	0.302	310.0
138	2,2',3,4,4',5'-	35065-28-2	360.878	80	0.289	310.0
139	2,2',3,4,4',6-	56030-56-9	360.878			310.0
140	2,2',3,4,4',6'-	59291-64-4	360.878			310.0
141	2,2,3,4,5,5'-	52712-04-6	360.878	85	0.258	310.0
142	2,2',3,4,5,6-	41411-61-4	360.878	136	0.0815	310.0
143	2,2',3,4,5,6'-	68194-15-0	360.878			310.0
144	2,2',3,4,5',6-	68194-14-9	360.878			310.0
145	2,2',3,4,6,6'-	74472-40-5	360.878			310.0
146	2,2',3,4',5,5'-	51908-16-8	360.878			310.0
147	2,2',3,4',5,6-	68194-13-8	360.878			310.0
148	2,2',3,4',5,6'-	74472-42-7	360.878			310.0
149	2,2',3,4',5',6-	38380-04-0	360.878	oil	1	310.0
150	2,2',3,4',6,6'-	68194-08-1	360.878			310.0
151	2,2',3,5,5',6-	52663-63-5	360.878	101	0.180	310.0
152	2,2',3,5,6,6'-	68194-09-2	360.878			310.0
153	2,2',4,4',5,5'-	35065-27-1	360.878	103.5	0.170	310.0
154	2,2',4,4',5,6'-	60145-22-4	360.878	oil	1	310.0
155	2,2',4,4',6,6'-	33979-03-2	360.878	112.5	0.139	310.0
156	2,3,3',4,4',5-	38380-08-4	360.878	127	0.100	310.0
157	2,3,3',4,4',5'-	69782-90-7	360.878			310.0
158	2,3,3',4,4',6	74472-42-7	360.878	107	0.157	310.0
159	2,3,3',4,5,5'-	39635-35-3	360.878			310.0
160	2,3,3',4,5,6-	41411-62-5	360.878	99	0.188	310.0
161	2,3,3',4,5',6-	74472-43-8	360.878			310.0
162	2,3,3',4',5,5'-	39635-34-2	360.878			310.0
163	2,3,3',4',5,6-	74472-44-9	360.878			310.0
164	2,3,3',4',5',6-	74472-45-0	360.878			310.0
165	2,3,3',5,5',6-	74472-46-1	360.878			310.0
166	2,3,4,4',5,6-	41411-63-6	360.878	163	0.0433	310.0
167	2,3',4,4',5,5'-	52663-72-6	360.878			310.0
168	2,3',4,4',5',6-	59291-65-5	360.878	110-111	0.145	310.0
169	3,3',4,4',5,5'-	32774-16-6	360.878	202	0.0183	310.0
170	2,2',3,3',4,4',5-	35065-30-6	395.323	135	0.0833	330.9

(Continued)

TABLE 7.2.1
Summary of physical-chemical properties of some PCB congeners

IUPAC no.	Congener	CAS no.	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume, V _M (cm ³ /mol)
171	2,2',3,3',4,4',6-	52663-71-5	395.323	117.5		0.124	330.9
172	2,2',3,3',4,5,5'-	52663-74-8	395.323				330.9
173	2,2',3,3',4,5,6-	68194-16-1	395.323				330.9
174	2,2',3,3',4,5,6'-	38411-25-5	395.323	130.6		0.0920	330.9
175	2,2',3,3',4,5',6-	40186-70-7	395.323				330.9
176	2,2',3,3',4,5,6'-	52663-65-7	395.323				330.9
177	2,2',3,3',4',5,6-	52663-70-4	395.323				330.9
178	2,2',3,3',5,5',6-	52663-67-9	395.323				330.9
179	2,2',3,3',5,6,6'-	52663-64-6	395.323				330.9
180	2,2',3,4,4',5,5'-	35065-29-3	395.323	110		0.147	330.9
181	2,2',3,4,4',5,6-	74472-47-2	395.323				330.9
182	2,2',3,4,4',5,6'-	60145-23-5	395.323	152		0.0567	330.9
183	2,2',3,4,4',5',6-	52663-69-1	395.323	83		0.270	330.9
184	2,2',3,4,4',6,6'-	74472-48-3	395.323				330.9
185	2,2',3,4,5,5',6-	52712-05-7	395.323	149		0.0607	330.9
186	2,2',3,4,5,6,6'-	74472-49-4	395.323				330.9
187	2,2',3,4',5,5',6-	52663-68-0	395.323	149		0.0607	330.9
188	2,2',3,4',5,6,6'-	74487-85-7	395.323				330.9
189	2,3,3',4,4',5,5'-	39635-31-9	395.323	170		0.0378	330.9
190	2,3,3',4,4',5,6-	41411-64-7	395.323	117		0.125	330.9
191	2,3,3',4,4',5',6-	74472-50-7	395.323				330.9
192	2,3,3',4,5,5',6-	74472-51-8	395.323				330.9
193	2,3,3',4',5,5',6-	69782-91-8	395.323				330.9
194	2,2',3,3',4,4',5,5'-	35694-08-7	429.768	159		0.0484	351.8
195	2,2',3,3',4,4',5,6-	52663-78-2	429.768				351.8
196	2,2',3,3',4,4',5,6'-	42740-50-1	429.768				351.8
197	2,2',3,3',4,4',6,6'-	33091-17-7	429.768	132		0.0892	351.8
198	2,2',3,3',4,5,5',6-	68194-17-2	429.768				351.8
199	2,2',3,3',4,5,5',6'-	52663-75-9	429.768				1.759
200	2,2',3,3',4,5,6,6'-	52663-73-7	429.768				351.8
201	2,2',3,3',4,5',6,6'-	40186-71-8	429.768				351.8

202	2,2',3,3',5,5',6,6'-	2136-99-4	429.768	161	0.0463	351.8
203	2,2',3,4,4',5,5',6-	52663-76-0	429.768			351.8
204	2,2',3,4,4',5,6,6'-	74472-52-9	429.768			351.8
205	2,3,3',4,4',5,5',6-	74472-53-0	429.768			351.8
206	2,2',3,3',4,4',5,5',6-	40186-72-9	464.213	206	0.0168	372.7
207	2,2',3,3',4,4',5,6,6'-	52663-79-3	464.213			372.7
208	2,2',3,3',4,5,5',6,6'-	52663-77-1	464.213	180.5	0.0298	372.7
209	2,2',3,3',4,4',5,5',6,6'-	2051-24-3	498.658	309	0.00164	393.6

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

TABLE 7.2.2

Summary of selected physical-chemical properties of some PCB congeners at 25 °C

		Selected properties:						Henry's law const. H/(Pa·m³/mol) calculated P/C
IUPAC no.	Congener	Vapor pressure		Solubility			log K _{OW}	
		P ^s /Pa	P _L /Pa	S/(g/m³)	C ^s /(mmol/m³)	C _L /(mmol/m³)		
0	Biphenyl	1.3	3.50	7	45.39	122.4	3.9	28.64
1	2-	2.04	2.5	5.5	29.15	35.73	4.3	69.97
2	3-	1	1	2.5	13.25	13.24	4.6	75.46
3	4-	0.271	0.91	1.2	6.36	21.42	4.5	42.60
4	2,2'-	0.265	0.59	1	4.482	10.00	4.9	59.12
7	2,4-	0.254	0.254	1.25	5.603	5.603	5.0	45.33
8	2,4'-			1	4.482	6.730	5.1	
9	2,5-	0.18	0.18	2	8.960	8.960	5.1	20.08
10	2,6-			1.4	6.275	7.840	5.0	
11	3,3'-	0.027	0.030	0.354	1.587	1.736	5.3	17.02
12	3,4-			0.008	0.0358	0.0617		
14	3,5-	0.105	0.120					
15	4,4'-	0.0048	0.080	0.06	0.269	4.460	5.3	17.84
18	2,2',5-	0.143	0.220	0.4	1.553	2.386	5.6	92.07
26	2,3',5-			0.251	0.975	1.382		
28	2,4,4'-			0.16	0.621	1.281	5.8	
29	2,4,5-	0.132	0.441	0.14	0.544	1.818	5.6	242.8
30	2,4,6-	0.0384	0.090	0.2	0.777	1.810	5.5	49.45
33	2,3',4'-	0.0136	0.003	0.08	0.311	0.684	5.8	43.78
37	3,4,4'-			0.015	0.0582	0.237	5.9	
40	2,2',3,3v-	0.00225	0.0197	0.03	0.103	0.901	5.6	21.90
44	2,2',3,5'-			0.1	0.342	0.563	6.0	
47	2,2',4,4'-	0.0054	0.02	0.09	0.308	1.142	5.9	17.52
49	2,2',4,5'-			0.016	0.0548	0.149	6.1	
52	2,2',5,5'-	0.0049	0.02	0.03	0.103	0.418	6.1	47.69
53	2,2',5,6'-						5.5	
54	2,2',6,6'-						5.48	
60	2,3,4,4'-						6.31	
61	2,3,4,5-			0.02	0.0685	0.313	5.9	
65	2,3,5,6-						5.94	
66	2,3',4,4'-			0.04	0.137	1.280	5.8	

75	2,4,4',6-			0.091	0.312		6.21	
77	3,3',4,4'-	5.88×10^{-5}	0.002	0.001	0.00342	0.114	6.5	17.16
80	3,3',5,5'-			0.0012	0.0041	0.0949		
86	2,2',3,4,5-	0.00927	0.0504	0.02	0.0613	0.333	6.2	151.3
87	2,2',3,4,5'-	0.000304	0.00227	0.004	0.0123	0.0914	6.5	24.81
88	2,2',3,4,6-			0.012	0.0368	0.200	6.5	
101	2,2',4,5,5'-	0.00109	0.00364	0.01	0.0306	0.102	6.4	35.58
104	2,2',4,6,6'-		0.00434	0.0156	0.0478	0.185		23.43
105	2,3,3',4,4'-						6.0	
110	2,3,3',4',6-			0.004	0.0123		6.3	
116	2,3,4,5,6-			0.008	0.0245	0.227	6.3	
128	2,2',3,3',4,4'-	1.98×10^{-5}	0.00034	0.0006	0.00166	0.0286	7.0	11.91
129	2,2',3,3',4,5-			0.0006	0.00166	0.0064	7.3	
134	2,2',3,3',5,6-			0.0004	0.00111	0.0060	7.3	
136	2,2',3,3',6,6'-			0.0008	0.00222	0.0167	6.7	
153	2,2',4,4',5,5'-	0.000119	0.0007	0.001	0.00277	0.0163	6.9	42.94
155	2,2',4,4',6,6'-	0.00048	0.00345	0.002	0.00554	0.0399	7.0	86.62
171	2,2',3,3',4,4',6-	2.73×10^{-5}	0.00022	0.002	0.00506	0.0408	6.7	5.396
185	2,2',3,4,5,5',6-			0.00045	0.00114	0.0188	7.0	
194	2,2',3,3',4,4',5,5'-			0.0002	0.00047	0.00962	7.4	
202	2,2',3,3',5,5',6,6'-	2.66×10^{-5}	0.0006	0.0003	0.0007	0.0158	7.1	38.11
206	2,2',3,3',4,4',5,5',6-	1.96×10^{-7}	1.17×10^{-5}	0.00011	0.000237	0.0141	7.2	0.8271
207	2,2',3,3',4,4',5,6,6'-						7.52	
208	2,2',3,3',4,5,5',6,6'-			1.8×10^{-5}	3.88×10^{-5}	0.00130	8.16	
209	2,2',3,3',4,4',5,5',6,6'-	5.02×10^{-8}	3.06×10^{-5}	1.0×10^{-6}	2.00×10^{-6}	0.0122	8.26	25.03

TABLE 7.2.3

Summary of physical properties of PCB isomer groups and Aroclor mixtures

PCB isomer group	CAS no.	Molecular weight, MW g/mol	Cl no.	m.p. °C	Fugacity ratio, F range at 25°C	Le Bas molar volume, V_M (cm ³ /mol)
Biphenyl	92-52-4	154.2	0	71	0.352	184.6
Monochloro-	27323-18-8	188.7	1	25.1–78	0.299–1.0	205.5
Dichloro-	25512-42-9	223.1	2	24.4–149	0.0594–1.0	226.4
Trichloro-	25323-68-6	257.5	3	28.1–102	0.173–0.932	247.3
Tetrachloro-	26914-33-0	292.0	4	47–164	0.042–0.606	268.2
Pentachloro-	25429-29-2	326.4	5	76.5–123	0.107–0.310	289.1
Hexachloro-	26601-64-9	360.9	6	70–201	0.0182–0.359	310
Heptachloro-	28655-71-2	395.3	7	109–162	0.0596–0.148	330.9
Octachloro-	31472-83-0	429.8	8	132–161	0.0452–0.0874474	351.8
Nonachloro-	53742-07-7	464.2	9	205–206	0.0163–0.0276	372.7
Decachloro-	2051-24-3	498.7	10	305	0.00167	393.6

Aroclor mixture	CAS no.	Molecular weight, MW g/mol	% Cl	No. of Cl/molecule	Fugacity ratio, F at 25°C	Density g/cm ³ at 25°C	Distillation range °C
Aroclor 1016	12674-11-2	257	41	3	1.0	1.33	323–356
Aroclor 1221	111-042-82	192	20.5–21.5	1.15	1.0	1.15	275–320
Aroclor 1232	111-411-65	221	31.4–32.5	2.04	1.0	1.24	290–325
Aroclor 1242	534-692-19	261	42	3.1	1.0	1.35	325–366
Aroclor 1248	126-722-96	288	48	3.9	1.0	1.41	340–375
Aroclor 1254	110-976-91	327	54	4.96	1.0	1.5	365–390
Aroclor 1260	110-968-25	372	60	6.3	1.0	1.58	385–420

TABLE 7.2.4

Summary of selected physical-chemical properties of PCB isomer groups and Aroclor mixtures at 20–25°C

PCB isomer group	Aqueous solubility range			Vapor pressure range		Henry's law const.	log K _{OW} range
	S/(g/m ³)	C _S /(mmol/m ³)	C _L /(mmol/m ³)	P _S /Pa	P _L /Pa	H/(Pa·m ³ /mol) calculated P/C	
Biphenyl	7.0	45.39	129.7	1.30	3.69	28.64	3.90
Monochloro-	1.21–5.50	6.36-29.15	1 13.24-35.66	0.271-2.04	0.9-2.5	42.56-75.55	4.3-4.60
Dichloro-	0.060–2.0	0.269-8.96	4.56-10.14	0.0048-0.279	0.008-0.60	17.0-92.21	4.9-5.30
Trichloro-	0.015–0.40	0.0582-1.55	0.24-2.39	0.0136-0.143	0.003-0.22	24.29-92.21	5.5-5.90
Tetrachloro-	0.0043–0.010	0.0147-0.342	0.133-1.30	0.000059-.0054	0.002	1.72-47.59	5.6-6.50
Pentachloro-	0.004–0.020	0.0123-0.0613	0.093-0.337	0.000304-0.0093	0.0023-0.051	24.8-151.4	6.2-6.50
Hexachloro-	0.0004–0.0007	0.0011-0.002	0.0061-0.0286	0.000020-0.00159	0.0007- 0.012	11.9-818	6.7-7.30
Heptachloro-	0.000045–0.0002	0.00114-0.0051	0.0191-0.046	0.0000273	0.00025	5.40	6.7-7.0
Octachloro-	0.0002–0.0003	0.00047-0.0007	0.0098-0.0158	0.0000266	0.0006	38.08	7.10
Nonachloro-	0.00018–0.0012	0.000038-0.00024	0.00141-0.0146	-	-	-	7.2-8.16
Decachloro-	0.000761	0.0000024	0.0144	0.00000005	0.00003	20.84	8.26

Aroclor mixture	Aqueous solubility range		Vapor pressure range		Henry's law const.	log K _{OW} range
	S/(g/m ³)	C _L /(mmol/m ³)	P _L /Pa		H/(Pa·m ³ /mol) calculated P/C	
Aroclor 1016	0.22-0.84	0.856-0.216	0.06-0.2		70-900	4.4-5.8
Aroclor 1221	0.59-5.0	0.307-26.0	0.89-2.0		34-450	4.1-4.7
Aroclor 1232	1.45	6.56-2.0	0.54		82-270	4.5-5.2
Aroclor 1242	0.1-0.75	0.383-2.87	0.05-0.13		45-130	4.5-5.8
Aroclor 1248	0.1-0.5	0.347-1.74	0.0085-0.11		5-300	5.8-6.3
Aroclor 1254	0.01-0.30	0.306-0.92	0.008-0.02		20-260	6.1-6.8*
Aroclor 1260	0.003-0.08	0.00806-0.215	0.0002-0.012		20-60	6.3-6.8*

* See discussion by Linkov et al. 2005.

TABLE 7.2.5
Suggested half-life classes of polychlorinated biphenyls (PCBs) in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Biphenyl	3	4	5	6
Monochloro-	4	7	8	8
Dichloro-	4	7	8	8
Trichloro-	5	8	9	9
Tetrachloro-	6	9	9	9
Pentachloro-	6	9	9	9
Hexachloro-	7	9	9	9
Heptachloro-	7	9	9	9
Octachloro-	8	9	9	9
Nonachloro-	8	9	9	9
Decachloro-	9	9	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

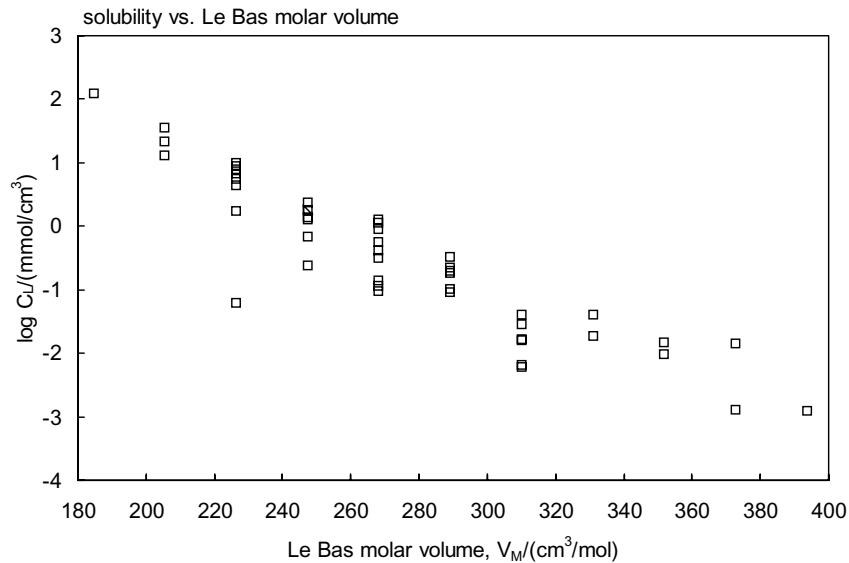


FIGURE 7.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated biphenyls.

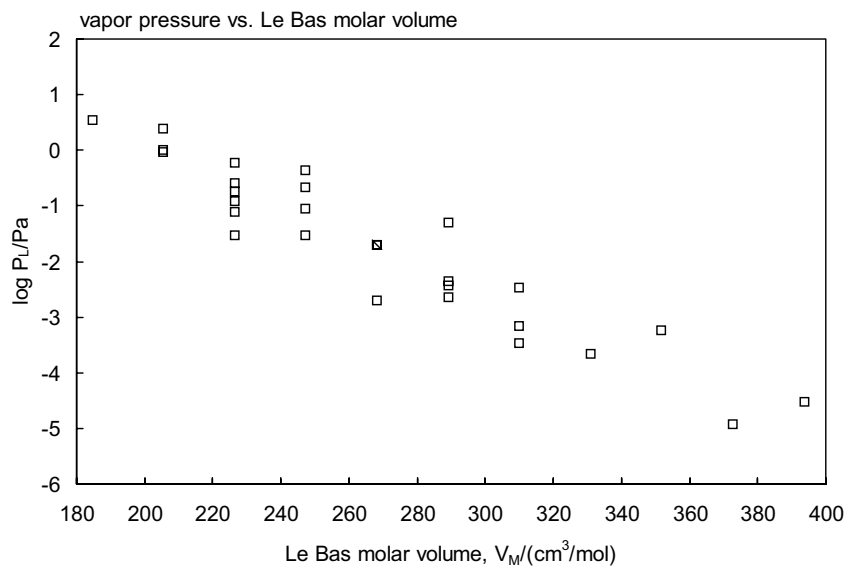


FIGURE 7.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated biphenyls.

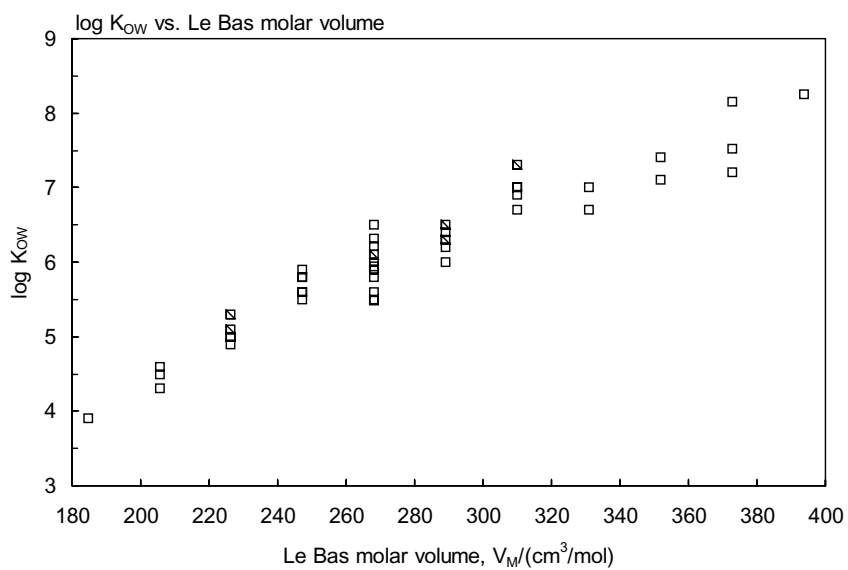


FIGURE 7.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated biphenyls.

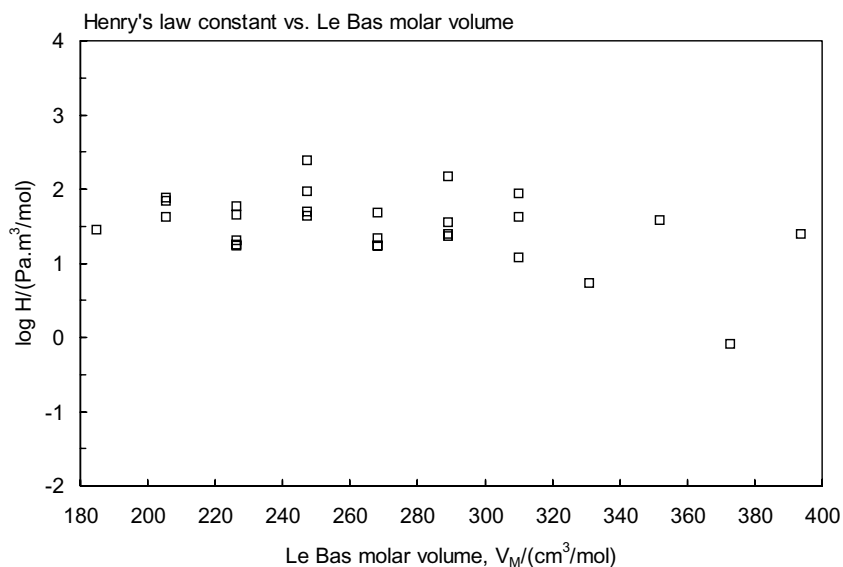


FIGURE 7.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated biphenyls.

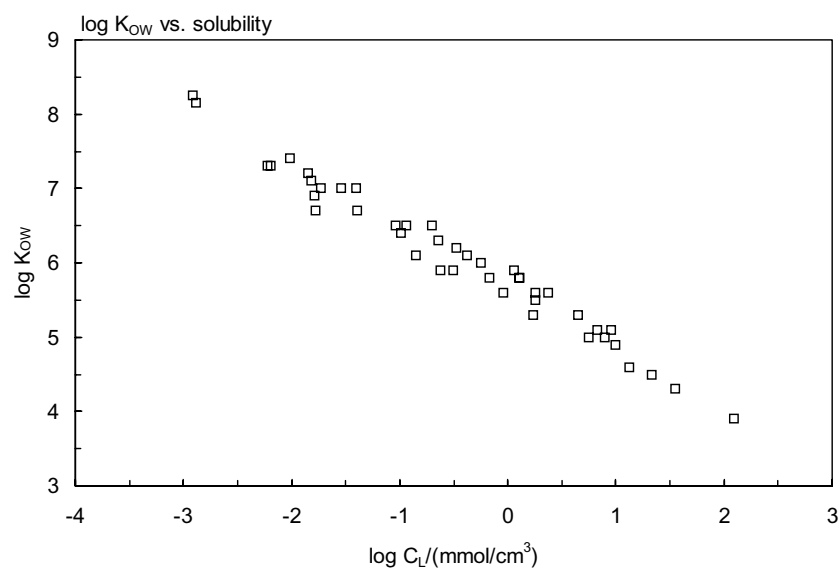


FIGURE 7.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated biphenyls.

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8 Chlorinated Dibenzo-*p*-dioxins

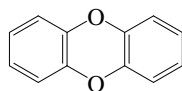
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8.1 LIST OF CHEMICALS AND DATA COMPILATIONS

8.1.1 DIBENZO-*p*-DIOXIN AND CHLORINATED DIBENZO-*p*-DIOXINS

8.1.1.1 Dibenzo-*p*-dioxin



Common Name: Dibenzo-*p*-dioxin

Synonym: dibenzo-1,4-dioxin

Chemical Name: dibenzo-*p*-dioxin

CAS Registry No: 262-12-4

Molecular Formula: C₆H₄O₂C₆H₄

Molecular Weight: 184.191

Melting Point (°C):

120.5 (Lide 2003)

Boiling Point (°C):

266.0 (Rordorf 1986)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

143.82, 142.06 (calculated-liquid density, crystalline volume, Govers et al. 1990)

146.96 (liquid molar volume, Govers et al. 1995)

177.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

68.4 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

92.250 (Rordorf 1987)

93.6 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.2, 22.6 (obs., predicted, Rordorf 1986)

22.6 (Ruelle & Kesselring 1997)

23.2, 22.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

57 (Rordorf 1986, 1987, 1989)

58.63, 57.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.116 (mp at 120.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.842*, 0.90 (generator column-HPLC/UV, generator column-GC/ECD; Shiu et al. 1988)

0.90* (generator column-GC/ECD, measured range 4–25°C, Doucette & Andren 1988a)

0.90* (generator column-GC, measured range 4–40°C, Doucette & Andren 1988a)

S/(mol/L) = 8.85 × 10⁻⁷ exp(0.067·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a)

log x = -2541/(T/K) - 1.476; temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)

ln x = 4.1680 - 6087.88/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

7.16 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.055* (gas saturation-GC, Rordorf 1985ab, 1986, 1987, 1989)

0.050 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

0.512; 0.251 (supercooled liquid P_L, quoted exptl., calculated-SOFA Solubility-parameter-based-model, Govers & Krop 1998)

log (P/Pa) = 14.91018 - 4820.43/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.389; 0.251(GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

0.107* (30°C, Knudsen effusion method, measured range 30–60°C Li et al. 2002)

$\ln(P/\text{Pa}) = (34.944 \pm 0.444) - (11259 \pm 141)/(T/\text{K})$; temp range 303–333 K (Knudsen effusion technique, Li et al. 2002, 2004)

$\ln(P/\text{Pa}) = 34.319 - 11095/(T/\text{K})$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

12.40 (calculated-P/C, Shiu et al. 1987; 1988)

10.96 (calculated-SOFA model, Govers & Krop 1998)

15.85; 10.96 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

4.31, 4.48, 4.38; 4.38, 4.46, 4.52 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)

4.26, 4.65 (Doucette 1985)

4.17, 4.46 (HPLC-RT correlation, Sarna et al. 1984)

4.26, 4.01; 4.34, 4.17 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)

4.20 (HPLC-RT correlation, Burkhard & Kuehl 1986)

4.37 (generator column-GC, Doucette & Andren 1987)

4.18 (HPLC-RT correlation, Doucette & Andren 1988b)

4.38 (recommended, Hansch et al. 1995)

4.15 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C:

Bioconcentration Factor, $\log \text{BCF}$:

4.49; 4.68 (lipid based BCF, guppy, quoted exptl., calculated-SOFA Solubility-parameter-base-model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

4.34 (sediment/water, calculated-SOFA Solubility-parameter-base-model, Govers & Krop 1998)

4.01 (derived from soot-water distribution coeff., Bärning et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated *data at other temperatures see reference:

$k_{\text{OH}} = 4.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ corresponding to an atmospheric lifetime $\tau \sim 7 \text{ h}$ at room temp. (Atkinson 1987a)

$k_{\text{OH}}(\text{calc}) = 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987b)

$k_{\text{OH}} = 37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.4 \text{ d}$ based on the gas-phase reactions with OH radical and a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{\text{OH}} = 1.48 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime $\tau = 1.0 \text{ d}$, $k_{\text{NO}_3} = 3.9 \times 10^{-27} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetime $\tau = 4.9 \text{ d}$, and $k_{\text{O}_3} < 5 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau > 330 \text{ d}$ at $297 \pm 2 \text{ K}$ (Kwok et al. 1994)

$k_{\text{OH}}(\text{exptl}) = 14.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, corresponding to a tropospheric lifetime of 1.0 d (Kwok et al. 1995)

$k_{\text{OH}}^* = 12 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 345–385 K; and $k_{\text{OH}}(\text{calc}) = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime $\tau = 24 \text{ h}$ based on gas-phase OH reactions (Brubaker & Hites 1998)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: room temp. gas-phase reaction rate constant $k = 4.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical corresponding to an atmospheric lifetime of about 7 h (Atkinson 1987a)

tropospheric lifetime $\tau = 0.4 \text{ d}$ calculated for dibenzo-*p*-dioxin based on the gas-phase reaction with OH radical (Atkinson 1991);

tropospheric lifetimes: $\tau(\text{calc}) = 1.0 \text{ d}$, 4.9 d and >330 d for reactions with OH radical, NO_3 radical and O_3 , respectively at room temp. (Kwok et al. 1994);

tropospheric lifetime $\tau(\text{calc}) = 1.0 \text{ d}$ with respect to reaction with the OH radical (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 8.1.1.1.1

Reported aqueous solubilities and vapor pressures of dibenzo-*p*-dioxin at various temperatures and the reported temperature dependence equations

Aqueous solubility				Vapor pressure			
Shiu et al. 1988		Doucette & Andren 1988		Rordorf 1987, 1989		Li et al. 2002	
generator column-HPLC/UV		generator column-GC/ECD		gas saturation		Knudsen effusion	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa
5	0.205	4.1	0.212	25	0.055	30	0.107
15	0.460	25	0.90	50	0.98	35	0.215
25	0.842	40	2.392	75	12.0	40	0.358
35	1.762			100	97	45	0.628
45	3.262	ΔH _{sol} /(kJ mol ⁻¹) = 48.6		125	630	50	1.14
		at 25 °C				55	1.90
ΔH _{sol} /(kJ mol ⁻¹) = 50.68				ΔH _v /(kJ mol ⁻¹) = 68.4		60	3.08
for 5–45 °C		S/(mol/L) = a·exp[b(t/°C)]		ΔH _{subl} /(kJ mol ⁻¹) = 92.25			
		a	8.85 × 10 ⁻⁷	ΔH _{fus} /(kJ mol ⁻¹) = 22.6		ln (P/Pa) = A – B/(T/K)	
		b	0.067	ΔS _{fus} /(J mol ⁻¹ K ⁻¹) = 57		A	34.994
		OR:				B	11259
		ln x = A – B/(T/K)					
		A	–1.476				
		B	2541				

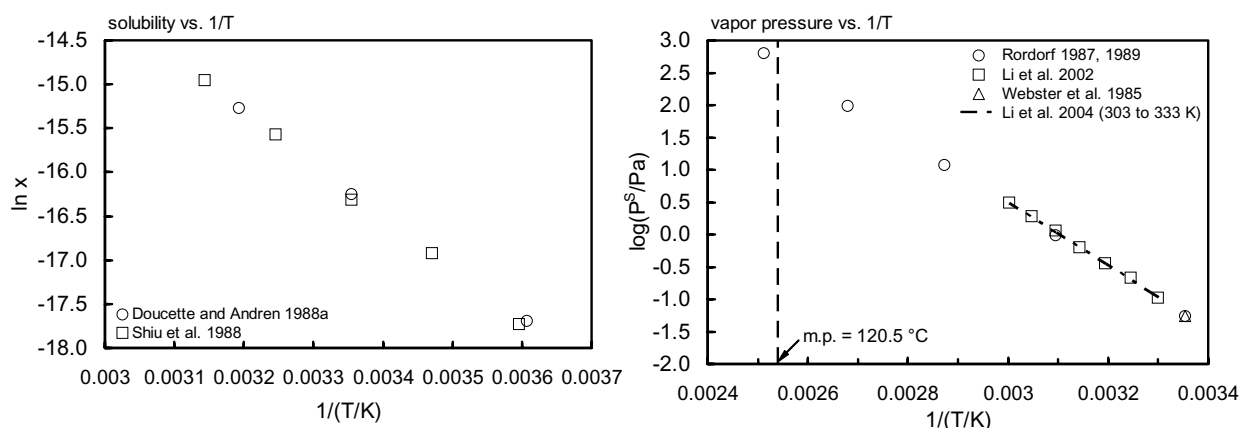
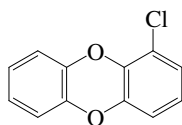


FIGURE 8.1.1.1.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for dibenzo-*p*-dioxin.

8.1.1.2 1-Chlorodibenzo-*p*-dioxin

Common Name: 1-Chlorodibenzo-*p*-dioxin

Synonym: 1-CDD, 1-MCDD

Chemical Name: 1-chlorodibenzo-*p*-dioxin

CAS Registry No: 39227-53-7

Molecular Formula: C₆H₄O₂C₆H₃Cl

Molecular Weight: 218.636

Melting Point (°C):

104.5–105.5 (Pohland & Yang 1972; quoted, Rordorf 1986,1987,1989)

Boiling Point (°C):

296.0 (Rordorf 1986)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

157.41, 158.07 (calculated-liquid density, crystalline volume, Govers et al. 1990)

156.19 (liquid molar volume, Govers et al. 1995)

197.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

76.2 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

98.55 (Rordorf 1987)

100.5 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.2, 21.4 (obs., predicted, Rordorf 1986)

23.2, 22.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.0 (Rordorf 1986,1987,1989)

61.34, 58.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.164 (mp at 105.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.417* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)

ln *x* = −0.68385 − 4912.15/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

1.51 (supercooled liquid S_L, GC-RI correlation; Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.012* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989; quoted, Shiu et al. 1988)

log (P/Pa) = 15.35327 − 5150.4/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.0275 (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)

ln (P/Pa) = 35.353 − 11859/(T/K); temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

ln (P/Pa) = (36.087 ± 0.293) − (12085 ± 96)/(T/K); temp range 308–343 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C):

8.38 (calculated-P/C, Shiu et al. 1988)

6.31; 4.57 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

7.76; 5.75 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 4.97, 5.20, 5.25; 5.05, 5.18, 5.23 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
4.91, 5.18 (HPLC-RT correlation, Sarna et al. 1984)
4.81, 4.52; 4.91, 5.74 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
4.75 (HPLC-RT correlation, Burkhard & Kuehl 1986)
5.05 (recommended, Hansch et al. 1995)
4.99 (GC-RI correlation; Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 7.86*; 8.34 (generator column-GC; calculated, Harner et al. 2000)
 $\log K_{OA} = -2.88 + 3200/(T/K)$; temp range 10–40°C (Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

- 5.17; 5.08 (lipid wt base, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.46 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5 \text{ d}$ based on the gas-phase reactions with OH radical and a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{exptl}) = 4.7 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, corresponding to a tropospheric lifetime of 1.0 d (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5 \text{ d}$ calculated for a mono-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime for mono-chlorinated dioxin was 3.0 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 8.1.1.2.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1-chlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure		log K _{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K _{OA}
5	0.205	25	0.012	10	8.466
15	0.460	50	0.26	20	8.018
25	0.842	75	3.60	30	7.628
35	1.762	100	36.0	40	7.396
45	3.262	125	260	25	7.86
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 40.85$ for 5–45°C		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 76.2$ $\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 98.55$ $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 21.4$ $\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 56.0$		$\log K_{\text{OA}} = a + b/(T/\text{K})$ a -2.88 b 3200	
				enthalpy of phase change $\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 61.30$	

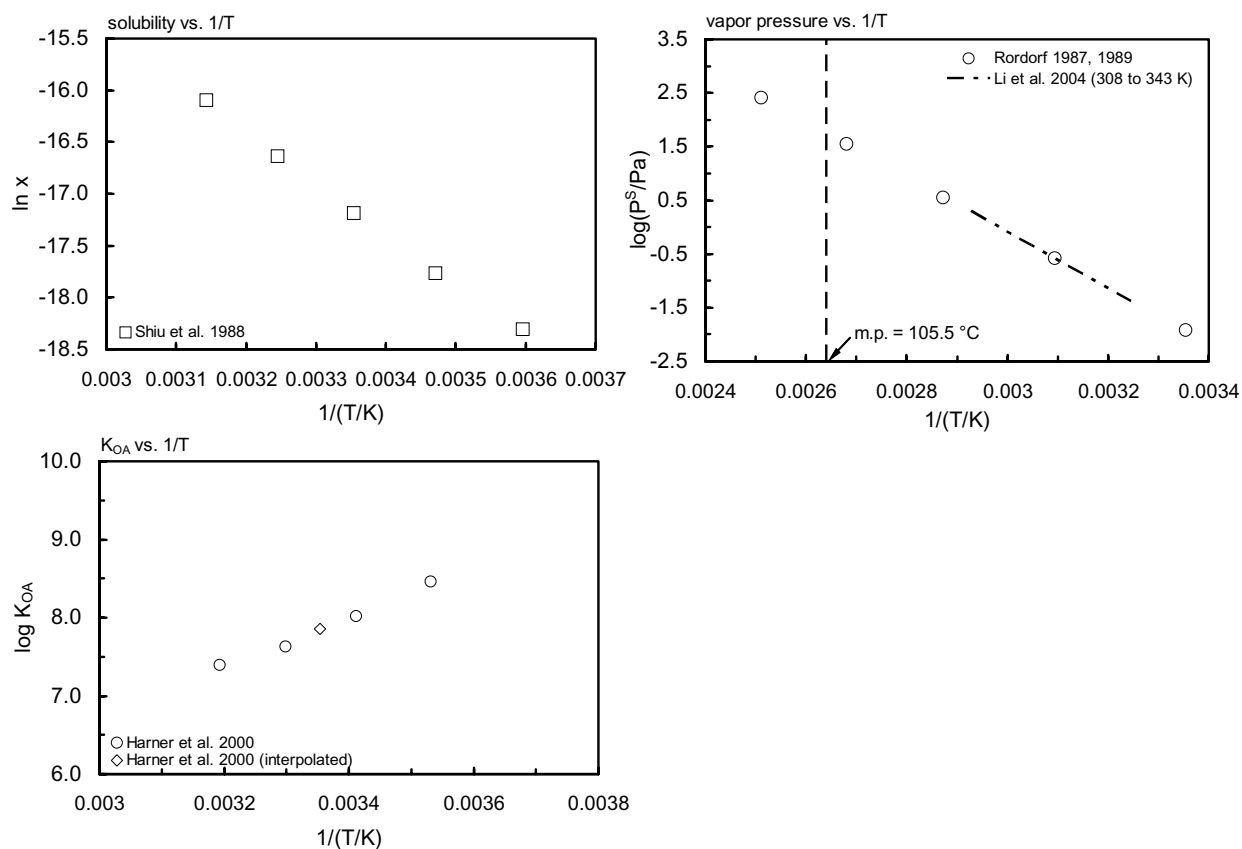
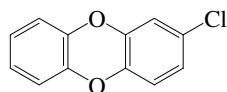


FIGURE 8.1.1.2.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1-chlorodibenzo-*p*-dioxin.

8.1.1.3 2-Chlorodibenzo-*p*-dioxin

Common Name: 2-Chlorodibenzo-*p*-dioxin

Synonym: 2-CDD, 2-MCDD

Chemical Name: 2-chlorodibenzo-*p*-dioxin

CAS Registry No: 39227-54-8

Molecular Formula: C₁₂H₈O₂Cl

Molecular Weight: 218.636

Melting Point (°C):

88–89 (Pohland & Yang 1972)

Boiling Point (°C):

298.0 (Rordorf 1986)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

154.85, 155.15 (calculated-liquid density, crystalline volume, Govers et al. 1990)

153.09 (liquid molar volume, Govers et al. 1995)

197.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.2 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

97.16 (Rordorf 1987)

98.1 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.1, 18.5 (obs., predicted, Rordorf 1986)

18.5 (Ruelle & Kesselring 1997)

23.1, 21.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

51 (Rordorf 1987, 1989)

63.78, 57.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.236 (mp at 89°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.278*, 0.319 (generator column-HPLC/UV, generator column-GC/ECD, measured range 5–45°C, Shiu et al. 1988)

0.319* (generator column-GC/ECD, measured range 3.9–39°C, Doucette & Andren 1988a)

S/(mol/L) = 4.88 × 10⁻⁷ exp(0.048·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or

log x = -1777/(T/K) - 1.566, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)

ln x = 4.093418 - 6448/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

1.44 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.017* (gas saturation-GC, Rordorf 1985a,b,1986,1987,1989)

0.016 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

log (P/Pa) = 15.2463 - 5071.88/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.0262 (GC-RI correlation, Wang & Wong 2002)

$\ln(P/\text{Pa}) = 35.106 - 11679/(T/\text{K})$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (35.549 \pm 0.415) - (11794 \pm 134)/(T/\text{K})$, temp range 308–343 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

14.82 (calculated-P/C, Shiu et al. 1988)
 12.60; 4.57 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 7.586; 4.57 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

5.36, 5.66, 5.71; 5.45, 5.64, 5.69 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 5.45, 5.64 (HPLC-RT correlation, Sarna et al. 1984)
 5.33, 5.00; 5.45, 5.29 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 5.08 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 4.94 (generator column-GC/ECD, Doucette & Andren 1987)
 4.98 (HPLC-RT correlation, Doucette & Andren 1988b)
 5.45 (recommended, Hansch et al. 1995)
 5.01 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

5.09 (guppy, Loonen et al. 1994)
 5.09; 5.12 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.92 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 5.35 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$

Volatilization:

Photolysis: photodegradation $t_{1/2} = 10$ min with simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988)
 photodegradation $k = 1.81 \text{ h}^{-1}$ with $t_{1/2} = 0.38$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5$ d for a mono-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{\text{OH}}(\text{exptl}) = 4.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 3.0$ d at room temp. (relative rate method, Kwok et al. 1995)

$k_{\text{OH}}(\text{calc}) = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Brubaker & Hites 1998)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5$ d calculated for a mono-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime for mono-chlorinated dioxin was 3.0 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

first-order photodegradation $k = 1.81 \text{ h}^{-1}$ with $t_{1/2} = 0.38$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: $t_{1/2} = 10$ min irradiated under simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 8.1.1.3.1

Reported aqueous solubilities and vapor pressures of 2-chlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure	
Shiu et al. 1988		Doucette & Andren 1988		Rordorf 1987, 1989	
generator column-HPLC/UV		generator column-GC/ECD		gas saturation-GC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
5	0.0603	3.9	0.133	25	0.017
15	0.137	25	0.319	50	0.36
25	0.278	39	0.7495	75	4.80
35	0.653			100	45.0
45	1.109			125	320

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 53.35$		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 34.0$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 78.1$	
5–45 $^{\circ}\text{C}$		4–32 $^{\circ}\text{C}$		$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 97.16$	
				$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.5$	
				$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 51$	

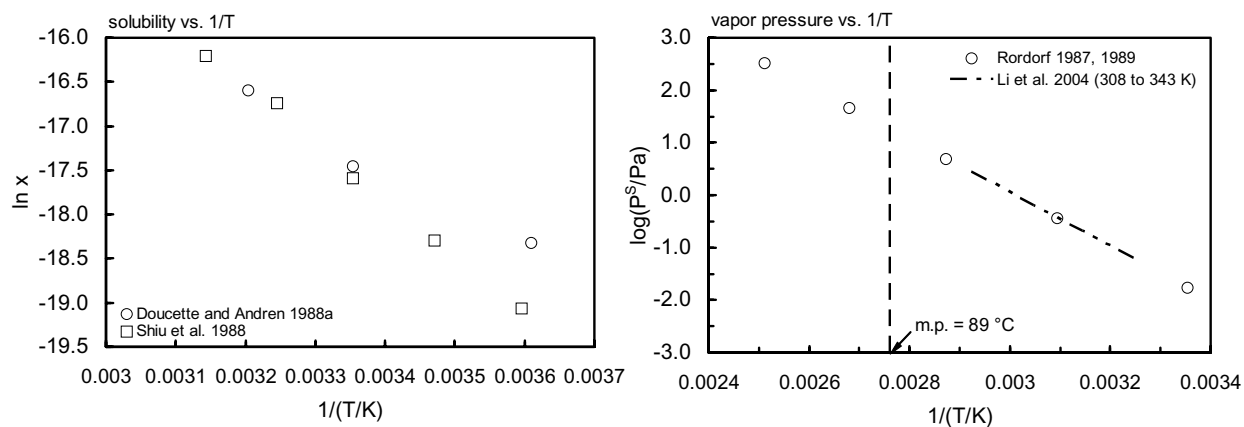
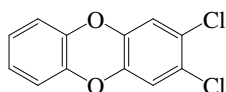


FIGURE 8.1.1.3.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2-chlorodibenzo-*p*-dioxin.

8.1.1.4 2,3-Dichlorodibenzo-*p*-dioxin

Common Name: 2,3-Dichlorodibenzo-*p*-dioxin

Synonym: 2,3-DCDD

Chemical Name: 2,3-dichlorodibenzo-*p*-dioxin

CAS Registry No: 29446-15-9

Molecular Formula: $C_{12}H_4O_2Cl_2$

Molecular Weight: 253.081

Melting Point ($^{\circ}C$):

163–164 (Pohland & Yang 1972)

Boiling Point ($^{\circ}C$):

358 (calculated, Rordorf 1986,1987,1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

164.07 (calculated-liquid density, Govers et al. 1990)

162.67 (liquid molar volume, Govers et al. 1995)

218.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.8 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

106.23 (Rordorf 1987)

106.2 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

26.7 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

61 (Rordorf 1986,1987,1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0433 (mp at $164^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0149* (generator column-HPLC/UV, measured range $5-45^{\circ}C$, Shiu et al. 1988)

$\ln x = 0.07859 - 6173.64/(T/K)$; temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.297 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00039* (gas saturation-GC, Rordorf 1985a,b, 1986,1989)

0.0004 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

0.0020 (GC-RI correlation, Wang & Wong 2002)

$\log (P_L/mmHg) = 48.98 - 6446/(T/K) - 12.569 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln (P/Pa) = 35.096 - 12804/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln (P/Pa) = (35.081 \pm 0.374) - (12771 \pm 134)/(T/K)$; temp range 338–378 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

6.61 (calculated-P/C, Shiu et al. 1988)

6.61; 2.51 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)

3.80; 2.51 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 4.70 (calculated, Kaiser 1983)
- 6.23, 5.60 (calculated-QSAR, quoted, Fiedler & Schramm 1990)
- 5.77 (calculated-SOFA model, Govers & Krop 1998)
- 5.738 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 5.80; 5.77 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 8.50 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 5.41 (lipid wt based, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{oc}$:

- 4.73 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
- 6.27 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (22 - 28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5\text{--}0.7$ d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (5.9 - 7.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.0\text{--}2.4$ d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

$k_{OH}(\text{calc}) = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Brubaker & Hites 1998)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.092 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5\text{--}0.7$ d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime $\tau = 2.0\text{--}2.4$ d for the reaction with OH radical (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: mean biological $t_{1/2} \sim 2$ d in rainbow trout (Niimi 1986);

biological $t_{1/2} = 7$ d in rainbow trout (Niimi & Oliver 1986);

biological $t_{1/2} = 2\text{--}7$ d in trout (Niimi 1987).

TABLE 8.1.1.4.1
Reported aqueous solubilities and vapor pressures of 2,3-dichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure	
Shiu et al. 1988		Rordorf 1987, 1989	
generator column-HPLC/UV		gas saturation-GC	
t/°C	S/g·m ⁻³	t/°C	P/Pa
5	0.00368	25	0.00039
15	0.00716	50	0.0011
25	0.0149	75	0.18
35	0.0304	100	2.20
45	0.0586	125	19.0

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 51.3$
5–45 °C

$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 77.8$
 $\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 106.23$
 $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 26.7$
 $\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 61$

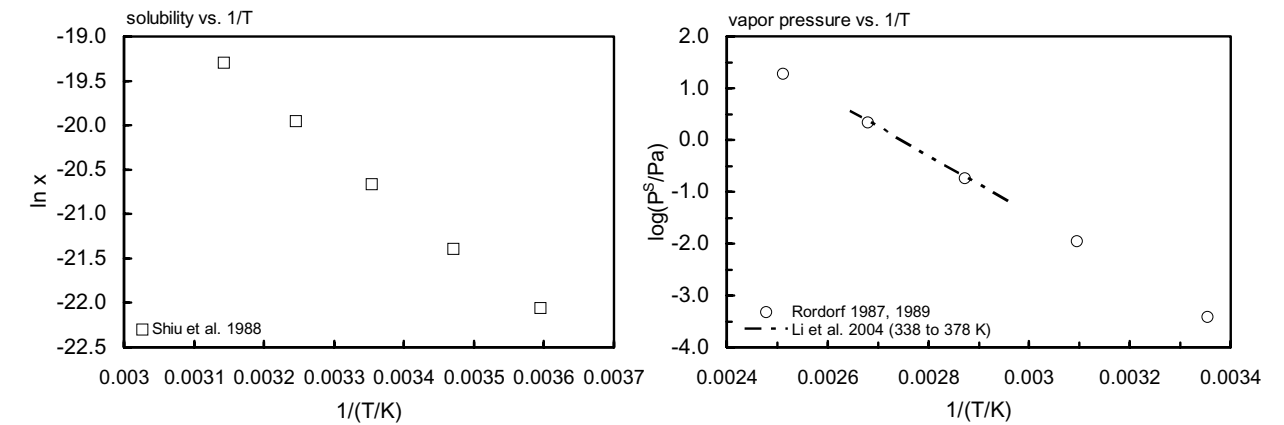
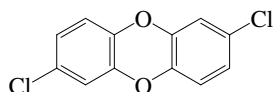


FIGURE 8.1.1.4.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,3-dichlorodibenzo-*p*-dioxin.

8.1.1.5 2,7-Dichlorodibenzo-*p*-dioxin

Common Name: 2,7-Dichlorodibenzo-*p*-dioxin

Synonym: 2,7-DCDD

Chemical Name: 2,7-dichlorodibenzo-*p*-dioxin

CAS Registry No: 33857-26-0

Molecular Formula: $\text{ClC}_6\text{H}_3\text{O}_2\text{C}_6\text{H}_3\text{Cl}$

Molecular Weight: 253.081

Melting Point ($^{\circ}\text{C}$):

210 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

374.5 (calculated, Rordorf 1987, 1989)

Density (g/cm^3):

1.647 (calculated, Boer et al. 1972)

Molar Volume (cm^3/mol):

165.88, 162.89 (calculated-liquid density, crystalline volume, Govers et al. 1990)

162.87 (liquid molar volume, Govers et al. 1995)

218.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

76.4 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

105.51 (Rordorf 1987)

113.8 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

26.8 (Rordorf 1986, 1987; Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

55 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.0188 (mp at 201°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00375* (generator column-HPLC/UV, Shiu et al. 1988)

0.00224 (generator column-GC/MS, Santl et al. 1994)

$\ln x = -3.48833 - 5543.9/(T/\text{K})$; temp range 5 – 50°C (regression eq. of literature data, Shiu & Ma 2000)

0.311 (GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00012* (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989; quoted, Shiu et al. 1988)

0.00013 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

$\log (P/\text{Pa}) = 14.60827 - 5523.34/(T/\text{K})$ temp range 5 – 50°C (regression eq. from literature data, Shiu & Ma 2000)

0.00219 (GC-RI correlation, Wang & Wong 2002)

$\log (P_L/\text{mmHg}) = 49.61 - 6624/(T/\text{K}) - 12.569 \cdot \log (T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln (P/\text{Pa}) = 33.637 - 12718/(T/\text{K})$; temp range 298 – 398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln (P/\text{Pa}) = (36.293 \pm 0.648) - (13686 \pm 245)/(T/\text{K})$; temp range 358 – 393 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C):

- 8.11 (calculated-P/C, Shiu et al. 1988)
- 6.98 (gas stripping-GC/MS, Santl et al. 1994)
- 8.13; 2.82 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 3.89; 2.82 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow}:

- 6.28, 6.64, 6.72; 6.38, 6.62, 6.71 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 6.62, 6.39 (HPLC-RT correlation, Sarna et al. 1984)
- 6.27, 5.86; 6.39, 6.17 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 5.75 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 6.38 (recommended, Sangster 1993)
- 6.38 (recommended, Hansch et al. 1995)
- 5.77 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 8.36*; 8.67 (generator column-GC; calculated, Harner et al. 2000)
- log K_{OA} = -3.74 + 3610/(T/K); temp range 10–40°C (Harner et al. 2000)
- 8.48 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 1.7, 2.9 (guppy, in whole fish, in lipid, Gobas et al. 1987)
- 2.56, 3.68 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
- 5.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{oc}:

- 6.15 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: photodegradation t_{1/2} = 46 min in an aqueous solution assisted by TiO₂ at 2.0 g/L under simulated sunlight (Barbeni et al. 1986)

photodegradation t_{1/2} = 1 h with irradiation under simulated sunlight in aerated aqueous suspension of semiconductor TiO₂ at 4.0 g/L and pH 3 (Pelizzetti et al. 1988)

photolysis k = 8.9 × 10⁻² min⁻¹ with t_{1/2} = 7.8 min in pure water, and rate constant k = 0.16 min⁻¹ with t_{1/2} = 4.3 min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:

k_{OH}(calc) = (26–28) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)

k_{OH} = (22–28) × 10⁻¹² cm³ molecule⁻¹ s⁻¹, calculated tropospheric lifetime τ = 0.5–0.7 d for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of 1.5 × 10⁶ molecule/cm³ (Atkinson 1991)

k_{OH}(calc) = (5.9–7.3) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with a calculated tropospheric lifetime τ = 2.0–2.4 d for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

k_{OH}(calc) = 4.1 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (Brubaker & Hites 1998)

k_{OH}* = 23 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K, measured temp range 355–395 K, and k_{OH}(calc) = 4.1 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, with a calculation lifetime τ = 65 h based on gas-phase OH reactions (Brubaker & Hites 1998)

Biodegradation:

Biotransformation: metabolic elimination k_m = 0.23 d⁻¹ (goldfish, 20°C, 96-h exposure, Sijm & Opperhuizen 1988)

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

k₂ = 0.462 d⁻¹ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

k₁ = 390 mL g⁻¹ d⁻¹; k₂ = 0.23 d⁻¹ (goldfish, 20°C, 96-h exposure, Sijm & Opperhuizen 1988)

k₁ = 543 d⁻¹; k₂ = 1.5 d⁻¹ (guppy, Gobas & Schrap 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5\text{--}0.7$ d calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric calculated lifetime $\tau = 2.0\text{--}2.4$ d for the reaction with OH radical (Kwok et al. 1995);

calculated lifetime $\tau = 65$ h based on gas-phase OH reactions (Brubaker & Hites 1998).

Surface water: photodegradation $t_{1/2} = 1$ h with irradiation under simulated sunlight in aerated aqueous suspension of semiconductor TiO_2 at 4.0 g/L and pH 3 (Pelizzetti et al. 1988);

photolysis rate constant $k = 8.9 \times 10^{-2} \text{ min}^{-1}$ with $t_{1/2} = 7.8$ min in pure water, and $k = 1.6 \times 10^{-1} \text{ min}^{-1}$ with $t_{1/2} = 4.3$ min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000).

Groundwater:

Sediment:

Soil:

Biota: mean biological $t_{1/2} \sim 2$ d in rainbow trout (Niimi 1986);

biological $t_{1/2} = 2$ d in rainbow trout (Niimi & Oliver 1986);

biological $t_{1/2} = 2\text{--}7$ d in trout (Niimi 1987).

TABLE 8.1.1.5.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,7-dichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure		log K_{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K_{OA}
5	0.00109	25	0.0001	10	9.020
15	0.00201	50	0.0033	20	8.564
25	0.00375	75	0.056	30	8.106
35	0.00727	100	0.64	40	7.818
45	0.0134	125	5.4	25	7.36
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 50.68$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 76.4$		$\log K_{OA} = a + b/(T/K)$	
25 °C		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 105.51$		a	-3.74
		$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 26.8$		b	3610
		$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 55$		enthalpy of phase change	
				$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 69.0$	

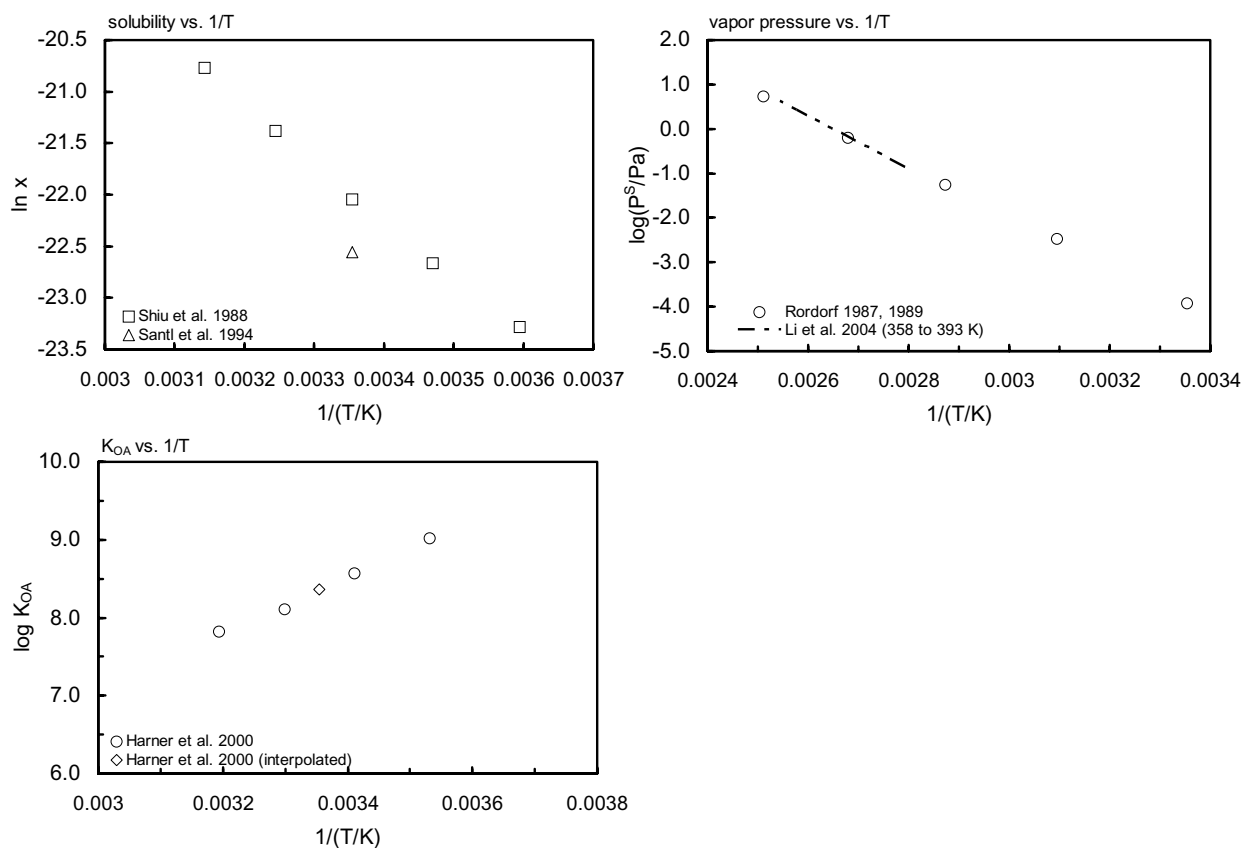
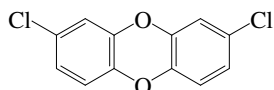


FIGURE 8.1.1.5.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,7-dichlorodibenzo-*p*-dioxin.

8.1.1.6 2,8-Dichlorodibenzo-*p*-dioxin

Common Name: 2,8-Dichlorodibenzo-*p*-dioxin

Synonym: 2,8-TCDD

Chemical Name: 2,8-dichlorodibenzo-*p*-dioxin

CAS Registry No: 38964-22-6

Molecular Formula: $\text{ClC}_6\text{H}_3\text{O}_2\text{C}_6\text{H}_3\text{Cl}$

Molecular Weight: 253.081

Melting Point ($^{\circ}\text{C}$):

150.5–151 (Pohland & Yang 1972; Rordorf 1986,1987,1989)

Boiling Point ($^{\circ}\text{C}$):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

165.88, 167.2 (calculated-liquid density, crystalline volume, Govers et al. 1990)

160.63 (liquid molar volume, Govers et al. 1995)

218.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.1 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

109.01 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.2 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

55 (Rordorf 1986,1987,1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, $F: 0.058$ (mp at 151°C))

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0167* (generator column-GC/ECD, measured range $5\text{--}45^{\circ}\text{C}$, Shiu et al. 1988)

$\ln x = -2.54177 - 5379/(T/\text{K})$; temp range $5\text{--}50^{\circ}\text{C}$ (regression eq. of literature data, Shiu & Ma 2000)

0.311 (supercooled liquid S_L , GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00014* (gas saturation-GC, Rordorf 1985a,b, 1986,1987,1989)

0.00013 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

$\log (P/\text{Pa}) = 15.25386 - 5699.96/(T/\text{K})$; temp range $5\text{--}50^{\circ}\text{C}$ (regression eq. from literature data, Shiu & Ma 2000)

0.00219 (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

0.00150 (solid P_S , gas saturation-GC/MS, Mader & Pankow 2003)

0.0260 (supercooled liquid P_L , calculated from P_S assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, Mader & Pankow 2003)

$\log (P_L/\text{mmHg}) = 49.89 - 6705/(T/\text{K}) - 12.569 \cdot \log (T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

2.13 (calculated- P/C , Shiu et al. 1988)

2.14; 2.29 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)

3.89; 2.29 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow} :

- 4.70 (calculated, Kaiser 1983)
- 5.60 (selected, Shiu et al. 1988)
- 5.68 (calculated-SOFA model, Govers & Krop 1998)
- 5.638 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 5.77; 5.68 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
- 5.34, 5.50, 5.75, 5.58 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 8.36*; 8.65 (generator column-GC; measured range 10–40°C; calculated, Harner et al. 2000)
- log $K_{OA} = -3.74 + 3610/(T/K)$; temp range 10–40°C, (Harner et al. 2000)
- 8.48 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 2.77, 2.82 (goldfish: treated with metabolic inhibitor PBO, untreated, Sijm & Opperhuizen 1988)
- 5.42 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} :

- 6.14 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (26-28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (22-28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.5-0.7 \text{ d}$ for a di-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (5.9-7.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.0-2.4 \text{ d}$ for a di-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation: metabolic elimination rate constant from goldfish was estimated to be 0.35 d^{-1} (Sijm & Opperhuizen 1988).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 390 \text{ L kg}^{-1} \cdot \text{d}^{-1}$; $k_2 = 0.23 \text{ d}^{-1}$ (goldfish, Opperhuizen & Sijm 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.5 - 0.7 \text{ d}$ calculated for a di-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime $\tau = 2.0 - 2.4 \text{ d}$ for the reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: mean biological $t_{1/2} \sim 2 \text{ d}$ in rainbow trout (Niimi 1986);

biological $t_{1/2} = 2-7 \text{ d}$ in trout (Niimi 1987).

TABLE 8.1.1.6.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 2,8-dichlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility		Vapor pressure		log K _{OA}	
Shiu et al. 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m ⁻³			t/°C	log K _{OA}
5	0.00422	25	0.0001	10	9.020
15	0.00859	50	0.0042	20	8.564
25	0.0167	75	0.078	30	8.106
35	0.0275	100	0.97	40	7.818
45	0.0515	125	8.80	25	8.36
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 50.04$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 84.1$		$\log K_{\text{OA}} = a + b/(T/\text{K})$	
5–45 °C		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 109.01$		a	
		$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 23.3$		b	
		$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 55$		enthalpy of phase change	
				$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 69.0$	

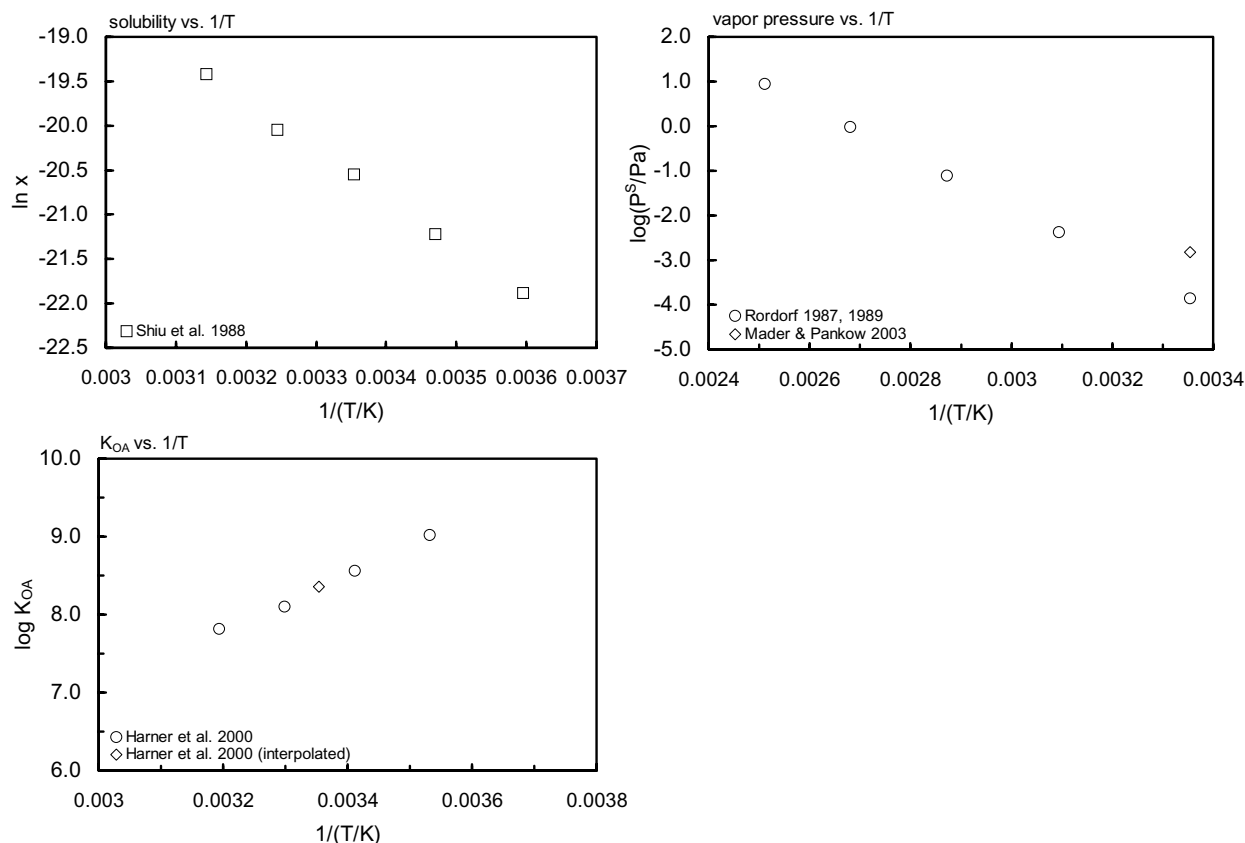
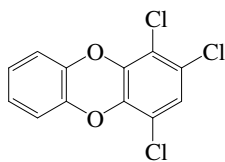


FIGURE 8.1.1.6.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 2,8-dichlorodibenzo-*p*-dioxin.

8.1.1.7 1,2,4-Trichlorodibenzo-*p*-dioxin

Common Name: 1,2,4-Trichlorodibenzo-*p*-dioxin

Synonym: 1,2,4-TCDD

Chemical Name: 1,2,4-trichlorodibenzo-*p*-dioxin

CAS Registry No: 39227-58-2

Molecular Formula: $C_{12}H_5Cl_3O_2$, $C_6H_4O_2C_6HCl_3$

Molecular Weight: 287.526

Melting Point (°C):

128–129 (Pohland & Yang 1972; quoted, Rordorf 1986, 1987, 1989)

Boiling Point (°C):

375.0 (calculated, Rordorf 1986, 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

179.66 (calculated-liquid density, Govers et al. 1990)

173.60 (liquid molar volume, Govers et al. 1995)

239.7 (calculated-Le Bas method at normal boiling)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.9 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

118.79 (Rordorf 1987)

121.0 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

33.9 (Rordorf 1986, 1987)

Entropy of Fusion, ΔS_{fus} (J/mol K):

67 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.0954 (mp at 129°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00841* (generator column-HPLC/UV, measured range 5–45°C, Shiu et al. 1988)

0.00695 (generator column-GC/MS, Santl et al. 1994)

$\ln x = -2.4909 - 5626.95/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

0.091 (supercooled liquid S_L , GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0001* (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)

0.0001 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

$\log(P/\text{Pa}) = 16.9148 - 6235.45/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.000324 (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

5.07×10^{-4} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

5.43×10^{-3} (supercooled liquid P_L , calculated from measured P_s assuming $\Delta S_{\text{fus}} = 56$ J/mol K, Mader & Pankow 2003)

$\log(P_L/\text{mmHg}) = 47.18 - 6479/(T/K) - 12.028 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/\text{Pa}) = 38.948 - 14358/(T/\text{K})$; temp range 298 – 398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (39.303 \pm 0.605) - (14550 \pm 221)/(T/\text{K})$; temp range 348–383 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 3.84 (calculated-P/C, Shiu et al. 1988)
- 3.64 (gas stripping-GC/MS, Santl et al. 1994)
- 3.72; 1.82 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 2.29; 1.82 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 7.40, 7.77, 7.69; 7.47, 7.76, 7.68 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 7.45, 7.76 (HPLC-RT correlation, Sarna et al. 1984)
- 7.36, 6.86; 7.45, 7.11 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 6.45 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 7.47 (recommended, Hansch et al. 1995)
- 6.34 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

- 8.97 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 1.90, 3.10 (guppy, in whole fish, in lipid, Gobas et al. 1987)
- 2.82, 3.95 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)
- 5.42 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{oc}$:

- 7.01 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 5.87 (derived from soot-water distribution coeff., Bärning et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is $1.27 \times 10^6 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{OH}(\text{calc}) = (21\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (17\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (4.5\text{--}5.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.5\text{--}3.3 \text{ d}$ for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_2 = 0.058 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)
- $k_1 = 601 \text{ d}^{-1}$; $k_2 = 0.91 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radical (Atkinson 1991); the calculated tropospheric lifetime $\tau = 2.5\text{--}3.3 \text{ d}$ for the gas phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone $k = 1.27 \times 10^6 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987).

Sediment:

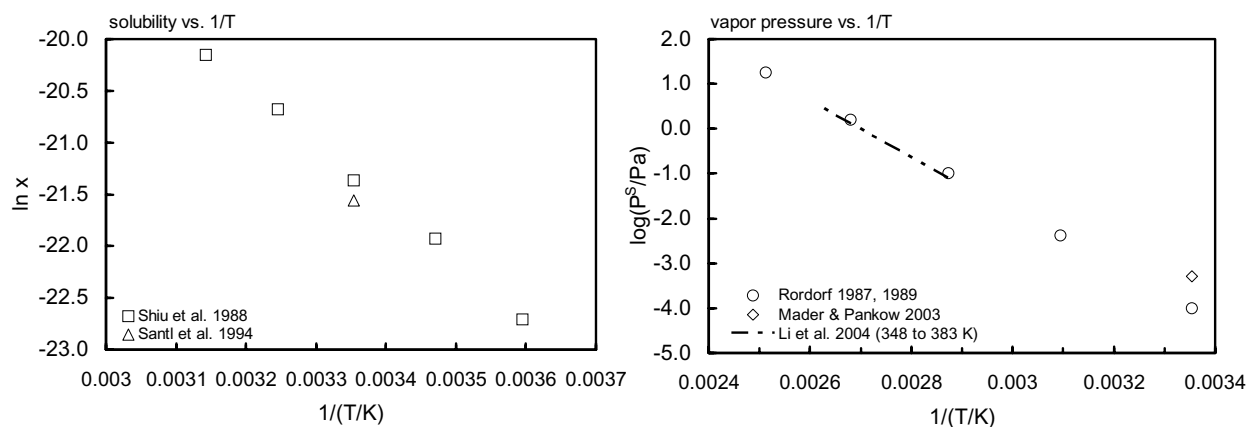
Soil:

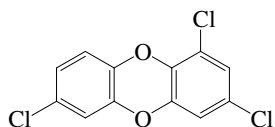
Biota: mean biological $t_{1/2} \sim 10$ d in rainbow trout (Niimi 1986); $t_{1/2} = 12$ d in rainbow trout (Niimi & Oliver 1986);biological $t_{1/2} = 12$ d in trout (Niimi 1987)**TABLE 8.1.1.7.1****Reported aqueous solubilities and vapor pressures of 1,2,4-trichlorodibenzo-*p*-dioxin at various temperatures**

Aqueous solubility		Vapor pressure	
Shiu et al. 1988		Rordorf 1987, 1989	
generator column-HPLC/UV		gas saturation-GC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
5	0.00219	25	0.0001
15	0.00477	50	0.0042
25	0.00841	75	0.1
35	0.0167	100	1.6
45	0.0282	125	18

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 46.62$
 $5\text{--}45^{\circ}\text{C}$

$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 83.9$
 $\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 118.79$
 $\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 33.9$
 $\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 84$

**FIGURE 8.1.1.7.1** Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,4-trichlorodibenzo-*p*-dioxin.

8.1.1.8 1,3,7-Trichlorodibenzo-*p*-dioxin

Common Name: 1,3,7-Trichlorodibenzo-*p*-dioxin

Synonym: 1,3,7-TCDD

Chemical Name: 1,3,7-trichlorodibenzo-*p*-dioxin

CAS Registry No: 67026-17-5

Molecular Formula: $C_{12}H_5Cl_3O_2$, $ClC_6H_3O_2C_6H_2Cl_2$

Molecular Weight: 287.526

Melting Point ($^{\circ}C$):

148.5 (Rordorf 1986, 1987, 1989)

Boiling Point ($^{\circ}C$):

398 (calculated, Rordorf 1986, 1987, 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

170.18 (liquid molar volume, Govers et al. 1995)

239.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.4 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

116.2 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.4 (Rordorf 1986, 1987)

30.8, 25.7 (reported exptl., calculated, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

67 (Rordorf 1986, 1987, 1989)

73.04, 61.0 (reported exptl., calculated, Chickos 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S = 56$ J/mol K), F: 0.0614 (mp at $148.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0974 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0997; 0.0974 (supercooled liquid S_L , GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3.60×10^{-5} * (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)

3.63×10^{-4} (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

$\log(P_L/mmHg) = 48.01 - 6714/(T/K) - 12.028 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1.48 (calculated-SOFA model, Govers & Krop 1998)

2.34, 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.19 (calculated-SOFA model, Govers & Krop 1998)

6.31; 6.19 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

5.55 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} :

6.85 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is $1.27 \times 10^6 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987)

$k_{OH}(\text{calc}) = (21\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (17\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (4.5\text{--}5.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.5\text{--}3.3 \text{ d}$ for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); the calculated tropospheric lifetime $\tau = .5\text{--}3.3 \text{ d}$ for the gas phase reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone $k = 1.27 \times 10^6 \text{ L} \cdot \text{g}^{-1} \cdot \text{min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987).

Sediment:

Soil:

Biota:

TABLE 8.1.1.8.1

Reported vapor pressures of 1,3,7-trichlorodibenzo-*p*-dioxin at various temperatures

Rordorf 1987, 1989	
gas saturation-GC/ECD	
$t/^{\circ}\text{C}$	P/Pa
25	3.6×10^{-5}
50	1.4×10^{-3}
75	3.1×10^{-2}
100	0.45
125	4.70
$\Delta H_v/(\text{kJ mol}^{-1}) = 86.4$	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 116.2$	
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 28.4$	

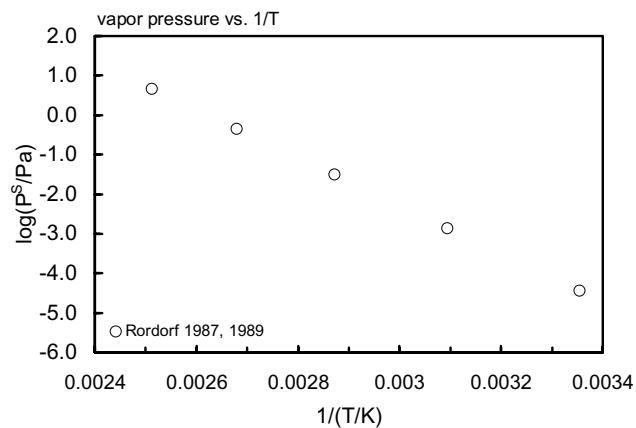
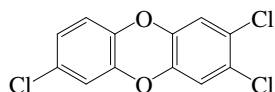


FIGURE 8.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3,7-trichlorodibenzo-*p*-dioxin.

8.1.1.9 2,3,7-Trichlorodibenzo-*p*-dioxin

Common Name: 2,3,7-Trichlorodibenzo-*p*-dioxin

Synonym: 2,3,7-TCDD

Chemical Name: 2,3,7-trichlorodibenzo-*p*-dioxin

CAS Registry No: 33857-28-2

Molecular Formula: $C_{12}H_5Cl_3O_2$, $ClC_6H_3O_2C_6H_2Cl_2$

Molecular Weight: 287.526

Melting Point ($^{\circ}C$):

162–163 (Rordorf 1986, 1987, 1989)

Boiling Point ($^{\circ}C$):

408.4 (calculated, Rordorf 1986, 1987, 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

179.11 (calculated-liquid density, Govers et al. 1990)

239.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.2 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

119.759 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.9 (Rordorf 1986, 1987)

Entropy of Fusion, ΔS_{fus} (J/mol K):

71 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0548 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0674; 0.0548 (supercooled liquid S_L , GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.000012* (calculated, Rordorf 1985a,b, 1986, 1987, 1989)

2.14×10^{-4} (supercooled liquid P_L , GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\log(P_L/mmHg) = 48.21 - 6829/(T/K) - 12.028 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1.78 (calculated-SOFA model, Govers & Krop 1998)

2.04; 1.78 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.33 (calculated-SOFA model, Govers & Krop 1998)

6.46; 6.33 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

6.47 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

9.14*, 9.28 (generator column-GC/ECD, measured range $0-40^{\circ}C$, calculated, Harner et al. 2000)

$\log K_{OA} = -5.35 + 4320/(T/K)$ (generator column-GC/ECD, measured range $0-40^{\circ}C$, Harner et al. 2000)

9.42 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, log BCF:

5.52 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} :

7.05 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolysis rate $k = 2.03 \times 10^{-4} \text{ s}^{-1}$ at 313 nm using a Hanovia 450-W mercury lamp in hexane solution (Dulin et al. 1986)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is $1.27 \times 10^6 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987)

$k_{OH}(\text{calc}) = (21\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (17\text{--}22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, calculated tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ for a tri-chlorinated dioxin with a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (4.5\text{--}5.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.5\text{--}3.3 \text{ d}$ for a tri-chlorinated DD at room temp. (relative rate method, Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.7\text{--}0.9 \text{ d}$ calculated for a tri-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric lifetime $\tau(\text{calc}) = 2.5\text{--}3.3 \text{ d}$ for the gas phase reaction with OH radical. (Kwok et al. 1995).

Surface water:

Groundwater: oxidative degradation rate of water dissolved PCDD by ozone $k = 1.27 \times 10^6 \text{ L g}^{-1} \cdot \text{min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987).

Sediment:

Soil:

Biota:

TABLE 8.1.1.9.1

Reported vapor pressures and octanol-air partition coefficients of 2,3,7-trichlorodibenzo-*p*-dioxin at various temperatures

Vapor pressure		log K_{OA}	
Rordorf 1987, 1989		Harner et al. 2000	
vapor pressure correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	K_{OA}
25	1.2×10^{-5}	0	10.573
50	5.2×10^{-4}	10	9.816
75	1.3×10^{-2}	20	9.313
100	0.21	30	8.935
125	2.3	40	8.497
		25	9.28
$\Delta H_v/(\text{kJ mol}^{-1}) = 87.2$		$\log K_{OA} = a + b/(T/K)$	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 119.76$		a	-5.35
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 30.9$		b	4320
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 82.7$	

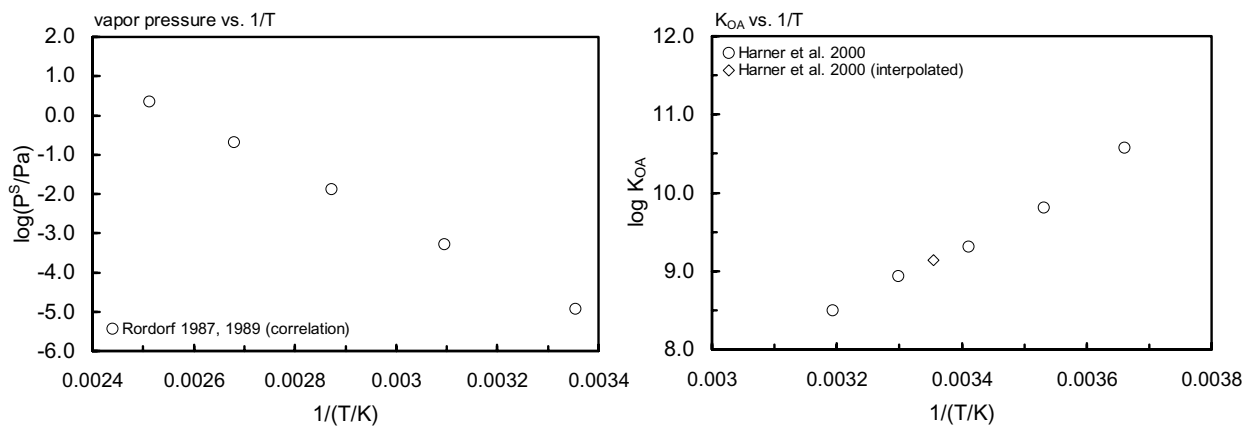
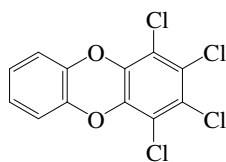


FIGURE 8.1.1.9.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 2,3,7-trichlorodibenzo-*p*-dioxin.

8.1.1.10 1,2,3,4-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4-TCDD

Chemical Name: 1,2,3,4-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 30746-58-8

Molecular Formula: C₁₂H₄O₂Cl₄

Molecular Weight: 321.971

Melting Point (°C):

189 (Pohland & Yang 1972; Rordorf 1986,1987,1989)

Boiling Point (°C):

419 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

186.71 (calculated-liquid density, Govers et al. 1990)

186.10 (liquid molar volume, Govers et al. 1995)

260.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.6 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

118.53 (Rordorf 1987)

111.3 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

31.2 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

68 (Rordorf 1986,1987,1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0246 (mp at 189°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00063*, 0.00047 (generator column-HPLC/UV, generator column-GC/ECD, Shiu et al. 1988)

0.00047* (generator column-GC/ECD, measured range 4–40°C, Doucette & Andren 1988a)

S/(mol/L) = 2.75 × 10⁻¹⁰ exp(0.065·t/°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a); or

log x = -2447/(T/K) - 2.373, temp range 4–40°C (generator column-GC/ECD, Doucette & Andren 1988a)

0.000388 (generator column-GC/MS, Santl et al. 1994)

ln x = -10.5076 - 3984/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

0.0165 (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0000064* (gas saturation-GC, Rordorf 1985a,b, 1986, 1987, 1989)

1.00 × 10⁻⁵ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

1.04 × 10⁻⁴ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)

6.30 × 10⁻⁶ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

6.37 × 10⁻⁴ (corrected supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1998)

2.48 × 10⁻⁶ (solid vapor pressure calculated from reported P_L, Delle Site 1997)

log (P/Pa) = 15.59851 - 6199.79/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

2.75 × 10⁻⁵ (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)

2.26×10^{-5} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

9.66×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56$ J/mol K, Mader & Pankow 2003)

$\log (P_L/\text{mmHg}) = 45.97 - 6777/(T/K) - 11.499 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln (P/\text{Pa}) = 35.917 - 14276/(T/K)$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln (P/\text{Pa}) = (33.217 \pm 0.442) - (13386 \pm 173)/(T/K)$; temp range 378–403 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

3.77 (calculated-P/C, Shiu et al. 1988)

2.02 (gas stripping-GC/MS, Santl et al. 1994)

3.02; 1.35 (quoted exptl., calculated-SOFA model, Govers & Krop 1998)

1.15; 1.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.65, 8.90, 8.96; 8.66, 8.91, 8.97 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)

8.64, 8.91 (HPLC-RT correlation, Sarna et al. 1984)

8.63, 8.02; 8.64, 8.07 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)

7.18, 7.08 (HPLC-RT correlation, Burkhard & Kuehl 1986)

6.20 (generator column-GC/ECD, Doucette & Andren 1987)

6.85 (HPLC-RT correlation, Doucette & Andren 1988b)

6.48 (shake flask/slow stirring method-GC/ECD, mixture from fly-ash extract, Sijm et al. 1989a)

7.18 (recommended, Sangster 1993)

7.18 (recommended, Hansch et al. 1995)

7.04 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

9.410 (calculated- K_{ow}/K_{aw} , Paterson et al. 1991)

9.70*; 9.86 (generator column-GC; calculated, Harner et al. 2000)

$\log K_{OA} = -4.96 + 4370/(T/K)$; temp range 10–40°C (Harner et al. 2000)

9.64 (GC-retention time indices, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

2.20, 3.40 (guppy, in whole fish, in lipid, Gobas et al. 1987)

2.90, 4.02 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990)

5.52 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

7.88 (sediment/water., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Photolysis: solution photolysis $t_{1/2} = 1294$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 560$ min on a clean glass surface under the same conditions (Nestrick et al. 1980)

sunlight induced photolysis $t_{1/2} = 380$ min in isooctane solution and sunlight induced solid phase $t_{1/2} = 65$ h of TCDD dispersed as solid films (Buser 1988);

photodegradation $t_{1/2} = 88$ h for 1,2,3,4-TCDD adsorbed to clean silica gels in a rotary photo-reactor by filtered <290 nm of light (Koester & Hites 1992);

first-order photodegradation $k = 0.98$ h⁻¹ with $t_{1/2} = 0.71$ h when loaded on TiO₂ film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is 4.73×10^5 L g⁻¹ min⁻¹ under alkaline condition at pH 10 and 20°C (Palaschek & Scholz 1987)

$k_{OH}(\text{calc}) = (16 - 19) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0 \text{ d}$ based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ at room temp. (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.0 - 5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2 \text{ d}$ for a tri-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

$k_{\text{OH}}^* = 8.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 306 – 366 K (Brubaker & Hites 1997)

$k_{\text{OH}}(\text{calc}) = 8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Brubaker & Hites 1998)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.016 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986)

$k_1 = 953 \text{ d}^{-1}$; $k_2 = 1.20 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

$k_1 = 35 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 > 0.23 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, $104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.802.0 \text{ d}$ calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

calculated tropospheric lifetime $\tau = 2.8\text{--}7.2 \text{ d}$ for the gas phase reaction with OH radical (Kwok et al. 1995);

first-order photodegradation $k = 0.98 \text{ h}^{-1}$ with $t_{1/2} = 0.71 \text{ h}$ when loaded on TiO_2 film under UV ($\lambda > 300 \text{ nm}$) or solar light irradiation in the air (Choi et al. 2000).

Surface water: sunlight induced photolysis $t_{1/2} = 380 \text{ min}$ in isooctane min and $t_{1/2} = 65 \text{ h}$ dispersed as solid films (Buser 1988).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ (estimated, Suzuki et al. 2000).

Biota: mean $t_{1/2} \sim 43 \text{ d}$ in rainbow trout (Niimi 1986);

biological $t_{1/2} = 43 \text{ d}$ in rainbow trout (Niimi & Oliver 1986);

biological $t_{1/2} = 5\text{--}14 \text{ d}$ in trout (Niimi 1987);

$t_{1/2} < 0.3 \text{ d}$ for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993)

TABLE 8.1.1.10.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4-tetrachlorodibenzo-p-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Shiu et al. 1988		Doucette & Andren 1988		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/UV		generator column-GC/ECD		gas saturation-GC/ECD		generator column-GC/ECD	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	log K_{OA}
5	0.00034	4	0.00011	25	6.4×10^{-6}	0	11.131
15	0.00045	25	0.00047	50	2.6×10^{-4}	10	10.400
25	0.00063	40	0.00117	75	6.2×10^{-3}	20	9.896
35	0.00114			100	9.2×10^{-2}	30	9.455
45	0.002085			125	1.1	40	9.057
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 46.8$				25	9.70
		4–40 $^{\circ}\text{C}$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 85.6$			
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 33.36$				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 118.53$		log $K_{\text{OA}} = a + b/(T/\text{K})$	
5–45 $^{\circ}\text{C}$				$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 31.2$		a	–4.96
				$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 68$		b	4370
						enthalpy of phase change	
						$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 83.60$	

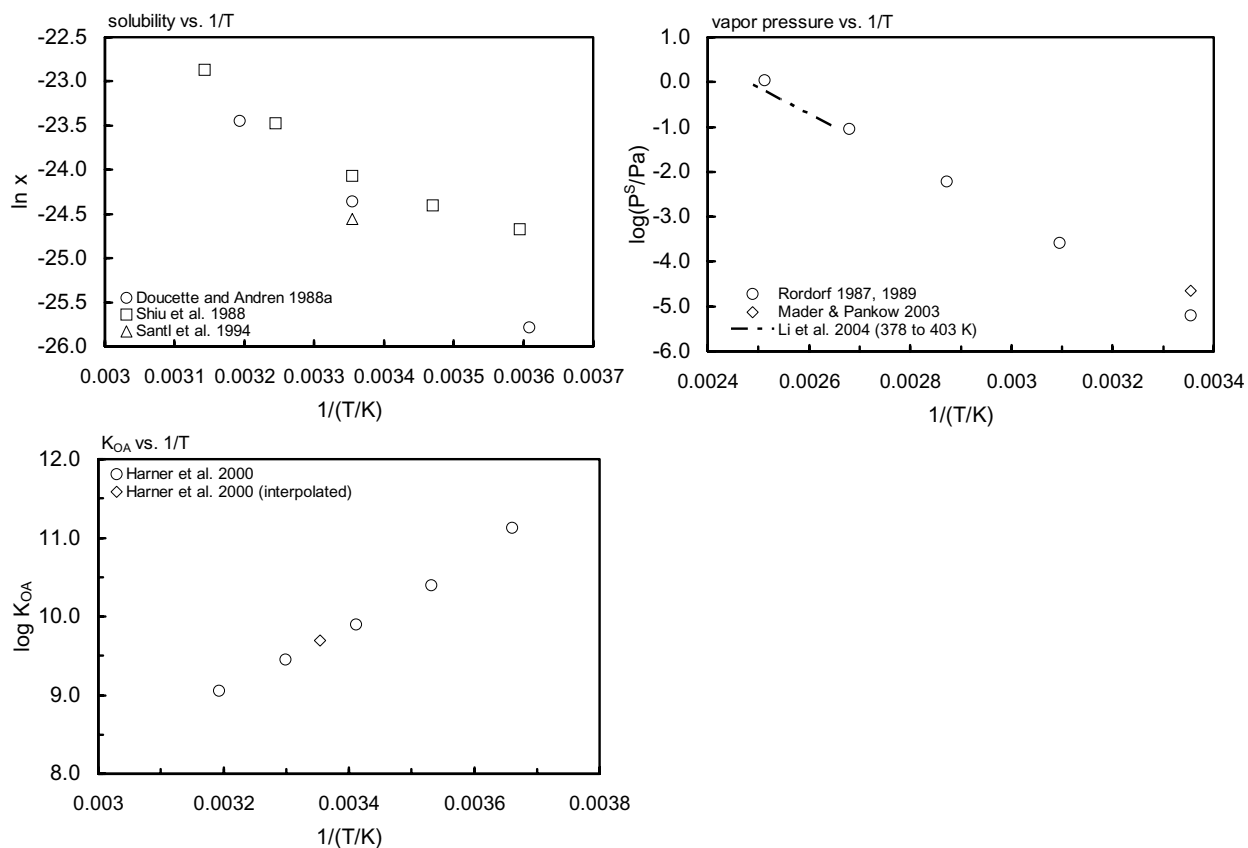
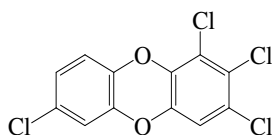


FIGURE 8.1.1.10.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4-tetrachlorodibenzo-*p*-dioxin.

8.1.1.11 1,2,3,7-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,7-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,7-TCDD

Chemical Name: 1,2,3,7-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 67028-18-6

Molecular Formula: $\text{ClC}_6\text{H}_3\text{O}_2\text{C}_6\text{HCl}_3$

Molecular Weight: 321.971

Melting Point (°C):

172–175 (Friesen et al. 1985)

Boiling Point (°C):

438.3 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

186.52 (calculated-liquid density, Govers et al. 1990)

260.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

90.9 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

129.41 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

25.31 (Friesen & Webster 1990)

Entropy of Fusion, ΔS_{fus} (J/mol K):

82 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S = 56$ J/mol K), F: 0.0361 (mp at 172°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00042* (20°C, ¹⁴C labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)

0.00043* (20°C, generator column-HPLC/LSC, measured range 20–40°C, Webster et al. 1985)

0.00028 (20°C, ¹⁴C labeled, generator column-HPLC/LSC, Webster et al. 1986)

0.00048* (21°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)

0.0161; 0.0131 (supercooled liquid S_L , GC-RI correlation, method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.0×10^{-6} * (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1986,1989)

7.0×10^{-6} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

5.0×10^{-6} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

2.69×10^{-5} (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

$\log (P_L/\text{mmHg}) = 46.64 - 6978/(T/K) - 11.503 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant (Pa m³/mol at 25°C):

0.77 (calculated-P/C, Shiu et al. 1988)

1.78 (calculated-SOFA model, Govers & Krop 1998)

1.15; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow} :

- 8.19, 8.59, 8.81; 8.22, 8.60, 8.81 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 8.18, 8.60 (HPLC-RT correlation, Sarna et al. 1984)
 8.15, 7.58; 8.19, 7.72 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 6.91 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 6.48 (shake flask/slow stirring method-GC/ECD, mixture from fly-ash extract, Sijm et al. 1989a)
 8.22 (recommended, Sangster 1993)
 8.22 (recommended, Hansch et al. 1995)
 7.05 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

- 3.17 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
 3.44 (fathead minnow, steady-state, wet weight, Muir et al. 1985)
 3.44, 4.44 (fathead minnow, wet wt. based, lipid based, Gobas & Schrap 1990)
 3.17, 4.17 (rainbow trout, wet wt. based, lipid based, Gobas & Schrap 1990)
 3.18, 2.90 (rainbow trout, Opperhuizen & Sijm 1990)
 3.30, 3.38 (fathead minnow, Opperhuizen & Sijm 1990)
 3.09, 3.02–3.14; 3.35, 3.30–3.37 (rainbow trout, range; fathead minnow, range, De Voogt et al. 1990)
 5.50 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 4.26 (DOC, Muir et al. 1985)
 5.39, 5.45, 5.59 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986)
 5.98, 5.97, 5.91 (20, 30, 40°C, humic acid from peat bog, Webster et al. 1986)
 6.55, 6.32, 6.44 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986)
 7.87 (sediment/water., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 563$ min for solution photolysis in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and
 $t_{1/2} = 156$ min for surface photolysis on a clean soft glass surface under the same conditions (Nestrick et al. 1980);

first order $k = 18.13 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 10.69$ h in water-acetonitrile (2:3 v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 33.52 \times 10^2 \text{ d}^{-1}$ with direct sunlight photolysis $t_{1/2} = 2.08$ d in spring, $k = 39.41 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 1.77$ d in summer, $k = 21.77 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 3.20$ d in autumn, $k = 12.86 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 8.73$ d in winter, in aquatic bodies at latitude 40°N and $t_{1/2} = 8.73$ d averaged over full year (Choudhary & Webster 1986, 1989).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is $4.73 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{OH}(\text{calc}) = (16\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime of 0.8–2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.0\text{--}5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 2.8–7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation: rate constant $k = 0.096 \text{ d}^{-1}$ for rainbow trout (Sijm et al. 1990).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 317 \text{ d}^{-1}$; $k_2 = 0.26 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_1 = 529 \text{ d}^{-1}$; $k_2 = 0.25 \text{ d}^{-1}$ (fathead minnow, flow-through system, Muir et al. 1985)
 $k_2 = 0.178, 0.163 \text{ d}^{-1}$ (rainbow trout, fathead minnow exposed to dioxins in their diets, Muir & Yarechewski 1988; quoted, Opperhuizen & Sijm 1990; Sijm et al. 1990)
 $k_1 = 420 \text{ to } 213 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.278 \text{ to } 0.250 \text{ d}^{-1}$ (rainbow trout exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
 $k_1 = 650 \text{ to } 408 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.322 \text{ to } 0.170 \text{ d}^{-1}$ (fathead minnow exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
 $k_2 = 9.5 \times 10^{-2}, 19.1 \times 10^{-2} \text{ d}^{-1}$ (metabolic inhibitor PBO-treated rainbow trout, control fish, 2–21 d exposure: Sijm et al. 1990)
 $k_1 = 35 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 > 0.23 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish after 120-h exposure, Sijm et al. 1993)
 $k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radical to be 0.8–2.0 d (Atkinson 1991); calculated tropospheric lifetime was 2.8–7.2 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water: direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 2.08 \text{ d}$ in spring, $t_{1/2} = 1.77 \text{ d}$ in summer, $t_{1/2} = 3.20 \text{ d}$ in fall, $t_{1/2} = 5.42 \text{ d}$ in winter, and $t_{1/2} = 8.73 \text{ d}$ averaged over a full year (Choudhary & Webster 1986);

$t_{1/2} = 10.69 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude: $t_{1/2} = 2.1 \text{ d}$ in spring, $t_{1/2} = 1.8 \text{ d}$ in summer, $t_{1/2} = 3.2 \text{ d}$ in fall and $t_{1/2} = 5.4 \text{ d}$ in winter (Choudhary & Webster 1986).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ (estimated, Suzuki et al. 2000).

Biota: elimination $t_{1/2} = 2.7 \text{ d}$ (Adams et al. 1986);

$t_{1/2} = 4 \text{ d}$ in whole body of rainbow trout (Muir & Yarechewski 1988);

$t_{1/2} < 0.3 \text{ d}$ for PBO treated gold fish in 120-h exposure studies (Sijm et al. 1993).

TABLE 8.1.1.11.1

Reported aqueous solubilities and vapor pressures of 1,2,3,7-tetrachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility						Vapor pressure	
Webster et al. 1985		Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989	
generator column-HPLC/LSC		generator column-GC/ECD		gen. col.-HPLC/LSC		vapor pressure correlation	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa
20	4.30×10^{-4}	20	4.30×10^{-4}	7.0	2.43×10^{-4}	25	1.0×10^{-6}
40	1.27×10^{-3}	40	1.27×10^{-3}	11.5	2.61×10^{-4}	50	5.9×10^{-5}
				17	4.03×10^{-4}	75	1.9×10^{-3}
				21	4.80×10^{-4}	100	3.7×10^{-2}
				26	7.28×10^{-4}	125	0.57
				41	1.39×10^{-3}		
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 50.68$						$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 90.9$	
25 °C						$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 129.41$	
						$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 36.6$	
						$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 82$	

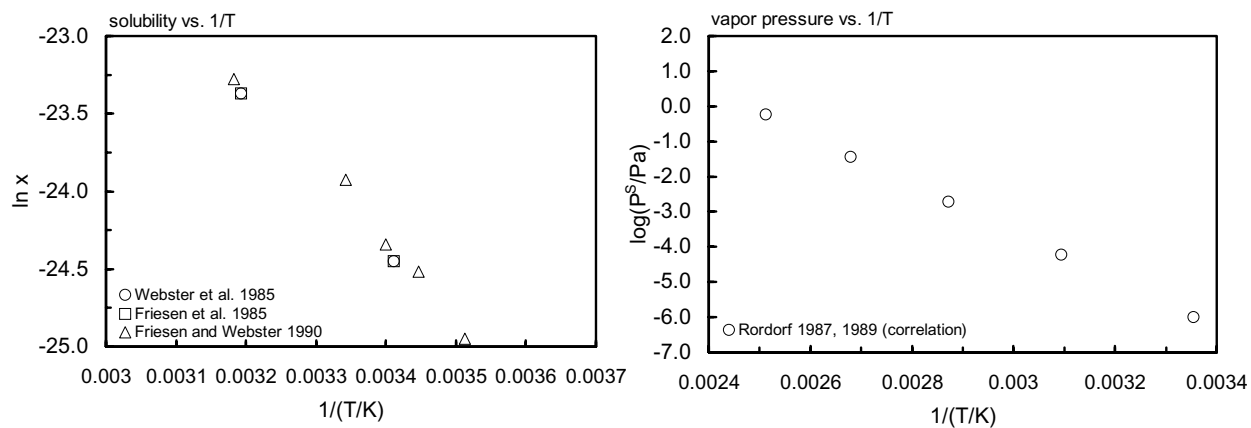
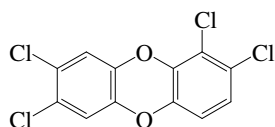


FIGURE 8.1.1.11.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,2,3,7-tetrachlorodibenzo-*p*-dioxin.

8.1.1.12 1,2,7,8-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,2,7,8-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,2,7,8-TCDD

Chemical Name: 1,2,7,8-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 34816-53-0

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

Melting Point ($^{\circ}\text{C}$):

Boiling Point ($^{\circ}\text{C}$):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

186.88 (calculated-liquid density, Govers et al. 1990)

260.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.00908 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

00223, 0.00908 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):

4.37×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

4.17×10^{-5} ; 4.37×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\log(P_L/\text{mmHg}) = 46.50 - 6956/(T/\text{K}) - 11.503 \cdot \log(T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1.48 (calculated-SOFA model, Govers & Krop 1998)

1.29; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

6.38 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989a)

6.99 (calculated-SOFA model, Govers & Krop 1998)

6.93; 6.99 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.35, 6.30, 6.30, 6.44 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

5.51 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

7.99 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: solution photolysis $t_{1/2} = 491$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 350$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate of water dissolved PCDD by ozone) is $4.73 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palaushek & Scholz 1987)

$k_{OH}(\text{calc}) = 7.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.0\text{--}5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 38 \text{ L kg}^{-1} \text{ d}^{-1}$; $49 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 > 0.9 \text{ d}^{-1}$; $> 0.3 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, $104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8\text{--}2.0$ d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991);

tropospheric lifetime $\tau(\text{calc}) = 2.8\text{--}7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

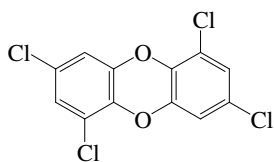
Surface water:

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100$ yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} < 0.7$ d for PBO treated and $t_{1/2} < 2.1$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.13 1,3,6,8-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,3,6,8-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,3,6,8-TCDD

Chemical Name: 1,3,6,8-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 33423-92-6

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

Melting Point ($^{\circ}\text{C}$):

219–219.5 (Pohland & Yang 1972; Rordorf 1987,1989; Delle Site 1997)

Boiling Point ($^{\circ}\text{C}$):

438.3 (calculated, Rordorf 1987, 1989)

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

192.34 (calculated-liquid density, Govers et al. 1990)

260.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.5 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

125.793 (Rordorf 1987)

118.6 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

74 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S = 56 \text{ J}/\text{mol K}$), F: 0.0125 (mp at 219°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00032* (20°C , ^{14}C -labeled, generator column-HPLC/LSC, measured range 20 – 40°C , Webster et al. 1985)

0.000317* (20°C , ^{14}C -labeled, generator column-HPLC/LSC, measured range 20 – 40°C , Friesen et al. 1985)

0.000283, 0.000326, 0.000366, 0.000328 (^{14}C -labeled/LSC, Milli-Q treated water, lake water, simulated lake water, Milli-Q water, Servos & Muir 1989a)

0.0322 (supercooled liquid S_L , GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.000537* (20°C , gas saturation, measured range 20 – 100°C , Webster et al. 1985)

7.0×10^{-7} * (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1986,1987,1989)

6.76×10^{-5} (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)

$\log (P_L/\text{mmHg}) = 46.99 - 6976/(T/K) - 11.503 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln (P/\text{Pa}) = 36.564 - 15127/(T/K)$, temp range 298 – 398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln (P/\text{Pa}) = (35.818 \pm 0.968) - (14262 \pm 380)/(T/K)$, temp range 378 – 408 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

6.90 (23°C , batch stripping, Webster et al. 1985)

3.77 (calculated-P/C, Shiu et al. 1988)

1.15 (calculated-SOFA model, Govers & Krop 1998)

1.48; 1.15 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow} :

8.72, 9.00, 9.42; 8.72, 9.02, 9.43 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 8.70, 9.02 (HPLC-RT correlation, Sarna et al. 1984)
 8.70, 8.08; 8.70, 8.12 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 7.20, 7.13 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 7.13 (corrected HPLC-RT value, Burkhard & Kuehl 1986)
 6.29 (shake flask/slow stirring method-GC/MS, Sijm et al. 1989a)
 7.18 (recommended, Sangster 1993)
 6.29 (recommended, Hansch et al. 1995)
 6.79 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

3.03, 2.67 (fathead minnow, rainbow trout, Corbet et al. 1983, 1988)
 3.39 (rainbow trout, steady-state, wet weight basis, Muir et al. 1985)
 3.83 (fathead minnow, steady-state, wet weight basis, Muir et al. 1985)
 3.39, 3.83 (rainbow trout average, fathead minnow average, Muir et al. 1986)
 3.39, 3.32, 3.57 (*Oncorhynchus mykiss*, Servos et al. 1989)
 1.08–3.75, 2.14, 1.76–1.93 (Amphipod in lake water, in simulated lake water, in water with Aldrich humic acid, Servos & Muir 1989a)
 4.20, 4.20 (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)
 5.00 (goldfish after 6 d exposure: metabolic inhibitor PBO-treated, Sijm et al. 1989b)
 3.76, 3.54–3.90; 3.32, 3.23–3.40 (fathead minnow, range; rainbow trout, range, De Voogt et al. 1990)
 3.83, 4.83 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 3.39, 4.39 (rainbow trout, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 3.46, 3.30, 3.15 (quoted, rainbow trout exposed to different concentrations, Opperhuizen & Sijm 1990)
 3.76, 3.75 (fathead minnow exposed to different concentrations, quoted, Opperhuizen & Sijm 1990)
 3.70 (10.1 ng/L for 0–10 d, predicted for biota held in lake enclosures, Servos et al. 1992b)
 3.12 (17.7 ng/L for 0–10 d, invertebrates, Servos et al. 1992b)
 3.20 (21.4 ng/L for 0–10 d, unionid clams & white suckers gill, Servos et al. 1992b)
 2.36 (3.1 ng/L for 0–10 d, white suckers carcass, Servos et al. 1992b)
 3.21 (1.6 ng/L for 14–24 d, invertebrates, Servos et al. 1992b)
 2.95 (0.9 ng/L for 14–24 d, unionid clams, Servos et al. 1992b)
 3.32 (2.1 ng/L for 14–24 d, white suckers gill, Servos et al. 1992b)
 2.70 (1.0 ng/L for 14–24 d, white suckers carcass, Servos et al. 1992b)
 4.54 (3.5 ng/L for 0–104 d, white suckers gill, Servos et al. 1992b)
 4.26 (1.8 ng/L for 0–104 d, white suckers carcass, Servos et al. 1992b)
 3.13 (gold fish, PBO-treated, 120-h exposure, Sijm et al. 1993)
 5.53 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} :

4.36 (DOC, De Voogt et al. 1990)
 6.74 (calculated- K_{ow} , Corbet et al. 1988)
 2.11–3.75, 2.39, 2.05–2.38 (DOC partition coeff., lake water, simulated lake water, Aldrich humic acid, Servos & Muir 1989a)
 5.98–6.23 (sediment, Servos & Muir 1989b)
 7.50 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 6.23 (derived from soot-water distribution coeff., Barring et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Volatilization: 3.9 d in water of 0.5 m depth in a small pond (Corbet et al. 1988)

Photolysis: solution photolysis $t_{1/2} = 507$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis on a clean glass surface under the same conditions with $t_{1/2} = 264$ min (Nestrick et al. 1980; quoted, Muto et al. 1991);

first-order $k = 59.57 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 0.35$ d in spring, $t_{1/2} = 0.31$ d in summer, $t_{1/2} = 0.53$ d in fall, $t_{1/2} = 0.84$ d in winter and $t_{1/2} = 1.47$ d averaged over full year (Choudhary & Webster 1986; quoted, Muto et al. 1991)

$t_{1/2} = 14.0$ – 28.5 h in outdoor pool and $t_{1/2} = 6.3$ – 8.0 d in natural water in a Pyrex flask under sunlight (Corbet et al. 1988)

$t_{1/2} = 25$ h in water column (Corbet et al. 1983)

$t_{1/2} = 6.3$ – 8.0 d for natural water under sunlight and photodegradation $t_{1/2} = 0.3$ d in summer sunlight at 40°N and $t_{1/2} = 7$ d in a 1-L flask (Corbet et al. 1988)

photolysis $k = 59.57 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 3.24$ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 198.13 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 0.35$ d in spring, $k = 226.99 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 0.31$ d in summer, $k = 130.91 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 0.53$ d in fall, $k = 82.85 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 0.84$ d in winter; while experimentally determined sunlight photolysis $t_{1/2} = 3.5$ d for ^{14}C labeled 1,3,6,8-TCDD in pond water (Choudhary & Webster 1989)

$t_{1/2} = 78.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation may be an important path of transformation (Corbet et al. 1988)

k (oxidative degradation rate of water dissolved PCDD by ozone) is $3.21 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = (16\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (7.6\text{--}19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8$ – 2.0 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.0\text{--}5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8$ – 7.2 d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 184 \text{ d}^{-1}$; $k_2 = 0.10 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_1 = 574 \text{ d}^{-1}$; $k_2 = 0.10 \text{ d}^{-1}$ (fathead minnow, Muir et al. 1985; quoted, Adams et al. 1986)

$k_1 = 225, 221, 106 \text{ d}^{-1}$ (rainbow trout fry, exposed to concn of 4, 74, 211 ng/L, 5-d uptake study, Muir et al. 1986)

$k_2 = 0.074, 0.110, 0.111 \text{ d}^{-1}$ (rainbow trout fry, exposed to 4, 74, 211 ng/L, 24 to 48-d depuration study, Muir et al. 1986)

$k_1 = 526, 621 \text{ d}^{-1}$ (fathead minnow, exposed to concn of 10, 41 ng/L, 5-d uptake study, Muir et al. 1986)

$k_2 = 0.08, 0.122 \text{ d}^{-1}$ (fathead minnow, exposed to concn of 10, 41 ng/L, 24 to 48-d depuration study, Muir et al. 1986)

$k_1 = 225, 97 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)

$k_2 = 0.211 \text{ d}^{-1}$ (fathead minnow, calculated, Corbet et al. 1983; quoted, Opperhuizen & Sijm 1990)

$k_2 = 0.158 \text{ d}^{-1}$ (rainbow trout, calculated, Corbet et al. 1983; quoted, Opperhuizen & Sijm 1990)

$k_1 = 225, 221, 106 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.074, 0.110, 0.110 \text{ d}^{-1}$ (rainbow trout exposed to different concentrations in a flow system, quoted, Opperhuizen & Sijm 1990)

$k_1 = 526, 621 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.080, 0.122 \text{ d}^{-1}$ (fathead minnow exposed to different concentrations in a flow system, quoted, Opperhuizen & Sijm 1990)

$k_1 = 1200 \text{ d}^{-1}$; $k_2 = 0.06 \text{ d}^{-1}$ (filter-feeder, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

$k_1 = 285 \text{ d}^{-1}$; $k_2 = 0.12 \text{ d}^{-1}$ (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

$k_1 = 142, 116 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.14, > 0.24 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8\text{--}2.0 \text{ d}$ calculated for a tetra-chlorinated dioxin based on the gas-phase reaction rate with OH radicals (Atkinson 1991);

calculated tropospheric lifetime $\tau = 2.8\text{--}7.2 \text{ d}$ for with OH radical (Kwok et al. 1995).

Surface water: direct sunlight photolysis in aquatic bodies at latitude 40°N for various seasons with half-lives: 0.35 d in spring, 0.31 d in summer, 0.53 d in fall, 0.84 d in winter and 1.47 d averaged over full year (Choudhary & Webster 1986);

$t_{1/2} = 14.0\text{--}28.5 \text{ h}$ for outdoor pool and $t_{1/2} = 6.3\text{--}8.0 \text{ d}$ for natural water in a Pyrex flask under sunlight (Corbet et al. 1988);

$t_{1/2} = 3.24 \text{ h}$ for photolysis in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude calculated to be: $t_{1/2} = 0.35 \text{ d}$ in spring, $t_{1/2} = 0.31 \text{ d}$ in summer, $t_{1/2} = 0.53 \text{ d}$ in fall, and $t_{1/2} = 0.84 \text{ d}$ in winter (Choudhary & Webster 1989);

calculated transformation rate constant in simulated lake enclosure of $9.4 \times 10^{-2} \text{ h}^{-1}$ (Servos et al. 1992a).

Groundwater:

Sediment: $t_{1/2} = 51.2\text{--}69.2 \text{ d}$ (Corbet et al. 1988);

calculated $t_{1/2} = 10 \text{ yr}$ with a transformation rate constant $k = 7.9 \times 10^{-6} \text{ h}^{-1}$ (Servos et al. 1992a);

degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ (estimated, Suzuki et al. 2000).

Biota: $t_{1/2} = 4 \text{ d}$ in rainbow trout (Neely 1979; quoted, Niimi & Oliver, 1983,1986);

$t_{1/2} = 4 \text{ d}$ in rainbow trout (Corbet et al. 1983; quoted, Niimi & Oliver 1986);

$t_{1/2} = 2 \text{ d}$ in rainbow trout (Muir et al. 1984);

$t_{1/2} = 6\text{--}9 \text{ d}$ for both rainbow trout fry and fathead minnow (Muir et al. 1986);

$t_{1/2} = 6.90 \text{ d}$ in fathead minnow (Adams et al. 1986);

$t_{1/2} = 41 \text{ to } 44 \text{ d}$ in rooted vegetable (Corbet et al. 1988);

$t_{1/2} = 15 \text{ d}$ in whole body of rainbow trout (Muir et al. 1990);

half-lives in gold fish: $t_{1/2} = 4.8 \text{ d}$ for PBO treated and $t_{1/2} < 0.3 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993)

TABLE 8.1.1.13.1

Reported aqueous solubilities and vapor pressures of 1,3,6,8-tetrachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure			
Webster et al. 1985		Friesen et al. 1985		Webster et al. 1985		Rordorf 1987, 1989	
generator column-HPLC/LSC		generator column-GC/ECD		gas saturation-GC		vapor pressure correlation	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
20	3.20×10^{-4}	20	3.20×10^{-4}	20	5.37×10^{-4}	25	7.0×10^{-7}
40	3.90×10^{-3}	40	3.90×10^{-3}	50	1.32×10^{-3}	50	3.6×10^{-5}
				100	1.12×10^{-2}	75	1.0×10^{-3}
						100	1.9×10^{-2}
						125	0.24
				$\Delta H_v/(\text{kJ mol}^{-1}) = 86.5$			
				$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 125.794$			
				$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 36.6$			
				$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 74$			

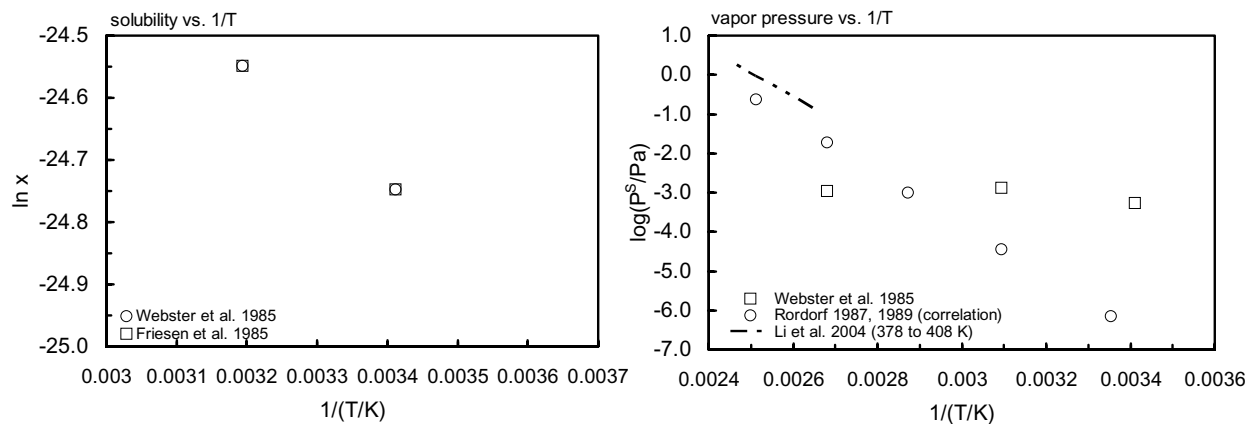
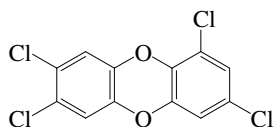


FIGURE 8.1.1.13.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 1,3,6,8-tetrachlorodibenzo-*p*-dioxin.

8.1.1.14 1,3,7,8-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,3,7,8-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,3,7,8-TCDD

Chemical Name: 1,3,7,8-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 50585-46-1

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

Melting Point ($^{\circ}\text{C}$):

193.5–195 (Rordorf 1986, 1987, 1989)

Boiling Point ($^{\circ}\text{C}$):

438.3 (calculated, Rordorf 1986, 1987, 1989)

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

188.33 (calculated-liquid density, Govers et al. 1990)

260.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.9 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

127.77 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1987)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

78 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0203 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

00223, 0.0203 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

8.4×10^{-7} , 4.5×10^{-5} , 1.4×10^{-3} , 2.6×10^{-2} , 0.35 (25, 50, 75, 100, 125°C , predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

8.32×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

4.17×10^{-5} ; 8.32×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\log(P_L/\text{mmHg}) = 46.80 - 6977/(T/\text{K}) - 11.503 \cdot \log(T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1.26 (calculated-SOFA model, Govers & Krop 1998)

1.29; 1.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

6.80 (calculated-SOFA model, Govers & Krop 1998)

6.93; 6.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.30; 6.29, 6.28, 6.40, 6.44 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

5.52 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

7.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: solution photolysis $t_{1/2} = 153$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 160$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

$t_{1/2} = 86.6$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 13 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.0 - 5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d at for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 57 \text{ L kg}^{-1} \text{ d}^{-1}$; $99 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.14 \text{ d}^{-1}$; $> 0.24 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, $104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8\text{--}2.0$ d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

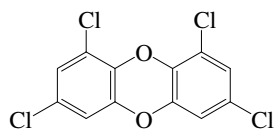
Surface water:

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100$ yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 2.1$ d for PBO treated and $t_{1/2} < 0.4$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.15 1,3,7,9-Tetrachlorodibenzo-*p*-dioxin

Common Name: 1,3,7,9-Tetrachlorodibenzo-*p*-dioxin

Synonym: 1,3,7,9-TCDD

Chemical Name: 1,3,7,9-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 62470-53-5

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

Melting Point ($^{\circ}\text{C}$):

Boiling Point ($^{\circ}\text{C}$):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

192.34 (calculated-liquid density, Govers et al. 1990)

260.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

123.6 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F:

Water Solubility (g/m^3 or mg/L at 25°C):

0.0294 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

00294, 0.0294 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

5.50×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

5.89×10^{-5} ; 5.50×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\log(P_L/\text{mmHg}) = 46.86 - 6956/(T/\text{K}) - 11.503 \cdot \log(T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/\text{Pa}) = (37.221 \pm 0.469) - (14864 \pm 185)/(T/\text{K})$; temp range 383–408 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.589 (calculated-SOFA model, Govers & Krop 1998)

1.42; 0.589 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.39 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)

6.68 (calculated-SOFA model, Govers & Krop 1998)

6.83; 6.68 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.28, 6.12, 6.47, 6.44 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

5.67 (lipid wt. base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

7.51 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: solution photolysis $t_{1/2} = 499$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 169$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984)

$t_{1/2} = 79.7$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (16 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.0\text{--}5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 54 \text{ L kg}^{-1} \text{ d}^{-1}$, $98 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1 \text{ d}^{-1}$, $> 2.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish; control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}$, $104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 0.8\text{--}2.0$ d calculated for a tetra-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

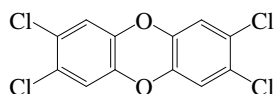
Surface water:

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100$ yr (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} > 7$ d for PBO treated and $t_{1/2} < 0.3$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.16 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin

Common Name: 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin

Synonym: 2,3,6,7-tetrachlorodibenzo-*p*-dioxin, TCDD, TCDBD, 2,3,6,7- TCDD, 2,3,7,8-TCDD, dioxin

Chemical Name: 2,3,7,8-tetrachlorodibenzo-*p*-dioxin

CAS Registry No: 1746-01-6

Molecular Formula: $\text{Cl}_2\text{C}_6\text{H}_2\text{O}_2\text{C}_6\text{H}_2\text{Cl}_2$

Molecular Weight: 321.971

Melting Point (°C):

295 (Lide 2003)

Boiling Point (°C):

421.2 (Schroy et al. 1985a)

Density (g/cm³ at 20°C):

1.827 (solid at 25°C, Boer et al. 1972; Schroy et al. 1985a)

1.021 (liquid at normal boiling point, Schroy et al. 1985a)

Molar Volume (cm³/mol):

184.32, 184.97 (calculated-liquid density, crystalline volume, Govers et al. 1990)

188.34 (liquid molar volume, Govers et al. 1990)

260.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

71.71 (at normal bp, Schroy et al. 1985a)

79.9 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

123.91 (Schroy et al. 1985b)

124.001 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

38.91 (Boer et al. 1972; Schroy et al. 1985a,b; Ruelle & Kesselring 1997)

38.9, 36.6 (Obs., predicted, Rordorf 1986, 1987)

Entropy of Fusion, ΔS_{fus} (J/mol K):

69 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.00244 (mp at 295°C)

0.0017 (Shiu et al. 1988)

4.07×10^{-4} (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):

0.0002 (shake flask-GC/ECD, Crummett & Stehl 1973)

3.17×10^{-4} (¹⁴C-labeled, generator column-HPLC/LSC, Webster et al. 1983)

1.93×10^{-5} (shake flask-GC/MS, Marple et al. 1986a)

7.91×10^{-6} (¹⁴C-labeled, Adams & Blaine 1986)

1.29×10^{-5} , 4.83×10^{-4} (4.3, 17.3°C, generator column-GC/MS, Lodge 1989)

$\log [S_L/(\text{mol/L})] = 0.190 - 2089/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

0.0158 (supercooled liquid S_L , GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.0×10^{-7} (¹⁴C-gas saturation method, Jaber & Podoll 1983)

$(4.50 \pm 2) \times 10^{-6}$ (gas saturation-GC, Rordorf 1985a)

$(3.5-6.3) \times 10^{-6}$, $(1.3-3.1) \times 10^{-4}$, $(2.8-8.9) \times 10^{-2}$, $(3.9-15.9) \times 10^{-2}$, $(4.4-21.9) \times 10^{-1}$ (25, 50, 75, 100, 125°C, predicted using estimated ΔH_{sub} and ΔS_{sub} for tetra-chloro isomers, Rordorf 1985a)

$4.61 \times 10^{-7*}$ (30.1°C, gas saturation-GC/MS, measured range 30.1–71.1°C Schroy et al. 1985a,b)

$\log (P/\text{mmHg}) = 12.89784 - 6477.132/(273.15 + t/^\circ\text{C})$; temp range 10–305°C (Antoine eq., from gas saturation-GC/MS, Schroy et al. 1985b)

$\log (P/\text{mmHg}) = 8.78307 - 4098.173/(273.15 + t/^{\circ}\text{C})$; temp range 305–420 $^{\circ}\text{C}$ (Antoine eq., from gas saturation-GC/MS, Schroy et al. 1985b)
 $2.02 \times 10^{-7*}$, 4.60×10^{-7} , 9.65×10^{-6} , 4.58×10^{-5} , 1.59×10^{-4} (25, 30, 50, 62, 71 $^{\circ}\text{C}$, results derived from Antoine eq., gas saturation-GC/MS, Schroy et al. 1985b)
 $\ln (P/\text{Pa}) = 34.570834 - [14903.438/(T/\text{K})]$, temp range: 283.15–578.15 K (gas saturation, Schroy et al. 1985a)
 $\ln (P/\text{Pa}) = 25.104351 - 93430.391/(T/\text{K})$, temp range: 578.15–703.15 K (gas saturation, Schroy et al. 1985a)
 $8.71 \times 10^{-6*}$ (20 $^{\circ}\text{C}$, gas saturation-LSC, measured range 20–100 $^{\circ}\text{C}$, Webster et al. 1985)
 9.87×10^{-8} (^{14}C -gas saturation, Podoll et al. 1986)
 8.14×10^{-8} , 6.0×10^{-5} (20 $^{\circ}\text{C}$, quoted: solid P_s , supercooled liquid P_L , Bidleman & Foreman 1987)
 $2.0 \times 10^{-7*}$ (gas saturation-GC, measured range 25–125 $^{\circ}\text{C}$, Rordorf 1987, 1989)
 6.20×10^{-7} , 2.6×10^{-5} , 6.1×10^{-4} , 9.7×10^{-3} , 1.1×10^{-1} (25, 50, 75, 100, 125 $^{\circ}\text{C}$, predicted-vapor pressure correlation method, Rordorf 1987, 1989)
 6.17×10^{-4} ; 2.51×10^{-7} (supercooled liquid P_L ; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)
 $\log (P_s/\text{Pa}) = 12.66 - 5739/(T/\text{K})$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 9.05 - 3663/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)
 1.17×10^{-4} ; 5.75×10^{-5} (supercooled liquid P_L , quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 $\log (P_s/\text{Pa}) = 15.0391 - 6482.7/(T/\text{K})$; temp range 5–50 $^{\circ}\text{C}$ (regression eq. from literature data, Shiu & Ma 2000)
 5.25×10^{-4} (supercooled liquid P_L , Harner et al. 2000)
 2.57×10^{-5} ; 5.75×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
 5.56×10^{-7} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)
 3.35×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$, Mader & Pankow 2003)
 $\log (P_L/\text{mmHg}) = 49.89 - 6705/(T/\text{K}) - 12.569 \cdot \log (T/\text{K})$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$ and reported temperature dependence equations):

0.0021 (calculated-P/C, Mabey et al. 1982)
 0.152 (calculated-P/C, Crosby 1985)
 0.212 (calculated-P/C, Schroy et al. 1985)
 1.64 (calculated-P/C, Podoll et al. 1986)
 1.63, 3.34, 10.34 (calculated-P/C, Shiu et al. 1988)
 7.93 (calculated-P/C, Jury et al. 1990)
 1.62 (calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 8.86 - 1574/(T/\text{K})$ (Passivirta et al. 1999)
 1.12; 1.62 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

5.38 (Crummett & Stehl 1973)
 6.19 (Neely 1979; Veith et al. 1979; Corbet et al. 1983)
 6.15 (Kenaga 1980;)
 8.93 (HPLC-RT correlation, Sarna et al. 1984)
 7.02 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 6.64 (shake flask-GC/MS, Marple et al. 1986b)
 6.42 (shake flask/slow stirring method-GC/MS, Sijm et al. 1989a)
 7.02 (recommended, Sangster 1993)
 6.53 (recommended, Hansch et al. 1995)
 7.06 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25 $^{\circ}\text{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

9.70 (calculated- $K_{\text{OW}}/K_{\text{AW}}$, Wania & Mackay 1996)
 10.05*; 9.91 (generator column-GC; calculated, Harner et al. 2000)
 11.04 (7 $^{\circ}\text{C}$, GC-retention time correlation, Harner et al. 2000)
 $\log K_{\text{OA}} = -6.19 + 4840/(T/\text{K})$; temp range 10–50 $^{\circ}\text{C}$ (generator column-GC/ECD, Harner et al. 2000)
 9.95 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 1.69, 2.34, 2.08 (*daphnia*, ostracod, brine shrimp, ^{14}C -labeled-LSC, Matsumura & Benezet 1973)
 4.30–4.41; 3.6–3.95 (snail, *gambusia*, *daphnids*; duckweed, algae, catfish; Isensee & Jones 1975)
 3.96 (rainbow trout, Branson et al. 1985)
 3.90 (fathead minnow, steady-state, wet weight, Adams et al. 1986)
 3.73, 4.55 (fish: flowing water test, static ecosystem test, Kenaga & Goring 1980, Kenaga 1980)
 3.97 (rainbow trout, Branson et al. 1983)
 3.97, 3.67 (rainbow trout: whole body, muscle, Branson et al. 1985)
 1.38–1.60 (rhesus monkey, Geyer et al. 1986)
 4.11 (guppy, Opperhuizen et al. 1986)
 4.43, 4.59 (rainbow trout: measured average, estimated BCF at steady-state, for 28-d exposure, Mehrle et al. 1988)
 4.30, 5.0 (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989b)
 3.89, 4.59 (fathead minnow, rainbow trout, De Voogt et al. 1990)
 5.80, 5.90 (goldfish after 6 d exposure: PBO-treated, control, Sijm et al. 1989b)
 4.11, 5.64 (guppy, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 3.97, 4.70; 4.97, 5.70 (rainbow trout, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 4.63, 4.40 (pine needle/air BCF values, Reissinger et al. 1989)
 4.59, 4.58, 4.93, 4.57, 3.97 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
 4.11, 3.90, 3.78 (guppy, fathead minnow, mosquito fish, quoted, Opperhuizen & Sijm 1990)
 2.62 (human, Webster & Connett 1991)
 5.24; 4.91 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 5.24; 4.83; 5.02 (guppies, 21-d exposure, lipid wt basis: measured- $C_{\text{fish}}/C_{\text{W}}$; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 5.24; 5.48 (lipid wt. base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 5.71, 6.71 (fish medaka 10% lipid: BCF_{W} , BCF_{L} , Geyer et al. 2000)
 6.02, 6.05 (fish muscle log BCF_{L} calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 5.67 (organic carbon soil, calculated- K_{OW} , Kenaga 1980)
 6.95, 7.39–7.58 (calculated- K_{OW} , 10 soils from Missouri & New Jersey, Jackson et al. 1985)
 6.22–6.54; 5.96–6.09 (red clay soil from Missouri, Alluvial soil from Missouri, Marple et al. 1986)
 4.83 (hydroxy aluminum-clay, Srinivasan & Fogler 1987)
 6.60 (^{14}C -labeled, soil, batch equilibrium-sorption isotherm, GC/ECD, Walters & Guiseppi-Elie 1988)
 3.06 (soil, Eduljee 1987)
 6.30; 7.59; 7.25 (Lake Ontario sediment; solids; DOC dissolved organic carbon; batch equilibrium-sorption isotherm, Lodge & Cook 1989)
 6.24, 6.10, 5.10 (Eglin Air Force Base soil/water with 0.01% surfactant from Florida at pH 4, 7, 8.5, batch equilibrium-GC, Puri et al. 1989)
 6.50, 5.86, 4.81 (Time Beach soil/water with 0.01% surfactant from Missouri at pH 4, 7, 8.5, Puri et al. 1989)
 5.70, 5.09, 4.76 (Visalia soil/water with 0.01% surfactant from California at pH 4, 7, 8.5, Puri et al. 1989)
 6.44, 6.66 (batch equilibrium-sorption isotherms: 2-d, 10-d isotherm, regression analysis for sorption of uncontaminated Time Beach soil from water, Walters et al. 1989)
 6.14 (soil, Jury et al. 1990)
 6.80 (Baltic sea particulate filed samples, concn distribution-GC/MS, Broman et al. 1991)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: probably not an important process (Callahan et al. 1979)

$t_{1/2} = 20\text{--}200$ d from water column which will be slowed down further by the fact that it is sorbed to the sediment and biota (Mill 1985)

$t_{1/2} \sim 32$ d for ponds and $t_{1/2} \sim 16$ d for rivers (Podoll et al. 1986)

$t_{1/2} = 104$ d from soil by calculation assuming diffusion of TCDD in soil is vapor-dominated up to volumetric water content of $0.3 \text{ m}^3/\text{m}^3$, and then liquid-dominated to saturation (Eduljee 1987)

$t_{1/2} = 190$ d (Thibodeaux & Lipsky 1985; quoted, Eduljee 1987)

$t_{1/2} = 365$ d for volatilization from below surface soil (Jury et al. 1990)

$k = 0.0054 \text{ h}^{-1}$ with $t_{1/2} = 128$ h from grass foliage (McCrary & Maggard 1993)

Photolysis:

stable to sunlight for at least 14 d in distilled water (Crosby et al. 1971; quoted, Dougherty et al. 1991)

$t_{1/2} = 3$ h in methanol solution in sunlight (Plimmer et al. 1973)

$t_{1/2} = 56$ min for vapor in sunlight (Peterson 1976; quoted, Mill 1985)

thin film of TCDD on glass plates showed transformation at about 6 h (Crosby & Wong 1977);

$t_{1/2}(\text{soln}) = 56.8$ min in *n*-hexadecane on a clean soft glass surface at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 140$ h on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984; Dougherty et al. 1991)

TCDD extracted from the aqueous sludge with hexane can be continuously degraded by a mercury arc of UV radiation (Exner et al. 1982; quoted, Crosby 1985)

$t_{1/2} \sim 1$ d in water, $t_{1/2} = 0.1$ d in vapor and $t_{1/2} = 1\text{--}100$ d in soil with $t_{1/2} = 50$ d for a small fraction in water column in equilibrium with sediment sorbed with TCDD (Mill 1985)

$k_p = 6.94 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 27$ h in a 90:10 mixture of distilled water and acetonitrile under summer sunlight; $k_p = 0.15 \text{ d}^{-1}$ with $t_{1/2} = 6$ d in summer sunlight at 40°L surface waters (Dulin et al. 1986)

$t_{1/2} = 81$ h after adjusting for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)

$k = 0.14 \text{ d}^{-1}$ with $t_{1/2} = 118$ h in winter, $k = 0.61 \text{ d}^{-1}$ with $t_{1/2} = 27$ h in spring, $k = 0.78 \text{ d}^{-1}$ with $t_{1/2} = 21$ h in summer, and $k = 0.32 \text{ d}^{-1}$ with $t_{1/2} = 51$ h in autumn for aqueous dissolved TCDD in sunlight over four seasons at 40°N latitude (Podoll et al. 1986)

photodegradation $t_{1/2} = 10$ min, a very rapid process at soil surface during the day (Facchetti et al. 1986)

$t_{1/2} = 14$ min sunlight induced photolysis in isooctane solution and sunlight induced solid phase $t_{1/2} = 300$ h dispersed as solid films (Buser 1988)

$k = 5.9 \times 10^{-3} \text{ s}^{-1}$ rate constant for photolysis in air at 150–350°C (Orth et al. 1989)

$k = 0.15 \text{ min}^{-1}$ first-order photolysis rate constant in isooctane and over 90% was lost in 21 min of irradiation in isooctane whereas only greater than 55% TCDD remained in soil after 15 d of irradiation (Kieatiwong et al. 1990)

photolytic degradation $t_{1/2} = 4.5$ h in extract from fly ash exposed to UV light from a distance of 20 cm for native congener and $t_{1/2} = 5.2$ h for ^{13}C -labeled congener in tetradecane solution (Tysklind & Rappe 1991)

$t_{1/2} = 31$ min in hexadecane and $t_{1/2} = 27$ min in ethyl oleate (Dougherty et al. 1991)

photodegradation $k = 0.0156 \text{ h}^{-1}$ with $t_{1/2} = 44$ h for TCDD sorbed to grass foliage and exposed to natural sunlight (McCrary & Maggard 1993)

$t_{1/2} = 52$ h, direct sunlight photolysis in water-acetonitrile in midday of mid-summer at 40°N (quoted, Zepp 1991)

$t_{1/2} = 55.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 6 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 320$ h, estimated for the reaction with 3×10^{-15} mole OH radicals in vapor phase (Singh 1977; quoted, Mill 1985)

laboratory tests shown that 99.5% TCDD was oxidized in 21 s at 800°C while only 50% reacted at 700°C (Esposito et al. 1980; quoted, Crosby 1985)

$k_{\text{OH}} = 2 \times 10^8 \text{ mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 13$ d for oxidation in vapor phase (Mill 1985)

$k_{\text{OH}} > 1.0 \times 10^8 \text{ mol}^{-1} \text{ s}^{-1}$, $1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 200$ h (Podoll et al. 1986)

$k_{\text{OH}}(\text{calc}) = 9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an atmospheric lifetime $\tau \sim 3$ d (Atkinson 1987a)

$k_{\text{OH}}(\text{calc}) = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship Atkinson 1987b) photooxidation $t_{1/2} = 22.3\text{--}223$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k = 1.33 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$, the oxidative degradation of water dissolved TCDDs by ozone takes place only under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 7.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (7.6 - 19) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 0.8\text{--}2.0$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ at room temp. (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous solutions (Haag & Yao 1992)

$k_{\text{OH}}(\text{calc}) = (2.0 - 5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 2.8\text{--}7.2 \text{ d}$ for a tetra-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis: hydrolysis is not likely under environmental conditions (Callahan et al. 1979; Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 10032 \text{ h}$, based on soil die-away test data (Kearney et al. 1971; quoted, Howard et al. 1991) and $t_{1/2} = 14160 \text{ h}$, based on lake water and sediment dieaway test data (Ward & Matsumura 1978; quoted, Howard et al. 1991)

$t_{1/2} > 1.0 \text{ yr}$ (Callahan et al. 1979);

$t_{1/2}(\text{aq. anaerobic}) = 40128\text{--}56640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (estimated, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 4.64 \text{ mL g}^{-1} \text{ h}^{-1}$; $k_2 = 5.00 \times 10^{-4} \text{ h}^{-1}$ (rainbow trout, Neely 1979)

$k_1 = 108 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.012 \text{ d}^{-1}$ (rainbow trout, Branson et al. 1983, 1985)

$k_1 = 476 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.120 \text{ d}^{-1}$ (fathead minnow, Adams et al. 1986)

$k_1 = 600 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.046 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1986)

$k_1 = 1832, 1543, 1337, 1591 \text{ d}^{-1}$ and $k_2 = 0.047, 0.041, 0.015, 0.043 \text{ d}^{-1}$ (rainbow trout, exposed to 38 pg/L, 176 pg/L, 382 pg/L, 702 pg/L for 28 d, Mehrle et al. 1988)

$k_1 = 216, 604 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 8 h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1989)

$k_2 = 0.008 \text{ d}^{-1}$ (rainbow trout, quoted, Opperhuizen & Sijm 1990)

$k_1 = 381 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.048 \text{ d}^{-1}$ (fathead minnow, quoted, Opperhuizen & Sijm 1990)

$k_1 = 100 \text{ mL g}^{-1} \text{ d}^{-1}$ (mosquito fish, quoted, Opperhuizen & Sijm 1990)

$k_1 = 86 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish, 120-h exposure, metabolic inhibitor PBO-treated; Sijm et al. 1993)

$k_1 = 66 \text{ L kg}^{-1} \text{ d}^{-1}, 104 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 > 1.3 \text{ d}^{-1}; < 0.1 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated; control, Sijm et al. 1993)

$k_1 = 500 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.049 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0061 \text{ d}^{-1}$ with a biological $t_{1/2} = 49 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_2 = 0.0246 \text{ d}^{-1}$ with $t_{1/2} = 28 \text{ d}$ (newly contaminated oysters, Gardinali et al. 2004)

$k_2 = 0.0199 \text{ d}^{-1}$ with $t_{1/2} = 35 \text{ d}$ (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: dominant transformation process in the atmosphere (Atkinson et al. 1982)

$t_{1/2} = 200 \text{ h}$ for reaction with OH radical (Podoll et al. 1986)

atmospheric lifetime of $\sim 3 \text{ d}$ at room temp. (Atkinson 1987a)

$t_{1/2} = 22.3\text{--}223 \text{ h}$, based on estimated photooxidation half-life in air (Howard et al. 1991)

$t_{1/2} = 1 \text{ h}$, an upper limit, undergo rapid photolysis in vapor phase (Travis & Hattemer-Frey 1987)

atmospheric $k = 0.012 \text{ min}^{-1}$ with $t_{1/2} = 58 \text{ min}$ in summer sunlight at 40°N latitude (Buser 1988)

reaction rate constant $k \sim 0.02 \text{ h}^{-1}$ (Paterson et al. 1990)

tropospheric lifetime $\tau(\text{calc}) = 0.8\text{--}2.0 \text{ d}$ for reaction with OH radical (Atkinson 1991)

tropospheric lifetime $\tau(\text{calc}) = 2.8\text{--}7.2 \text{ d}$ for with OH radical (Kwok et al. 1995);

$t_{1/2} = 200 \text{ h}$ at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis $t_{1/2} = 3 \text{ h}$ in methanol solution under sunlight (Plimmer et al. 1973);

$t_{1/2} = 600 \text{ d}$ in a model aquatic environment (Ward & Matsumura 1978);

reaction rate constant estimated to be $2.6 \times 10^{-5} \text{ h}^{-1}$ (Mackay et al. 1985);

calculated sunlight photolysis half-lives over four seasons at 40°N latitude averaged over for 24 h exposure per day: $t_{1/2} = 130 \text{ h}$ in winter, $t_{1/2} = 28 \text{ h}$ in spring, $t_{1/2} = 20 \text{ h}$ in summer and $t_{1/2} = 52 \text{ h}$ in fall (Mill et al. 1982; quoted, Mill 1985);

calculated photolysis half-lives in sunlight at 40°N latitude: $t_{1/2} = 118 \text{ h}$ in winter, $t_{1/2} = 27 \text{ h}$ in spring, $t_{1/2} = 21 \text{ h}$ in summer and $t_{1/2} = 51 \text{ h}$ in fall (Podoll et al. 1986);

photolysis $t_{1/2} = 40 \text{ h}$ in near-surface waters is an important degradative pathway (Travis & Hattemer-Frey 1987);

$t_{1/2} = 14 \text{ min}$, sunlight-induced photolysis half-life in isooctane (Buser 1988);

reaction rate constant estimated to be 0.008 h^{-1} (Paterson et al. 1990);

- photolysis $t_{1/2} = 27\text{--}81$ h, aerobic $t_{1/2} = 1.15\text{--}1.62$ yr, anaerobe $t_{1/2} = 4.58\text{--}6.45$ yr (Howard et al. 1991)
 $t_{1/2} = 4000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
- Groundwater: $t_{1/2} = 20064\text{--}28320$ h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).
- Sediment: $t_{1/2} = 12000\text{--}14400$ h in aquatic sediment (Ward & Matsumura 1978; quoted, Quensen & Matsumura 1983)
 reaction rate constant $k \sim 8.0 \times 10^{-6} \text{ h}^{-1}$ (Mackay et al. 1985)
 $k \sim 1.5 \times 10^{-5} \text{ h}^{-1}$ (Paterson et al. 1990)
 $t_{1/2} > 1$ yr (O'Keefe et al. 1986)
 $t_{1/2} = 9.9\text{--}98$ yr (Geyer et al. 2000)
 degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000)
 $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).
- Soil: $t_{1/2} = 10032\text{--}14160$ h, based on soil dieaway test data for two soils (Howard et al. 1991);
 $t_{1/2} \sim 1$ yr (Kearney et al. 1973; quoted, Quensen & Matsumura 1983);
 degradation $t_{1/2} = 10\text{--}12$ yr in soil (De Dimenico et al. 1980, Kimbrough et al. 1984);
 $t_{1/2} \sim 1$ yr if applied to surface on soil with 2,4-D (Nash & Beall 1980);
 $k \sim 8.0 \times 10^{-6} \text{ h}^{-1}$ (Mackay et al. 1985)
 $k \sim 1.1 \times 10^{-5} \text{ h}^{-1}$ (Paterson et al. 1990)
 $t_{1/2} = 10$ min during the day, photodegradation is a rapid process at the soil surface (Facchetti et al. 1986);
 $t_{1/2} \sim 10$ yr in soil if TCDD is on or near the surface and $t_{1/2} = 100$ yr if TCDD is buried at greater depth (Nauman & Schaum 1987)
 calculated $t_{1/2} = 10$ yr (Edujee 1987)
 $t_{1/2} = 10$ yr or longer (Boddington et al. 1990)
 $t_{1/2} = 365$ d for volatilization to atmosphere below surface soil (Jury et al. 1990)
 $t_{1/2} = 10$ yr (Geyer et al. 2000)
 degradation $t_{1/2} = 10\text{--}100$ yr in soils (estimated, Suzuki et al. 2000)
 $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000)
- Biota: $t_{1/2} = 31$ d, estimated half-life in rat (Rose et al. 1976; quoted, Birnbaum 1985);
 $t_{1/2} = 11$ d, estimated half-life in hamster (Olsen et al. 1980; quoted, Birnbaum 1985)
 $t_{1/2} = 30$ d, estimated half-life in guinea pig (Decad et al. 1981a; quoted, Birnbaum 1985)
 $t_{1/2} = 11\text{--}24$ d, estimated half-life in mouse (Gasiewicz et al. 1983; quoted, Birnbaum 1985)
 depuration $t_{1/2} = 58$ d, total body burden of ^{14}C -TCDD in whole rainbow trout (Branson et al. 1983, 1985)
 $t_{1/2} = 17\text{--}37$ d in mouse, $t_{1/2} = 31$ d in rat and $t_{1/2} = 30$ d in guinea pig (quoted, Van den Berg et al. 1985)
 elimination $t_{1/2} = 14.5$ d from fathead minnow (Adams et al. 1986)
 $t_{1/2} = 105$ d in whole body of rainbow trout (Kleeman et al. 1986);
 $t_{1/2} = 300\text{--}325$ d in carp (Kuehl et al. 1986)
 biological $t_{1/2} = 58$ d for rainbow trout (Niimi & Oliver 1986)
 $t_{1/2} = 5.8$ yr in human (estimated, Poiger & Schlatter 1986)
 $t_{1/2} > 336$ d for carps in Lake Superior (Kuehl et al. 1987)
 $t_{1/2} = 6.7$ yr in human (estimated, Kissel & Robarge 1988)
 elimination $t_{1/2} = 15\text{--}48$ d from rainbow trout for exposures of different concn (Mehrle et al. 1988)
 $t_{1/2} = 7.1$ yr in human (estimated, Pirkle et al. 1989; quoted, Webster & Connett 1991)
 $t_{1/2} = 5\text{--}8$ yr for human, $t_{1/2} = 17.4\text{--}31$ d for rats, $t_{1/2} = 9.6\text{--}24.4$ d for mice, $t_{1/2} = 22\text{--}93.7$ d for guinea pigs,
 $t_{1/2} = 12.0\text{--}150$ d for hamsters, $t_{1/2} = 1$ yr for monkeys (Boddington et al. 1990)
 $t_{1/2} = 40.3$ d for lactating cows (Olling et al. 1991)
 $t_{1/2} = 5\text{--}10$ yr assumed half-life for human (Schecter & Ryan 1991)
 elimination $t_{1/2} = 35\text{--}37$ d from lake trout sac fry (Walker et al. 1991)
 $t_{1/2} = 4.4$ yr for a 70 kg non-lactating "reference" human (Webster & Connett 1991)
 $t_{1/2} < 0.5$ d for metabolic inhibitor PBO treated gold fish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993)
 elimination $t_{1/2} = 45$ d from soft-shell clam (Brown et al. 1994)
 biological $t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994)
 reported $t_{1/2} = 8\text{--}24.4$ d for mice, $t_{1/2} = 30.2$ and 93.7 d for guinea pigs, $t_{1/2} = 20\text{--}28.9$ d for rats and $t_{1/2} = 365\text{--}3470$ d for humans (Miniero et al. 2001).
 depuration $t_{1/2} = 28$ d for newly contaminated oysters, and $t_{1/2} = 35$ d for chronically contaminated oysters (Gardinali et al. 2004)

TABLE 8.1.1.16.1
Reported vapor pressures of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin at various temperatures

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Schroy et al. 1985a		Schroy et al. 1985b		Webster et al. 1985		Rordorf 1987, 1989	
gas saturation		gas saturation		gas saturation-LSC		gas saturation-GC/ECD	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30.1	4.61×10^{-7}	30	4.67×10^{-7}	20	8.71×10^{-6}	25	2.0×10^{-7}
30.2	5.19×10^{-7}	54.6	1.83×10^{-5}	50	1.12×10^{-5}	50	9.5×10^{-6}
30.3	8.73×10^{-7}	62	4.97×10^{-5}	100	1.72×10^{-5}	75	2.6×10^{-4}
54.6	2.06×10^{-5}	71	1.59×10^{-4}			100	4.6×10^{-3}
55	1.37×10^{-5}					125	5.7×10^{-2}
55.2	1.94×10^{-5}	Antoine eq. for 10–305 °C					
61.9	3.71×10^{-5}	eq. 2	P/mmHg			$\Delta H_v/(\text{kJ mol}^{-1}) = 79.9$	
62	4.58×10^{-5}	A	12.89784			$\Delta H_{\text{subl}}(\text{kJ mol}^{-1}) = 124.001$	
70.9	1.79×10^{-4}	B	6477.132			$\Delta H_{\text{fus}}(\text{kJ mol}^{-1}) = 39.9$	
71	1.58×10^{-4}	C	273.15			$\Delta S_{\text{fus}}(\text{J mol}^{-1} \text{ K}^{-1}) = 69$	
71.1	1.59×10^{-4}						
		Antoine eq. for 305–420 °C					
eq. 1	P/Pa	eq. 2	P/mmHg				
A	34.570834	A	8.78307				
B	14903.438	B	4098.173				
		C	273.15				

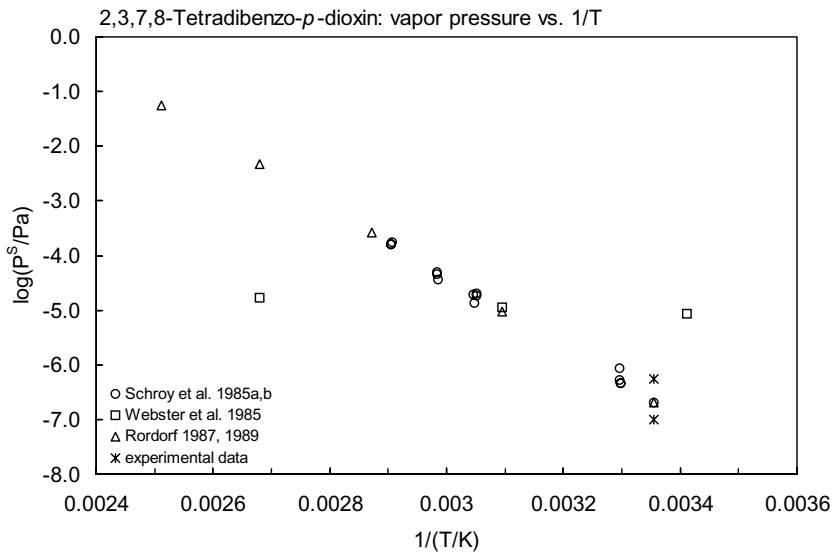


FIGURE 8.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.

TABLE 8.1.1.16.2
Reported octanol-air partition coefficients of 2,3,7,8-
tetrachlorodibenzo-*p*-dioxin at various temperatures

Harner et al. 2000	
generator column-GC/ECD	
$t/^{\circ}\text{C}$	K_{OA}
20	10.318
40	9.283
50	8.778
25	10.05
$\log K_{\text{OA}} = a + b/(T/\text{K})$	
a	-6.19
b	4840
enthalpy of phase change	
$\Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 92.60$	

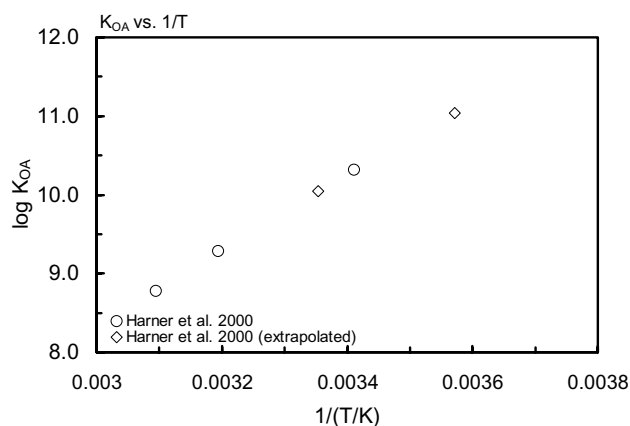
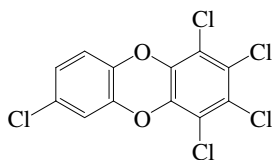


FIGURE 8.1.1.16.2 Logarithm of K_{OA} versus reciprocal temperature for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.

8.1.1.17 1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4,7-P₅CDD

Chemical Name: 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin

CAS Registry No: 39227-61-7

Molecular Formula: ClC₆H₃O₂C₆Cl₄

Molecular Weight: 356.416

Melting Point (°C):

195 (Lide 2003)

Boiling Point (°C):

464.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

197.74 (calculated-liquid density, Govers et al. 1990)

281.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

92.8 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.419 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

42.4 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

26 (Friesen & Webster 1990)

Entropy of Fusion, ΔS_{fus} (J/mol K):

90 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0215 (mp at 195°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

0.000118*; 0.0000855 (20°C, ¹⁴C-labelled, generator column-HPLC/LSC, measured range 20–40°C, calculated, Friesen et al. 1985)

0.0000955 (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, Webster et al. 1986)

1.23 × 10⁻⁴* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)

0.00428 (supercooled liquid P_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

8.80 × 10⁻⁸* (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.00 × 10⁻⁶ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

1.00 × 10⁻⁶ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

log (P/Pa) = 17.02207 – 7179.05/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

4.57 × 10⁻⁶ (supercooled liquid P_L, GC-RI correlation; Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol at 25°C):

0.264 (calculated-P/C, Shiu et al. 1988; quoted, Kaupp & McLachlan 1999)

0.224; 1.23 (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

0.691; 1.23 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow} :

- 9.44, 9.62, 10.02; 9.39, 9.65, 10.05 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 9.40, 9.65 (HPLC-RT correlation, Sarna et al. 1984)
 9.48, 8.80; 9.40, 8.64 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 9.65, 7.44 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 6.60 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)
 7.53 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

- 10.67*; 10.32 (generator column-GC; calculated, Harner et al. 2000)
 log K_{OA} = $-7.65 + 5460/(T/K)$, temp range 30–50°C (Harner et al. 2000)
 10.42 (GC-retention time correlation, Chen et al. 2002)

Bioconcentration Factor, log BCF:

- 3.26 (fathead minnow, steady-state, wet weight, Muir et al. 1985)
 2.50 (rainbow trout, steady-state, wet weight, Muir et al. 1985)
 3.16, 2.91 (fathead minnow, rainbow trout, De Voogt et al. 1990;)
 3.50, 4.50 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 5.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 4.85, 4.60, 4.50 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986b)
 5.80, 5.67, 5.90 (20, 30, 40°C, humic acid from Manitoba peat bog, Webster et al. 1986b)
 6.38, 6.39, 6.46 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986b)
 5.02 (DOC, De Voogt et al. 1990)
 8.57 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 4.31 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) at 313 nm and calculated half-lives under conditions of variable sunlight intensity at 40°N latitude: $t_{1/2} = 18.29 \text{ d}$ in spring with rate constant $k = 0.466 \times 10^{-6} \text{ s}^{-1}$, $t_{1/2} = 15.16 \text{ d}$ in summer with $k = 0.562 \times 10^{-6} \text{ s}^{-1}$, $t_{1/2} = 28.59 \text{ d}$ in fall with $k = 0.298 \times 10^{-6} \text{ s}^{-1}$, $t_{1/2} = 52.37 \text{ d}$ in winter with $k = 0.163 \times 10^{-6} \text{ s}^{-1}$, and $t_{1/2} = 76.82 \text{ d}$ averaged over full year with rate constant $k = 0.111 \times 10^{-6} \text{ s}^{-1}$ (Choudhary & Webster 1985a, 1986);

$k = 4.3115 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (3:3 v/v) at 313 nm (Choudhary & Webster 1985b);

photolysis $k = 4.31 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 45.86 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 4.03 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 18 \text{ d}$ in spring, $k = 4.86 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 15 \text{ d}$ in summer, $k = 2.58 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 29 \text{ d}$ in fall, $k = 1.41 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 52 \text{ d}$ in winter (Choudhary & Webster 1989);

$k = 0.74 \text{ d}^{-1}$ under mid-summer sunlight at 50°N latitude in filtered-sterilized natural water and $k = 0.058 \text{ d}^{-1}$ in (2:3, v/v) distilled water-acetonitrile (Friesen et al. 1990);

photolytic $t_{1/2} = 38 \text{ h}$ in fly-ash extract (Tysklind & Rappe 1991);

$t_{1/2} = 92 \text{ h}$ for photodegradation in a rotary photoreactor adsorbed to clean silica gel by filtered <290 nm of light (Koester & Hites 1992).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (12 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (6.5 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.1\text{--}2.4 \text{ d}$ based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.7 - 3.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 4.0\text{--}8.5 \text{ d}$ for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation: biotransformation rate constant $k = 0.014 \text{ d}^{-1}$ for rainbow trout (Sijm et al. 1990).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 285 \text{ d}^{-1}$; $k_2 = 0.22 \text{ d}^{-1}$ (fathead minnow, flow-through system, Muir et al. 1985)

$k_1 = 204 \text{ d}^{-1}$; $k_2 = 0.28 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_2 = 2.5 \times 10^{-2}$, $3.9 \times 10^{-2} \text{ d}^{-1}$ (rainbow trout for 2 to 21 d exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1990)

$k_1 = 509$, $162 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1$, $> 1.5 \text{ d}^{-1}$ (goldfish after 120-h exposure for metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 169 \text{ L kg}^{-1} \text{ d}^{-1}$, $251 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P₅CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime of 1.1–2.4 d calculated for the gas-phase with OH radicals using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, (Atkinson 1991);

photodegradation $t_{1/2} = 92 \text{ h}$ in a rotary photo-reactor adsorbed to clean silica gel by filtered $\lambda < 290 \text{ nm}$ of light (Koester & Hites 1992);

calculated tropospheric lifetime of 4.0–8.5 d for penta-chlorinated dioxin for the gas-phase reaction with OH radical at room temp. (Kwok et al. 1995);

suggested $t_{1/2} = 200 \text{ h}$ at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000).

Surface water: under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile solution (4:6, v/v): $t_{1/2} = 18.29 \text{ d}$ in spring, $t_{1/2} = 15.16 \text{ d}$ in summer, $t_{1/2} = 28.6 \text{ d}$ in fall, $t_{1/2} = 52.37 \text{ d}$ in winter, and $t_{1/2} = 76.82 \text{ d}$ averaged over full year (Choudhary & Webster 1985a, 1986);

photolysis $t_{1/2} = 45.86 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct phototransformation half-lives near water bodies at 40°N latitude: $t_{1/2} = 18.4 \text{ d}$ in spring, $t_{1/2} = 15 \text{ d}$ in summer, $t_{1/2} = 29 \text{ d}$ in fall and $t_{1/2} = 52 \text{ d}$ in winter (Choudhary & Webster 1989);

$t_{1/2} = 27 \text{ d}$ in sunlit surface water and $t_{1/2} = 0.94 \text{ d}$ in surface water of actual pond (Friesen et al. 1990).

Groundwater:

Sediment: degradation half-lives in sediment 20–200 yr for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation half-lives in soil 10–100 yr (estimated, Suzuki et al. 2000).

Biota: $t_{1/2} = 3.1 \text{ d}$ in fathead minnow (Adams et al. 1986);

$t_{1/2} = 2 \text{ d}$ in whole body of rainbow trout (Muir & Yarechewski 1988);

half-lives in gold fish: $t_{1/2} > 7 \text{ d}$ for PBO treated and $t_{1/2} < 0.5 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

TABLE 8.1.1.17.1

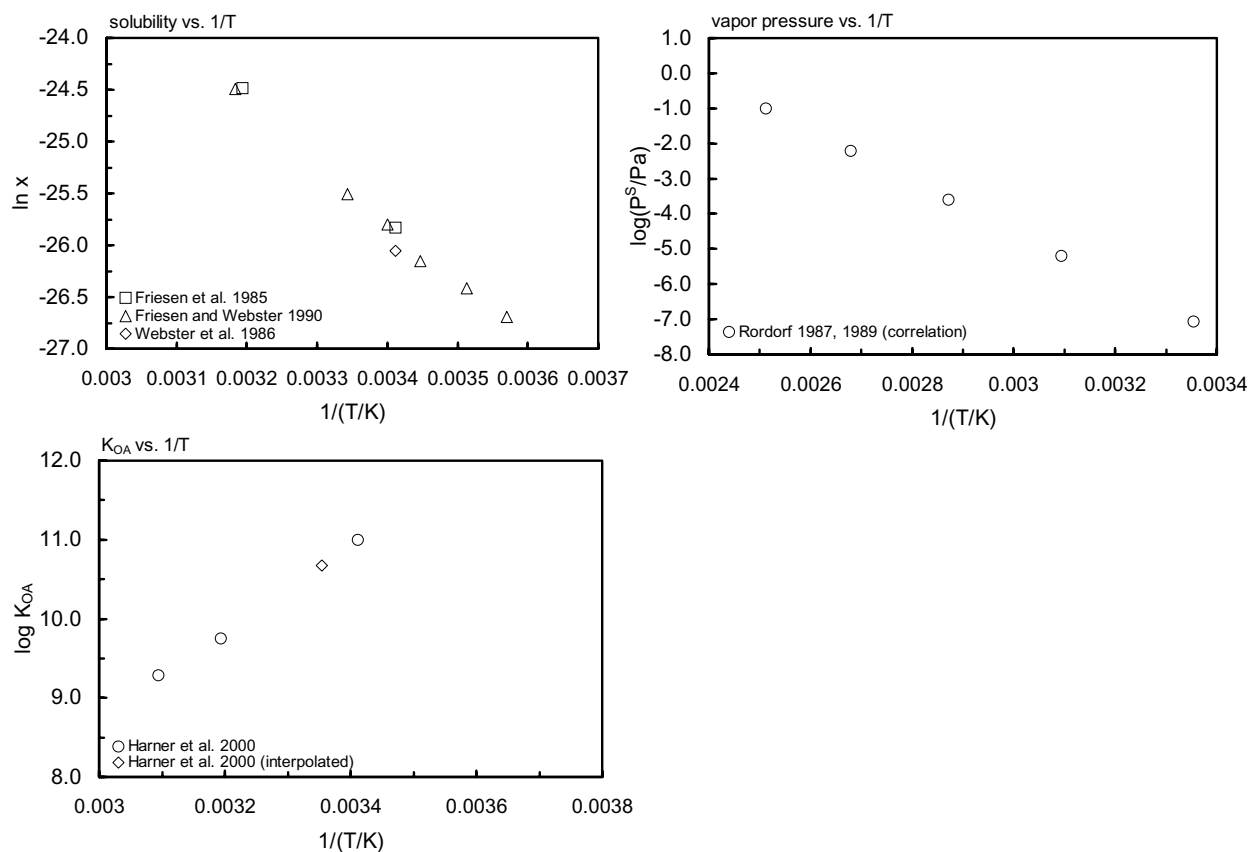
Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin at various temperatures

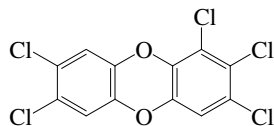
Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	log K_{OA}
20	1.20×10^{-4}	7	5.05×10^{-5}	25	8.8×10^{-8}	20	10.996
40	3.17×10^{-4}	11.5	6.70×10^{-5}	50	6.4×10^{-6}	40	9.751
		17	8.70×10^{-5}	75	2.5×10^{-4}	50	9.282
		21	1.24×10^{-4}	100	6.1×10^{-3}	25	10.67
		26	1.65×10^{-4}	125	9.8×10^{-2}		
		41	4.56×10^{-4}				
						log $K_{OA} = a + b/(T/K)$	

(Continued)

TABLE 8.1.1.17.1 (Continued)

Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K_{OA}
		$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 47.5$ 7–41 °C		$\Delta H_v/(\text{kJ mol}^{-1}) = 92.8$ $\Delta H_{subl}/(\text{kJ mol}^{-1}) = 131.42$ $\Delta H_{fus}/(\text{kJ mol}^{-1}) = 42.4$ $\Delta S_{fus}/(\text{J mol}^{-1} \text{K}^{-1}) = 90$		a	–7.65
						b	5460
						enthalpy of phase change $\Delta H_{OA}/(\text{kJ mol}^{-1}) = 104.0$	

FIGURE 8.1.1.17.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,7-pentachlorodibenzo-*p*-dioxin.

8.1.1.18 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,7,8-P₅CDD

Chemical Name: 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin

CAS Registry No: 40321-76-4

Molecular Formula: Cl₂C₆H₂O₂C₆HCl₃

Molecular Weight: 356.416

Melting Point (°C):

Boiling Point (°C):

464.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

195.74 (calculated-liquid density, Govers et al. 1990)

281.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.7 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

134.062 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

42.4 (Rordorf 1987)

Entropy of Fusion, ΔS_{fus} (J/mol K):

83 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

0.000722 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):

9.82×10^{-5} (calculated-QSAR, Fielder & Schramm 1990)

2.77×10^{-3} (supercooled liquid S_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(\text{mol/L})] = 0.445 - 2232/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

4.0×10^{-3} ; 2.77×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

5.80×10^{-8} * (calculated, Rordorf 1985a,b, 1987,1989; quoted, Kaupp & McLachlan 1999)

1.20×10^{-5} (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

1.71×10^{-4} ; 1.23×10^{-7} (supercooled liquid P_L; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.72 - 5850/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 8.38 - 3321/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

4.17×10^{-6} ; 1.20×10^{-5} (supercooled liquid P_L; GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

1.48 (calculated-SOFA model, Govers & Krop 1998)

$\log (H/(\text{Pa m}^3/\text{mol})) = 7.94 - 1089/(T/K)$ (Passivirta et al. 1999)

0.661; 1.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow}:

6.64 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989a)

7.50 (calculated-SOFA model, Govers & Krop 1998)

7.27 (estimated-solubility S_L and regression eq. using lit. K_{ow} values, Passivirta et al. 1999)

- 7.215 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 7.55; 7.50 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)
 6.78, 6.84, 6.49, 6.87 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 10.57*; 10.44 (generator column-GC; calculated, Harner et al. 2000)
 11.63 (7°C, GC-retention time correlation, Harner et al. 2000)
 $\log K_{OA} = -8.02 + 5540/(T/K)$; temp range 30–50°C (generator column-GC/ECD, Harner et al. 2000)
 10.46 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 3.20 (guppy, exposed to fly ash extract, Opperhuizen et al. 1986)
 3.93; 4.31 (goldfish: PBO treated; control, 120-h exposure, Sijm et al. 1993)
 5.27 (guppies, 21-d exposure, system-I absence of sediment, Loonen et al. 1994b)
 4.98 (guppies, 21-d exposure, system-II with sediment, Loonen et al. 1984b)
 5.34 (calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.91 (calculated-QSAR, Fiedler & Schramm 1990)
 6.80 (Baltic sea particulate field samples, concentration distribution-GC/MS, Broman et al. 1991)
 8.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: solution photolysis $t_{1/2} = 456$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 52.8$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984);

photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with $t_{1/2} = 33.6$ h for native congener and $t_{1/2} = 16.7$ h for ^{13}C -labeled congener in tetradecane solution (Tysklind & Rappe 1991);

$t_{1/2} = 57.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (6.5 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.1\text{--}2.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.7 - 3.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 4.0\text{--}8.5$ d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 700 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.090 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1986)

$k_1 = 127, 695 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.02, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure, Sijm et al. 1993)

$k_1 = 169 \text{ L kg}^{-1} \text{ d}^{-1}$, $251 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_3CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 952 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.030 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0051 \text{ d}^{-1}$ with $t_{1/2} = 50$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: for a penta-chlorinated dioxin, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime $\tau = 1.1\text{--}2.4$ d for the gas phase with OH radical (Atkinson 1991);

calculated tropospheric lifetime $\tau = 4.0\text{--}8.5$ d for reaction with OH radical (Kwok et al. 1995);

$t_{1/2} = 360$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 7200$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Groundwater:

Sediment: $t_{1/2} = 1000000$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000).

Soil: $t_{1/2} = 1,000,000$ h at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000);

degradation $t_{1/2} = 10\text{--}100$ yr in soil (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 32$ d for PBO treated and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.18.1

Reported vapor pressures and octanol-air partition coefficients of 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin at various temperatures

Vapor pressure		log K_{OA}	
Rordorf 1987, 1989		Harner et al. 2000	
vapor pressure correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	log K_{OA}
25	5.8×10^{-8}	20	10.867
50	3.8×10^{-6}	40	9.755
75	1.4×10^{-4}	50	9.083
100	3.0×10^{-3}	25	10.57
125	4.6×10^{-2}		
$\Delta H_v/(\text{kJ mol}^{-1}) = 88.7$		$\log K_{OA} = a + b/(T/K)$	
$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 138.062$		a	-8.02
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 42.4$		b	5540
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 106$	
		for GC-RT correlation	

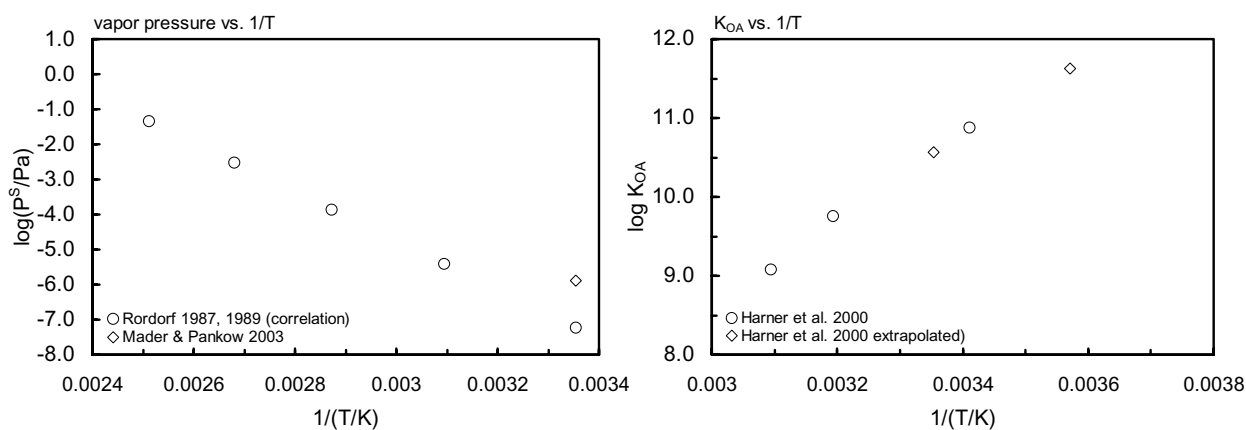
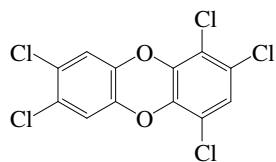


FIGURE 8.1.1.18.1 Logarithm of vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin.

8.1.1.19 1,2,4,7,8-Pentachlorodibenzo-*p*-dioxin

Common Name: 1,2,4,7,8-Pentachlorodibenzo-*p*-dioxin

Synonym: 1,2,4,7,8-P₅CDD

Chemical Name: 1,2,4,7,8-pentachlorodibenzo-*p*-dioxin

CAS Registry No: 58802-08-7

Molecular Formula: Cl₅C₆H₂O₂C₆HCl₃

Molecular Weight: 356.416

Melting Point (°C):

206 (Rordorf 1987)

Boiling Point (°C):

464.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

199.91 (calculated-liquid density, Govers et al. 1990)

281.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.8 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

136.636 (Rordorf 1987)

125.3 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

42.4 (Rordorf 1987)

Entropy of Fusion, ΔS_{fus} (J/mol K):

88 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0168 (mp at 206°C)

Water Solubility (g/m³ or mg/L at 25°C):

9.82×10^{-5} (calculated-QSAR, Fielder & Schramm 1990)

4.92×10^{-3} (supercooled liquid S_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

5.39×10^{-3} ; 4.92×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):

7.80×10^{-8} , 5.6×10^{-6} , 2.1×10^{-4} , 5.1×10^{-3} , 8.0×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.58×10^{-5} (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)

6.026×10^{-6} ; 1.58×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

$\ln(P/\text{Pa}) = 38.743 - 16431/(T/\text{K})$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln(P/\text{Pa}) = (36.472 \pm 0.679) - (15073 \pm 282)/(T/\text{K})$; temp range 403–428 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol):

1.096 (calculated-SOFA model, Govers & Krop 1998)

7.41; 1.096 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow}:

6.64 (shake flask/slow stirring-GC/MS, from mixture of fly-ash extract, Sijm et al. 1989)

8.41 (calculated-QSAR, Fiedler & Schramm 1990)

7.36 (calculated-SOFA model, Govers & Krop 1998)

7.46; 7.36 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.20; 6.71, 6.78, 6.55, 6.87 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

5.34 (calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

5.91 (calculated-QSAR, Fiedler & Schramm 1990)

8.72 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Volatilization:

Photolysis: $t_{1/2} = 81.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (6.5 - 14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime of 1.1 – 2.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.7 - 3.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime of 4.0–8.5 d for a penta-chlorinated dioxin at room temp. (relative rate method, Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 61, 164 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.21, > 1.9 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure, Sijm et al. 1993)

$k_1 = 169 \text{ L kg}^{-1} \text{ d}^{-1}$, $251 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime $\tau = 1.1\text{--}2.4$ d calculated for a penta-chlorinated dioxin based on the gas-phase reaction with OH radicals (Atkinson 1991); calculated tropospheric lifetime $\tau = 2.8\text{--}7.2$ d for the gas-phase reaction with OH radical (Kwok et al. 1995).

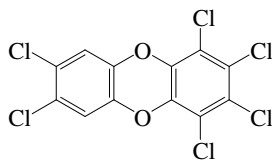
Surface water:

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100$ yr in soil (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 3.3$ d for PBO treated and $t_{1/2} > 1.9$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.20 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4,7,8-H₆CDD

Chemical Name: 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin

CAS Registry No: 39227-26-8

Molecular Formula: Cl₂C₆H₂O₂C₆Cl₄

Molecular Weight: 390.861

Melting Point (°C):

273–275 (Pohland & Yang 1972; Rordorf 1987,1989; Delle Site 1997)

Boiling Point (°C):

487.7 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

206.96 (calculated-liquid density, Govers et al. 1990)

302.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

89.1 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

140.782 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

30.21 (Friesen & Webster 1990)

Entropy of Fusion, ΔS_{fus} (J/mol K):

88 (Rordorf 1987, 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F: 0.00369 (assuming ΔS_{fus} = 56 J/mol K and mp at 273°C)

0.00352 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)

0.000148 (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4.40 × 10⁻⁶* (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)

5.70 × 10⁻⁶ (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, Webster et al. 1986b)

4.89 × 10⁻⁶* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)

log [S_L/(mol/L)] = 0.235 B 2515/(T/K) (supercooled liquid, Passivirta et al. 1999)

1.15 × 10⁻³ (supercooled liquid S_L; GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

5.10 × 10⁻⁹* (calculated-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

3.20 × 10⁻⁷ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

3.96 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)

5.43 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1989)

1.00 × 10⁻⁸ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

1.45 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Falconer & Bidleman 1994)

1.36 × 10⁻⁹, 1.87 × 10⁻⁹ (solid P_S, calculated from reported P_L, Delle Site 1997)

3.19 × 10⁻⁶ (corrected supercooled liquid P_L, Eitzer & Hites 1998)

5.20 × 10⁻⁵; 7.70 × 10⁻⁹ (supercooled liquid P_L; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.97 - 6282/(T/\text{K})$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 8.37 - 3769/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P/\text{Pa}) = 15.65106 - 7087.08/(T/\text{K})$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 3.72×10^{-5} (supercooled liquid P_L , Harner et al. 2000)
 8.91×10^{-7} (supercooled liquid P_L ; GC-RI correlation; Wang & Wong 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

0.452 (calculated-P/C, Shiu et al. 1988; quoted, Kaupp & McLachlan 1999)
 0.631; 1.45 (quoted lit., calculated-SOFA model, Govers & Krop 1998)
 $\log (H/(\text{Pa m}^3/\text{mol})) = 8.14 - 1254/(T/\text{K})$ (Passivirta et al. 1999)
 0.427; 1.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

10.36, 10.39, 10.89; 10.22, 10.44, 10.89 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 10.40, 9.65; 10.22, 9.19 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 10.44, 7.79 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 7.80 (selected, Shiu et al. 1988)
 8.0 (calculated-QSAR, Fiedler & Schramm 1990)
 7.30 (calculated, Broman et al. 1991)
 9.53 (HPLC-RT correlation, Chessells et al. 1991)
 9.13 (calculated-fragment const., Chessells et al. 1991)
 10.22 (quoted, Hansch et al. 1995)
 7.94 (calculated-SOFA model, Govers & Krop 1998)
 7.90 (estimated-solubility S_L and regression eq. using lit. K_{ow} values, Passivirta et al. 1999)
 7.628 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 7.94; 7.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
 7.80; 7.12, 7.12, 7.25, 7.30 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.50 (calculated- K_{ow}/K_{Aw} , Wania & Mackay 1996)
 11.17 (calculated, Finizio et al. 1997)
 11.11*; 10.88 (generator column-GC; calculated, Harner et al. 2000)
 12.20 (7°C, GC-retention time correlation, Harner et al. 2000)
 $\log K_{OA} = -6.20 + 5160/(T/\text{K})$; temp range 30–50°C (generator column-GC/ECD, Harner et al. 2000)
 10.95 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

3.73, 4.00 (rainbow trout, fathead minnow, steady-state, wet weight, Muir et al. 1985)
 4.00, 5.00 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 3.41, 3.76 (fathead minnow, quoted, Opperhuizen & Sijm 1990)
 3.45, 3.23 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
 3.45, 4.87 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
 5.01; 4.65 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 5.01; 5.01; 5.14 (guppy, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 5.01; 5.07 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 5.90, 5.98 (fish muscle $\log BCF_L$ calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, $\log K_{oc}$ at 25°C or as indicated:

5.41, 5.31, 5.13 (20, 30, 40°C, fulvic acid from a Manitoba soil, Webster et al. 1986)
 6.02, 6.15, 5.95 (20, 30, 40°C, humic acid from Manitoba peat bog, Webster et al. 1986)
 6.32, 6.27, 6.15 (20, 30, 40°C, Aldrich humic acid, Na salt, Webster et al. 1986b)
 5.02 (DOC, De Voogt et al. 1990)
 7.10 (Baltic Sea particulate field samples, concentration distribution-GC/MS, Broman et al. 1991)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

$k(\text{calc}) = 1.06 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 7.57 \text{ d}$ in spring, $k = 1.280 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 6.27 \text{ d}$ in summer, $k = 0.676 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 11.87 \text{ d}$ in autumn, $k = 0.37 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 21.57 \text{ d}$ in winter and the averaged $k = 0.252 \times 10^{-6} \text{ s}^{-1}$ over full year with $t_{1/2} = 31.85 \text{ d}$, under conditions of variable sunlight intensity at 40°N latitude in aqueous acetonitrile (4:6 v/v) solution (Choudhary & Webster 1985a,c, 1986)

$k = 7.86 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhary & Webster 1985b)

$k = 7.86 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 24.5 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons:

$k = 9.16 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 7.6 \text{ d}$ in spring, $k = 11.06 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 6.3 \text{ d}$ in summer, $k = 5.84 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 12.0 \text{ d}$ in fall, $k = 3.21 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 22.0 \text{ d}$ in winter (Choudhary & Webster 1989)

$k = 0.28 \text{ d}^{-1}$ in natural water and $k = 0.019 \text{ d}^{-1}$ in distilled water-acetonitrile (Friesen et al. 1990)

photolytic $t_{1/2}(\text{calc}) = 38 \text{ h}$ in the fly ash extract in tetradecane (Tysklind & Rappe 1991)

photodegradation $t_{1/2} = 140 \text{ h}$ in a rotary photoreactor absorbed to silica gel by filtered $< 290 \text{ nm}$ of light (Koester & Hites 1992)

$t_{1/2} = 91.8 \text{ h}$ on spruce needles surface under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved PCDD is $5.02 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (4.6 - 10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.5\text{--}3.4 \text{ d}$ based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 102 \text{ d}^{-1}$; $k_2 = 0.046 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_1 = 112 \text{ d}^{-1}$; $k_2 = 0.030 \text{ d}^{-1}$ (fathead minnow, Muir et al. 1985)

$k_2 = 0.030 \text{ d}^{-1}$ (fathead minnow, Muir et al. 1985)

$k_2 = 0.015 \text{ d}^{-1}$ (rainbow trout, Muir & Yarechewski 1988)

$k_2 = 0.0066 \text{ d}^{-1}$ (fathead minnow, Muir & Yarechewski 1988)

$k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}$, $299 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.29$, $> 0.02 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1993)

$k_1 = 868 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.065 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0105 \text{ d}^{-1}$ with $t_{1/2} = 29 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: estimated reaction rate constant, $k = 0.005 \text{ h}^{-1}$ (Paterson et al. 1990);

tropospheric lifetime $\tau = 1.5\text{--}3.4 \text{ d}$ for a hexa-chlorinated dioxin reaction with the OH radicals using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, (Atkinson 1991);

photodegradation $t_{1/2} = 140 \text{ h}$ in a rotary photoreactor adsorbed to clean silica gel by filtered $\lambda < 290 \text{ nm}$ of light, (Koester & Hites 1992);

suggested $t_{1/2} = 740 \text{ h}$ at 7°C for Baltic Proper environment (Sinkkonen & Passivirta 2000).

Surface water: under conditions of variable sunlight intensity at 40°N latitude: $t_{1/2} = 7.57 \text{ d}$ in spring, $t_{1/2} = 6.27 \text{ d}$ in summer, $t_{1/2} = 11.87 \text{ d}$ in fall, $t_{1/2} = 21.57 \text{ d}$ in winter, and $t_{1/2} = 76.8 \text{ d}$ averaged over full year (Choudhary & Webster 1985a, 1986);

photolysis $t_{1/2} = 24.5 \text{ h}$ in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, midseason direct phototransformation half-lives near water bodies at 40°N latitude: 7.6 d in spring, 6.3 d in summer, 12.0 d in fall and 22.0 d in winter (Choudhary & Webster 1989);

$t_{1/2} = 81 \text{ d}$ in sunlit surface water and $t_{1/2} = 2.5 \text{ d}$ in surface water of actual pond (Friesen et al. 1990);

estimated reaction rate constant, $k = 0.002 \text{ h}^{-1}$ (Paterson et al. 1990);

suggested $t_{1/2} = 14800 \text{ h}$ at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: estimated reaction rate constant $k = 4.0 \times 10^{-6} \text{ h}^{-1}$ (Paterson et al. 1990);

degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ in sediment for all homologues (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 2400000 \text{ h}$ at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: estimated reaction rate constant $k = 2.8 \times 10^{-6} \text{ h}^{-1}$ (Paterson et al. 1990);

degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ in soil for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 2400000 \text{ h}$ at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} = 43 \text{ d}$ in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);

half-lives in gold fish: $t_{1/2} = 2.4 \text{ d}$ for PBO treated and $t_{1/2} = 40 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 29 \text{ d}$ in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.20.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		vapor pressure correlation		generator column-GC/ECD	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	log K_{OA}
20	4.40×10^{-6}	7	2.31×10^{-6}	25	5.1×10^{-9}	20	11.403
40	1.90×10^{-5}	11.5	3.12×10^{-6}	50	4.1×10^{-7}	40	10.297
		17	4.18×10^{-6}	75	1.8×10^{-5}	50	9.762
		21	4.89×10^{-6}	100	4.6×10^{-4}	25	11.11
		26	7.90×10^{-6}	125	8.0×10^{-3}		
		41	1.90×10^{-5}				
		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 45.5$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 89.1$		log $K_{OA} = a + b/(T/K)$	
		7–41 $^\circ\text{C}$		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 140.78$		a	–6.20
				$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 48.1$		b	5160
				$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 88$		enthalpy of phase change	
						$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 98.70$	

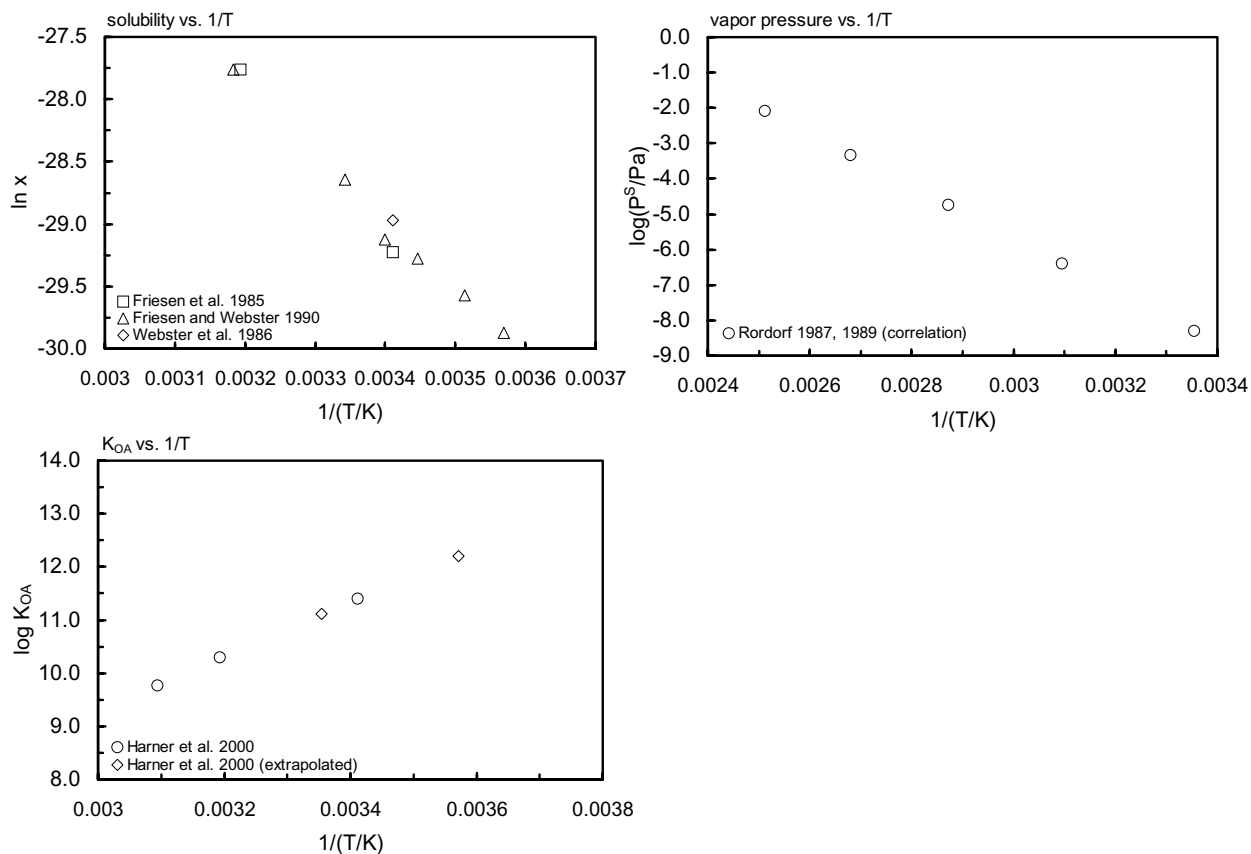
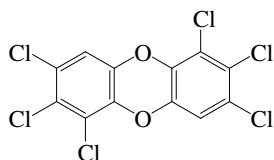


FIGURE 8.1.1.20.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin.

8.1.1.21 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,6,7,8-H₆CDD

Chemical Name: 1,2,3,6,7,8-hexachlorodibenzo-*p*-dioxin

CAS Registry No: 57653-85-7

Molecular Formula: Cl₃C₆HO₂C₆HCl₃

Molecular Weight: 390.861

Melting Point (°C):

285 (Lide 2003)

Boiling Point (°C):

487.7 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

207.16 (calculated-liquid density, Govers et al. 1990)

302.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.1 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

139.975 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1987)

Entropy of Fusion, ΔS_{fus} (J/mol K):

86 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C, F: 0.00281 (assuming ΔS_{fus} = 56 J/mol K and mp at 185°C)

0.000167 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):

8.75 × 10⁻⁴ (calculated-SOFA model, Govers & Krop 1998)

log [S_L/(mol/L)] = 0.125 – 2515/(T/K) (supercooled liquid, Passivirta et al. 1999)

1.10 × 10⁻³, 8.75 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations):

4.80 × 10⁻⁹, 3.80 × 10⁻⁷, 1.60 × 10⁻⁵, 4.0 × 10⁻⁴, 6.9 × 10⁻³ (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

3.31 × 10⁻⁶ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)

5.20 × 10⁻⁵; 8.69 × 10⁻⁹ (supercooled liquid P_L; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

log (P_s/Pa) = 12.96 – 6363/(T/K) (solid, Passivirta et al. 1999)

log (P_L/Pa) = 8.47 – 3751/(T/K) (supercooled liquid, Passivirta et al. 1999)

8.51 × 10⁻⁷, 3.31 × 10⁻⁶ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

1.45 (calculated-SOFA model, Govers & Krop 1998)

log [H/(Pa m³/mol)] = 8.35 – 1236/(T/K) (Passivirta et al. 1999)

0.417; 1.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow}:

9.13 (calculated-QSAR, Fiedler & Schramm 1990)

7.80 (calculated, Broman et al. 1991)

- 7.98 (calculated-SOFA model, Govers & Krop 1998)
- 7.96 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 7.639 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.94; 7.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
- 7.58 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.22 (7°C, GC-retention time correlation, Harner et al. 2000)
- 10.97 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 3.41, 4.61 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
- 4.94; 4.70 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
- 4.94; 5.05; 5.24 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
- 5.98 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)
- 5.56 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
- 7.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 9.42 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

- Photolysis: solution photolysis $t_{1/2} = 379$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 44100$ min on a clean glass surface under the same conditions (Nestrick et al. 1980; quoted, Mamantov 1984);
- photolytic degradation in extract from fly ash exposed to UV light from a distance of 20 cm with $t_{1/2} = 17.3$ h for native congener and $t_{1/2} = 14.2$ h for ^{13}C -labeled congener in tetradecane solution (Tysklind & Rappe 1991);
- $t_{1/2} = 76.2$ h on spruce needle surface under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

- $k_{OH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (4.6 - 10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.5\text{--}3.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- $k_1 = 432 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 120-h exposure, control fish, Sijm et al. 1993)
- $k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}$, $299 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for H_6CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- $k_2 = 0.23, < 0.1 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- $k_1 = 844 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.050 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)
- $k_2 = 0.0075 \text{ d}^{-1}$ with $t_{1/2} = 60$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

- Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991);

$t_{1/2} = 740$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 14800$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 550000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

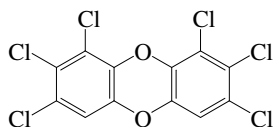
Soil: degradation $t_{1/2} = 10\text{--}100$ yr in soil for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 550\,000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: 43 d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);

$t_{1/2} = 3.0$ d for PBO treated gold fish, $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 40$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

8.1.1.22 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,7,8,9-H₆CDD OR 2,3,4,6,7,8-H₆CDD

Chemical Name: 1,2,3,7,8,9-hexachlorodibenzo-*p*-dioxin

CAS Registry No: 19408-74-3

Molecular Formula: Cl₃C₆HO₂C₆HCl₃

Molecular Weight: 390.861

Melting Point (°C):

243–244 (Rordorf 1987)

Boiling Point (°C):

487.7 (calculated, Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

207.16 (calculated-liquid density, Govers et al. 1990)

210.16 (liquid molar volume, Govers et al. 1995)

301.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.7 (Rordorf 1987)

103.9 (GC-RI correlation, Govers et al. 1995)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

142.922 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1987)

Entropy of Fusion, ΔS_{fus} (J/mol K):

93 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C, F:

0.00027 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C and the reported temperature dependence equations):

6.34×10^{-4} (calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(\text{mol/L})] = 0.491 - 2515/(T/K)$ (liquid, Passivirta et al. 1999)

1.10×10^{-3} , 6.34×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

6.50×10^{-9} , 5.60×10^{-7} , 2.60×10^{-5} , 7.00×10^{-4} , 1.30×10^{-2} (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.38×10^{-6} (calculated-SOFA model, Govers & Krop 1998)

4.51×10^{-5} ; 1.22×10^{-8} (supercooled liquid P_L; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 12.93 - 6211/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 8.07 - 3699/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

8.51×10^{-7} , 1.38×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

0.832 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(\text{Pa m}^3/\text{mol})] = 7.58 - 1184/(T/K)$ (Passivirta et al. 1999)

0.417; 0.832 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow}:

6.90 (calculated, Broman et al. 1991)

- 8.02 (calculated-SOFA model, Govers & Krop 1998)
- 7.76 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 7.61 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.95; 8.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
- 7.58 (calculated-QSPR: GRNN model General Regression Neural Network, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.26 (7°C, GC-retention time correlation, Harner et al. 2000)
- 11.01 (GC-retention time indices correlation, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$:

- 2.95 (guppy exposed to fly ash extract, Opperhuizen et al. 1986)
- 3.50, 4.02 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
- 4.93; 4.34 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
- 4.99; 4.94; 5.02 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from nonlinear regression analysis, Loonen et al. 1994b)
- 5.18 (calculated-SOFA model, Govers & Krop 1998)
- 5.29 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
- 6.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 9.45 (calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic $t_{1/2} = 5.4$ h when exposed to sunlight in hexane solution (Doobs & Grant 1979)

photolytic degradation $t_{1/2} = 17.1$ h in extract from fly ash exposed to UV light from a distance of 20 cm in tetradecane solution (Tysklind & Rappe 1991)

$t_{1/2} = 92.4$ h on spruce needle surface under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved PCDD) is $5.02 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{OH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (4.6 - 10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime of 1.5 – 3.4 d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 200 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.210 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1986)

$k_1 = 48, 433 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.44, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}$, $299 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_6\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 687 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.074 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0057 \text{ d}^{-1}$ with $t_{1/2} = 52 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of 1.5×10^6 molecule cm^{-3} , the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991)

$t_{1/2} = 740$ h at 7°C for Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_{1/2} = 14800$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000);

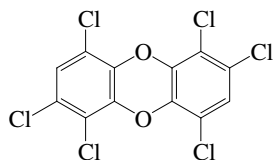
$t_{1/2} = 2400000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 10\text{--}100$ yr in soil for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 2400\,000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Biota: half-lives in gold fish: 1.6 d for PBO treated and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 52$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

8.1.1.23 1,2,4,6,7,9-Hexachlorodibenzo-*p*-dioxin

Common Name: 1,2,4,6,7,9-Hexachlorodibenzo-*p*-dioxin

Synonym: 1,2,4,6,7,9-H₆CDD

Chemical Name: 1,2,4,6,7,9-hexachlorodibenzo-*p*-dioxin

CAS Registry No: 39227-62-8

Molecular Formula: Cl₃C₆HO₂C₆HCl₃

Molecular Weight: 390.861

Melting Point (°C):

238–240 (Pohland & Yang 1972, Rordorf 1987)

Boiling Point (°C):

487.7 (calculated, Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

215.5 (calculated-liquid density, Govers et al. 1990)

302.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

92.1 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

143.238 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1987)

Entropy of Fusion, ΔS_{fus} (J/mol K):

94 (Rordorf 1987, 1989)

Fugacity Ratio at 25°C, F:

Water Solubility (g/m³ or mg/L at 25°C):

0.00187 (calculated-SOFA model, Govers & Krop 1998)

1.71 × 10⁻³, 1.87 × 10⁻³ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

6.80 × 10⁻⁹, 5.9 × 10⁻⁷, 2.7 × 10⁻⁵, 7.5 × 10⁻⁴, 1.40 × 10⁻² (25, 50, 75, 100, 125°C, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.41 × 10⁻⁶ (supercooled liquid P_L, calculated-SOFA model, Govers & Krop 1998)

1.35 × 10⁻⁶, 1.41 × 10⁻⁶ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol at 25°C):

0.0282 (calculated-SOFA model, Govers & Krop 1998)

0.479; 0.0282 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{ow}:

7.85 (shake flask/slow stirring-GC/MS, mixture of fly-ash extract, Sijm et al. 1989a)

7.73 (calculated-SOFA model, Govers & Krop 1998)

7.84; 7.73 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

6.85; 7.05, 7.26, 6.96, 7.30 (observed; calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

5.36 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC} :

8.99 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic $t_{1/2} = 47$ h when exposed to sunlight in hexane solution (Doobs & Grant 1979); solution photolysis $t_{1/2} = 764$ min in *n*-hexadecane at 1.0 m from a GE Model RS sunlamp and surface photolysis $t_{1/2} = 7870$ min on a clean glass surface under the same conditions (Nestrick et al. 1980)

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (4.6 - 5.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (4.6 - 10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 1.5\text{--}3.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dioxin at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 88, 82 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.62, > 0.8 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 58 \text{ L kg}^{-1} \text{ d}^{-1}$, $299 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_6\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a hexa-chlorinated dioxin was calculated to be 1.5–3.4 d for the gas-phase reaction with the OH radical (Atkinson 1991)

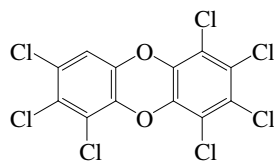
Surface water:

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}100$ yr in sediment for all homologues (estimated, Suzuki et al. 2000).

Soil: degradation $t_{1/2} = 10\text{--}100$ yr in soil or all homologues (estimated, Suzuki et al. 2000).

Biota: half-lives in gold fish: $t_{1/2} = 1.1$ d for PBO treated and $t_{1/2} < 0.9$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.24 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4,6,7,8-H₇CDD

Chemical Name: 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin

CAS Registry No: 35822-46-9

Molecular Formula: Cl₇C₆H₂O₂Cl₄

Molecular Weight: 425.308

Melting Point (°C):

264–265 (Rordorf 1987,1989; Delle Site 1997)

Boiling Point (°C):

507.2 (Rordorf 1987,1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

218.32 (calculated-liquid density, Govers et al. 1990)

323.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

92.5 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

149.792 (Rordorf 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

53.9 (Rordorf 1987; quoted, Ruelle & Kesselring 1997)

30.42 (Friesen & Webster 1990)

Entropy of Fusion, ΔS_{fus} (J/mol K):

100 (Rordorf 1987,1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25°C, F: 0.00442 (assuming ΔS_{fus} = 56 J/mol K and mp at 265°C)

0.00423 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)

6.11 × 10⁻⁵ (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.40 × 10⁻⁶*, 2.42 × 10⁻⁶ (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, calculated, Friesen et al. 1985)

2.30 × 10⁻⁶* (21°C, generator column-HPLC/LSC, measured range 7–41°C, Friesen & Webster 1990)

log [S_L/(mol/L)] = 0.391 – 2820/(T/K) (supercooled liquid, Passivirta et al. 1999)

3.15 × 10⁻⁴ (supercooled liquid S_L, GC-RI correlation, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7.5 × 10⁻¹⁰* (predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987,1989)

3.20 × 10⁻⁸ (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf et al. 1986)

1.02 × 10⁻⁶ (supercooled liquid P_L, GC-RT correlation, Eitzer & Hites 1988, 1991)

1.19 × 10⁻⁶ (supercooled liquid, GC/MS, Eitzer & Hites 1989)

3.20 × 10⁻⁹ (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

4.41 × 10⁻⁹, 5.15 × 10⁻⁹ (solid P_s, calculated from reported P_L, Delle Site 1997)

8.97 × 10⁻⁶ (corrected supercooled liquid P_L, Eitzer & Hites 1998)

6.03 × 10⁻⁷; 5.89 × 10⁻⁷ (supercooled liquid P_L, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

8.97 × 10⁻⁶; 6.79 × 10⁻¹⁰ (supercooled liquid P_L; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/\text{Pa}) = 13.18 - 6661/(T/\text{K})$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 7.95 - 3844/(T/\text{K})$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P/\text{Pa}) = 17.10357 - 7820.06/(T/\text{K})$ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 2.04×10^{-7} , 5.89×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C and the reported temperature dependence equations):

0.133 (calculated-P/C, Shiu et al. 1988)
 4.25 (computed-expert system SPARC, Kollig 1995)
 0.832 (calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 7.56 - 7024/(T/\text{K})$ (Passivirta et al. 1999)
 0.275; 0.832 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

11.29, 11.42, 11.90; 11.03, 11.50, 11.98 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
 11.05, 11.50 (HPLC-RT correlation, Sarna et al. 1984)
 11.38, 10.55; 11.05, 9.69 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
 8.20 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 11.03 (Hansch et al. 1995)
 8.85 (computed-expert system SPARC, Kollig 1995)
 8.40 (calculated-SOFA model, Govers & Krop 1998)
 8.31 (estimated-solubility S_L and regression eq. using lit. K_{ow} values, Passivirta et al. 1999)
 8.051 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 8.27; 8.40 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)
 7.66, 7.43, 8.18, 7.73 (calculated-QSPR: PLS, BPN GRNN, MOD models, Zheng et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.42*; 10.73 (generator column-GC, measured range 20–50°C, calculated, Harner et al. 2000)
 $\log K_{OA} = -3.51 + 4450/(T/\text{K})$; temp range 30–50°C (Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

3.32, 3.74 (fathead minnow, rainbow trout, steady-state, wet weight, Muir et al. 1985)
 3.32, 4.32 (fathead minnow, wet wt. based, lipid based, quoted, Gobas & Schrap 1990)
 2.92, 4.28 (goldfish: PBO treated, control fish, 120-h exposure, Sijm et al. 1993)
 4.68 (guppy, Loonen et al. 1994)
 4.68; 4.08 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.68; 4.68; 4.76 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.68; 4.79 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 6.11, 6.34 (fish muscle $\log BCF_L$ calculated from water, calculated from sediment, Wu et al. 2001)

Sorption Partition Coefficient, $\log K_{oc}$:

6.69 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 5.47 (DOC, De Voogt et al. 1990)
 7.80 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 10.95; 10.0 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

photolytic $t_{1/2} = 11$ h in *n*-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)
 solution photolysis $t_{1/2} = 1800$ min at 1.0 m from a GE Model sunlamp and surface photolysis $t_{1/2} = 3140$ min on clean soft glass surface under the same conditions (Nestrick et al. 1980)

$t_{1/2} = 30$ h in *n*-hexadecane solution (Mamantov 1984);

first order $k = 1.02 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 56.46$ d in spring; $t_{1/2} = 47.33$ d in summer; $t_{1/2} = 87.86$ d in autumn, $t_{1/2} = 155.79$ d in winter and averaged $t_{1/2}$ 2993 d over full year (Choudhary & Webster 1985b, 1986)

photolysis $k = 1.02 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 191$ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 1.24 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 57$ d in spring, $k = 1.48 \times 10^2 \text{ d}^{-1}$ $t_{1/2} = 47$ d in summer, $k = 0.80 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 88$ d in autumn, $k = 0.45 \times 10^2 \text{ d}^{-1}$ $t_{1/2} = 156$ d in winter (Choudhary & Webster 1989)

sunlight photolysis $k = 0.28 \text{ d}^{-1}$ in filtered and sterilized natural water and $k = 0.019 \text{ d}^{-1}$ in (2:32, v/v) distilled water-acetonitrile solution at 50°N (Friesen et al. 1990)

photolytic $t_{1/2} = 53.4$ for native congener and $t_{1/2} = 32.6$ h in ^{13}C -labeled congener in extract from fly ash (Tysklind & Rappe 1991)

tropospheric lifetime was calculated based on the gas-phase reaction rate constant $k = (4.6\text{--}10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with the OH radicals to be 1.5–2.4 d (Atkinson 1991)

photodegradation rate constant $k = 0.18 \text{ h}^{-1}$ with $t_{1/2} = 3.9$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000)

$t_{1/2} = 83.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved PCDD by ozone) is $5.46 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 3.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 4.4$ d based on gas phase OH reactions and a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a heptachlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 56 \text{ d}^{-1}$; $k_2 = 0.042 \text{ d}^{-1}$ (rainbow trout exposed to concn of 11, 55 pg/L, Muir et al. 1985)

$k_1 = 19 \text{ d}^{-1}$; $k_2 = 0.040 \text{ d}^{-1}$ (fathead minnow exposed to concn of 8, 39 pg/L, Muir et al. 1985)

$k_2 = 0.048 \text{ d}^{-1}$ (fathead minnow, Muir & Yarechewski 1988)

$k_2 = 0.0092 \text{ d}^{-1}$ (fathead minnow, quoted, Opperhuizen & Sijm 1990)

$k_2 = 0.0110 \text{ d}^{-1}$ (rainbow trout, quoted, Opperhuizen & Sijm 1990)

$k_1 = 32, 150 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.49, > 0.12 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated, control goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 23 \text{ L kg}^{-1} \text{ d}^{-1}$, $167 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_5CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 456 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.081 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

$k_2 = 0.0061 \text{ d}^{-1}$ with $t_{1/2} = 49$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime $\tau = 4.4$ d for a hepta-PCDD for the gas-phase reaction with OH radicals (Atkinson 1991);

suggested $t_{1/2} = 1500$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000);

first-order photodegradation $k = 0.19 \text{ h}^{-1}$ with $t_{1/2} = 3.9$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: $t_{1/2} = 11$ h in *n*-hexane solution to natural sunlight as well as to fluorescent black light (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982);

direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 56.46$ d in spring; $t_{1/2} = 47.33$ d in summer; $t_{1/2} = 87.86$ d in autumn; $t_{1/2} = 155.79$ d in winter and averaged $t_{1/2} = 2393$ d over full year (Choudhary & Webster 1985b, 1986);

photolysis $t_{1/2} = 190.97$ h in water-acetonitrile (2:3, v/v) at 313 nm and the calculated midday, mid-season direct phototransformation half-lives near water bodies at 40°N latitude: $t_{1/2} = 57$ d in spring, $t_{1/2} = 47$ d in summer, $t_{1/2} = 88$ d in fall and $t_{1/2} = 156$ d in winter (Choudhary & Webster 1989);

$t_{1/2} = 81$ d in sunlit filtered and sterilized surface water and $t_{1/2} = 2.5$ d in surface water of actual pond at 50°N latitude (Friesen et al. 1990);

$t_{1/2} = 53.4$ and 32.6 h in native and ^{13}C -labeled congeners, respectively, in extract from fly ash (Tysklind & Rappe 1991);

suggested $t_{1/2} = 30000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20$ –200 yr in sediment for all homologues (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 10$ –100 yr in soil (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 900000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} = 17.2$ d in fathead minnow (Adams et al. 1986);

$t_{1/2} > 336$ d in carp (Kuehl et al. 1987);

$t_{1/2} = 39$ d in whole body of rainbow trout (Muir et al. 1988; quoted, Muir et al. 1990);

$t_{1/2} = 27.2$ d in lactating cows (Olling et al. 1991);

half-lives in gold fish: $t_{1/2} = 1.4$ d for PBO treated and $t_{1/2} = 5.6$ d for control fish in 120-h exposure studies (Sijm et al. 1993);

$t_{1/2} = 49$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.24.1

Reported aqueous solubilities, vapor pressures and octanol-air partition coefficients of 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin at various temperatures

Aqueous solubility				Vapor pressure		log K_{OA}	
Friesen et al. 1985		Friesen & Webster 1990		Rordorf 1987, 1989		Harner et al. 2000	
generator column-HPLC/LSC		generator column-HPLC/LSC		gas saturation-GC		generator column-GC/ECD	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	log K_{OA}
20	2.40×10^{-6}	7	9.35×10^{-7}	25	7.5×10^{-10}	20	11.66
40	6.30×10^{-5}	11	1.14×10^{-6}	50	8.0×10^{-8}	40	10.774
		17	1.29×10^{-6}	75	4.4×10^{-6}	50	10.225
		21	2.30×10^{-6}	100	1.4×10^{-4}	25	11.42
		26	2.56×10^{-6}	125	2.9×10^{-3}		
		41	6.34×10^{-5}				
		$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 42.4$		$\Delta H_v/(\text{kJ mol}^{-1}) = 92.5$		$\log K_{OA} = a + b/(T/K)$	
		7–41 °C		$\Delta H_{subl}/(\text{kJ mol}^{-1}) = 149.79$		a	–3.51
				$\Delta H_{fus}/(\text{kJ mol}^{-1}) = 53.9$		b	4450
				$\Delta S_{fus}/(\text{J mol}^{-1} \text{K}^{-1}) = 100$		enthalpy of phase change	
						$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 85.10$	

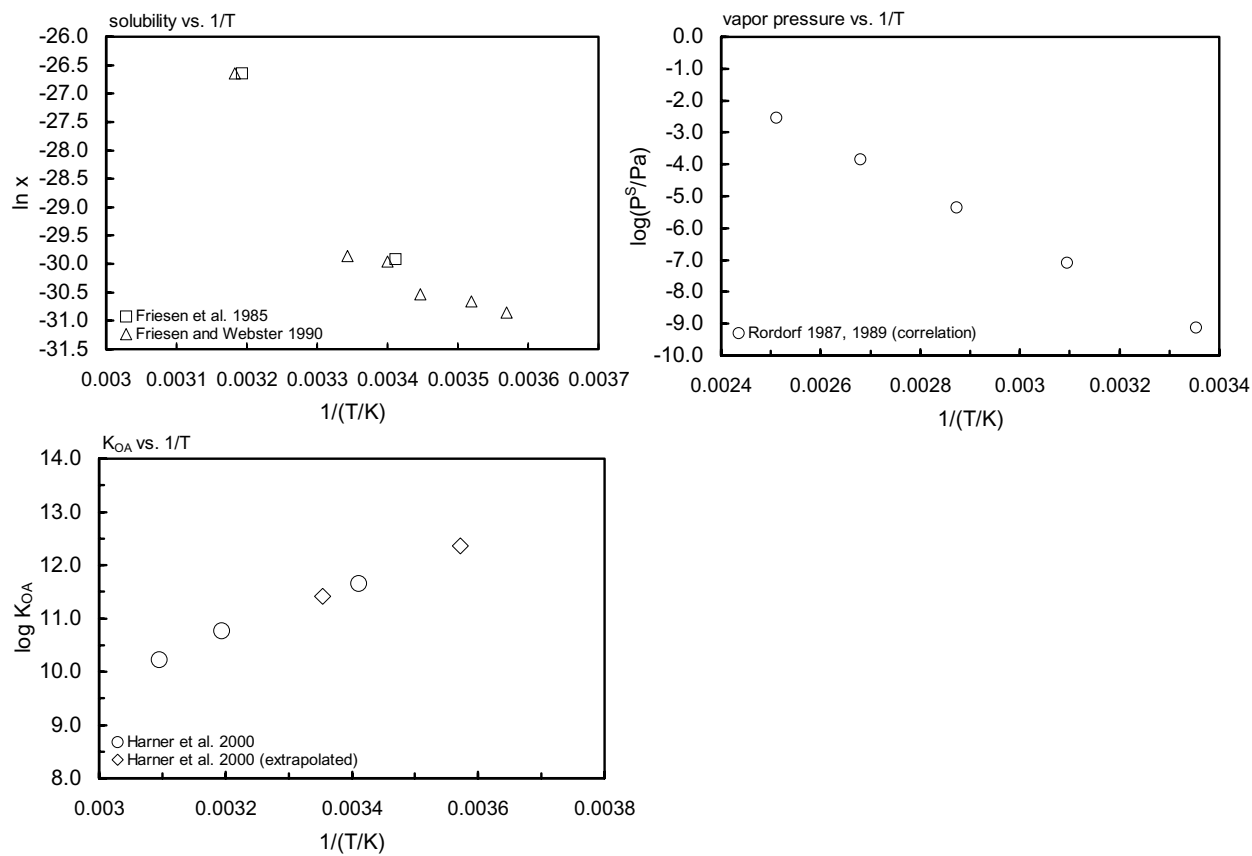
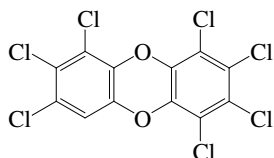


FIGURE 8.1.1.24.1 Logarithm of mole fraction solubility, vapor pressure and K_{OA} versus reciprocal temperature for 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin.

8.1.1.25 1,2,3,4,7,8,9-Heptachlorodibenzo-*p*-dioxin

Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzo-*p*-dioxin

Synonym: 1,2,3,4,7,8,9-H₇CDD

Chemical Name: 1,2,3,4,7,8,9-heptachlorodibenzo-*p*-dioxin

CAS Registry No:

Molecular Formula: Cl₇C₆H₂O₂Cl₄

Molecular Weight: 425.308

Melting Point (°C):

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

222.55 (calculated-liquid density, Govers et al. 1990)

323.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F:

Water Solubility (g/m³ or mg/L at 25°C):

4.57 × 10⁻⁴ (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)

3.97 × 10⁻⁴, 4.57 × 10⁻⁴ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at 25°C):

3.39 × 10⁻⁷ (supercooled liquid S_L, calculated-SOFA model, Govers & Krop 1998)

2.57 × 10⁻⁷, 3.39 × 10⁻⁷ (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Henry's Law Constant (Pa m³/mol):

0.309 (calculated-SOFA model, Govers & Krop 1998)

0.295; 0.309 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, log K_{OW}:

8.25 (calculated-SOFA model, Govers & Krop 1998)

8.22; 8.25 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

4.95 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, log K_{OC}:

9.75 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: photolytic t_{1/2} = 27 h when exposed to sunlight in hexane solution (Dobbs & Grant 1979)

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved PCDD by ozone) is $5.46 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 3.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 4.4 \text{ d}$ based on gas phase OH reactions and a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a heptachlorinated dioxin at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 12 \text{ L kg}^{-1} \text{ d}^{-1}$, $183 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 1.3 \text{ d}^{-1}$, $>3.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 22 \text{ L kg}^{-1} \text{ d}^{-1}$, $167 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for H_7CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a hepta-PCDD was calculated to be 4.4 d for the gas-phase reaction with OH radical (Atkinson 1991)

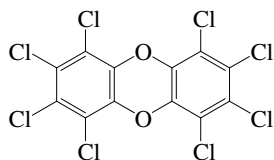
Surface water:

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ in sediment for all homologues (estimated, Suzuki et al. 2000)

Soil: degradation $t_{1/2} = 10\text{--}100 \text{ yr}$ in soil (estimated, Suzuki et al. 2000)

Biota: half-lives in gold fish: $t_{1/2} = 0.5 \text{ d}$ for PBO treated and $t_{1/2} < 0.2 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

8.1.1.26 Octachlorodibenzo-*p*-dioxin

Common Name: Octachlorodibenzo-*p*-dioxin

Synonym: O₈CDD, OCDD

Chemical Name: octachlorodibenzo-*p*-dioxin

CAS Registry No: 3268-87-9

Molecular Formula: C₁₂Cl₈O₂, Cl₄C₆O₂C₆Cl₄

Molecular Weight: 459.751

Melting Point (°C):

331 (Lide 2003)

Boiling Point (°C):

510 (Rordorf 1987, 1989)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

229.6, 229.11 (calculated-liquid density, crystalline volume, Govers et al. 1990)

237.21 (liquid molar volume, Govers et al. 1995)

344.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.7 (Rordorf 1987)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

151.13 (Rordorf 1987)

145.7 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

61.4 (Rordorf 1986, 1987; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

102 (Rordorf 1986, 1987, 1989; Passivirta et al. 1999)

Fugacity Ratio at 25°C, F: 0.000995 (assuming ΔS_{fus} = 56 J/mol K and mp at 331°C)

0.00107 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1987)

0.00115 (calculated-assuming ΔS_{fus} = 56 J/mol K, Shiu et al. 1988)

3.46 × 10⁻⁶ (calculated-ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.0 × 10⁻⁶ (Barrie et al. 1983)

4.0 × 10⁻⁷ (¹⁴C-labeled, generator column-HPLC/LSC, Webster et al. 1983)

4.0 × 10^{-7*} (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Friesen et al. 1985)

4.0 × 10^{-7*} (20°C, ¹⁴C-labeled, generator column-HPLC/LSC, measured range 20–40°C, Webster et al. 1985)

1.8 × 10⁻⁴ (Opperhuizen 1986)

1.0 × 10⁻⁷ (¹⁴C-labeled-LSC, Srinivasan & Fogler 1987)

7.4 × 10^{-8*} (extrapolated, generator column-GC/ECD, measured range 40–80°C, Doucette & Andren 1988a)

S/(mol/L) = 8.32 × 10⁻⁶ exp(0.041·t/°C) (generator column-GC/ECD, temp range 40–80°C, Doucette & Andren 1988a)

log x = -3891/(T/K) - 1.482; temp range 40–80°C (generator column-GC/ECD, Doucette & Andren 1988a)

log [S_L/(mol/L)] = -0.163 - 3212/(T/K) (supercooled liquid, Passivirta et al. 1999)

1.03 × 10⁻⁴ (supercooled liquid S_L, GC-RI correlation; Wang & Wong 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 2.40×10^{-5} , 1.8×10^{-5} (quoted, calculated-volatilization rate, Dobbs & Cull 1982)
- 8.70×10^{-6} (20°C, gas saturation, Webster et al. 1985)
- 1.10×10^{-10} * (gas saturation, Rordorf 1985a,b, 1986a,b, 1987, 1989)
- 2.51×10^{-10} (gas saturation, estimated from vapor pressure vs. temperature plot, Rordorf 1986)
- 2.74×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988)
- 2.77×10^{-7} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1991)
- 2.72×10^{-7} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)
- 0.000280* (120.1°C, average value, gas saturation-GC, measured range 120.1–199.7°C, Rordorf 1990)
- 1.60×10^{-10} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substituted no. plot, Rordorf et al. 1990)
- 2.62×10^{-10} , 2.56×10^{-10} (solid P_s , calculated from reported P_L , Delle Site 1997)
- 2.75×10^{-7} (correcting supercooled liquid P_L value of 1988, Eitzer & Hites. 1998)
- 1.82×10^{-7} ; 1.35×10^{-7} (supercooled liquid P_L , quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- 2.75×10^{-7} ; 4.92×10^{-12} (supercooled liquid P_L ; converted to solid P_s with fugacity ratio F , Passivirta et al. 1999)
- $\log (P/\text{Pa}) = 15.81886 - 7629.38/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.0912* (175°C, Knudsen effusion method, measured range, 175–220°C, Li et al. 2002)
- $\log (P_s/\text{Pa}) = 13.62 - 7429/(T/K)$ (solid, Passivirta et al. 1999)
- $\log (P_L/\text{Pa}) = 8.32 - 4221/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
- $\ln (P/\text{Pa}) = (32.825 \pm 0.153) - (15773 \pm 72)/(T/K)$; temp range 448–493 K (Knudsen effusion method, Li et al. 2002)
- 6.61×10^{-8} (supercooled liquid P_L , GC-RI correlation, Wang & Wong 2002)
- $\ln (P/\text{Pa}) = 38.156 - 16431/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)
- $\ln (P/\text{Pa}) = (36.461 \pm 1.020) - (17529 \pm 487)/(T/K)$; temp range 463–493 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C and the reported temperature dependence equations):

- 0.683 (calculated-P/C, Shiu et al. 1987, 1988)
- 1.32; 0.513 (supercooled liquid P_L , quoted exptl., calculated-SOFA model, Govers & Krop 1998)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 8.34 - 1009/(T/K)$ (Passivirta et al. 1999)
- 0.191; 0.513 (GC-RI correlation; calculated-SOFA, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 8.50 (Bruggeman et al. 1984; quoted, Opperhuizen 1986)
- 12.21, 12.60, 12.97; 11.82, 12.72, 13.08 (HPLC-RT correlation, linear; quadratic regressions, Sarna et al. 1984)
- 11.16, 12.72 (HPLC-RT correlation, Sarna et al. 1984)
- 10.56, 7.53 (calculated-TSA, Doucette 1985)
- 12.26, 11.35; 11.76, 10.07 (HPLC-RT correlation, linear; quadratic regressions, Webster et al. 1985)
- 8.60 (HPLC-RT correlation, Burkhard & Kuehl 1986)
- 7.59 (generator column-GC/ECD, Doucette & Andren 1987)
- 7.83 (HPLC-RT correlation, Doucette and Andren 1988b)
- 8.60 (calculated, Endicott & Cook 1994)
- 7.59, 8.60 (quoted, Hansch et al. 1995)
- 9.31 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 8.450 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 8.48 (GC-RI correlation, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.80 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
- 13.0 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

- 1.93, 3.35 (fathead minnow; rainbow trout, steady-state, wet weight, Muir et al. 1985, 1986)
- 1.53–2.13; 3.35 (fathead minnow, rainbow trout, Muir et al. 1986)

- 1.00, 2.05 (human fat, calculated-lipid base, Geyer et al. 1987)
 0.903, 1.93 (human fat, calculated-wet wt. base, Geyer et al. 1987)
 1.90, 3.10 (guppy: in whole fish, in lipid, Gobas et al. 1987)
 6.33; 5.85 (plant parts, calculated-vapor pressure; calculated-vapor pressure & HLC, Reischl et al. 1989)
 2.85, 3.97 (guppy: wet weight base, lipid weight base, Gobas & Schrap 1990; quoted, Devillers et al. 1996)
 2.85 (predicted for biota held in lake enclosures exposed to water concentration of 0.1 ng/g for 0–10 d, Servos et al. 1992b)
 2.15 (caged invertebrates exposed to water concn. 2.0 ng/L for 0–10 d, Servos et al. 1992b)
 2.32 (caged unionid clams exposed to water concn. 2.9 ng/L for 0–10 d, Servos et al. 1992b)
 2.32 (caged white suckers gill exposed to water concn. 2.9 ng/L for 0–10 d, Servos et al. 1992b)
 1.89 (caged white suckers carcass exposed to water concn. 1.1 ng/L for 0–10 d, Servos et al. 1992b)
 2.42 (caged invertebrates exposed to water concn. 0.6 ng/L for 14–24 d, Servos et al. 1992b)
 2.34 (caged unionid clams exposed to water concn. 0.5 ng/L for 14–24 d, Servos et al. 1992b)
 2.75 (caged white suckers gill exposed to water concn. 1.3 ng/L for 14–24 d, Servos et al. 1992b)
 2.24 (caged white suckers carcass exposed to water concn. 0.4 ng/L for 14–24 d, Servos et al. 1992b)
 3.97 (caged white suckers gill exposed to water concn. 2.8 ng/L for 0–104 d, Servos et al. 1992b)
 3.95 (caged white suckers carcass exposed to water concn. 2.7 ng/L for 0–104 d, Servos et al. 1992b)
 4.13; 3.38 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.13; 4.34; 4.38 (guppy, 21-d exposure, lipid wt basis: measured- $C_{\text{fish}}/C_{\text{W}}$; calculated; rate constant ratio k_1/k_2 from nonlinear regression analysis, Loonen et al. 1994b)
 3.38 (*Poecilia reticulata*, quoted, Devillers et al. 1996)
 4.13; 4.39 (lipid wt base, quoted exptl., calculated-SOFA model, Govers & Krop 1998)
 7.15, 8.45 (fish 5% lipid: BCF_{W} , BCF_{L} , Geyer et al. 2000)
 8.02, 7.53 (fish muscle log BCF_{L} calculated from water, sediment, Wu et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 5.92 (estimated DOC partition coeff., Muir et al. 1985)
 7.08 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 5.92 (DOC, De Voogt et al. 1990)
 7.90 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 10.96; 10.5 (sediment/water, quoted exptl., calculated-SOFA model, Govers & Krop 1998)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

- photolytic $t_{1/2} = 16$ h by both natural sunlight and fluorescent black light in hexane solution, (Dobbs & Grant 1979; quoted, Choudhary & Webster 1982)
 solution photolysis $t_{1/2} = 1460$ min at 1.0 m from a GE Model RS sunlamp and surface photolysis of 46900 min on clean soft glass surface under the same conditions (Nestrick et al. 1980);
 photolysis $t_{1/2} = 24.3$ h in hexadecane solution (Mamantov 1984)
 photolysis $k = 1.06 \times 10^{-6} \text{ s}^{-1}$ in water acetonitrile (2:3, v/v) solution at 313 nm and calculated direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 20.53$ d in spring; $t_{1/2} = 17.85$ d in summer; $t_{1/2} = 31.26$ d in autumn; $t_{1/2} = 50.45$ d in winter; and $t_{1/2} = 863$ d averaged over full year (Choudhary & Webster 1986; quoted, Muto et al. 1991)
 photolysis rate constant $k = 1.06 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 183.95$ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct sunlight photolysis first-order rate constant in aquatic bodies for various seasons: $k = 3.45 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 21$ d in spring, $k = 3.97 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 18$ d in summer, $k = 2.27 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 31$ d in fall, $k = 1.40 \times 10^2 \text{ d}^{-1}$ with $t_{1/2} = 50$ d in winter (Choudhary & Webster 1989)
 photolysis decay rate constants when irradiated with UV light at 254 nm: $k(\text{calc}) = 1.77 \times 10^{-5} \text{ s}^{-1}$, $4.62 \times 10^{-5} \text{ s}^{-1}$ for fly ash suspensions in distilled water, $k(\text{calc}) = 1.42 \times 10^{-5} \text{ s}^{-1}$ for fly ash suspensions in water-acetonitrile solution (2:3, v/v), and $k(\text{calc}) = 2.74 \times 10^{-5} \text{ s}^{-1}$ for fly ash suspensions in water-acetonitrile solution (2:3, v/v) with ozone (Muto et al. 1991);

photolytic $t_{1/2} = 37.3$ h-native congener, $t_{1/2} = 29.6$ h for ^{13}C -labeled congener in extract of fly ash and in tetradecane solution (Tysklind & Rappe 1991);

photolysis $k = 1.6 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 440$ min in pure water, and $k = 1.0 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 680$ min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000);

photodegradation $k = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 5.8$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000)

$t_{1/2} = 105$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved OCDD by ozone) is $1.51 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline condition at pH 10 and 20°C (Palauscek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 1.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and a calculated tropospheric lifetime $\tau = 9.6$ d based on gas phase OH reactions and a 12-h average daytime OH radical concentration of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for OCDD at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 142 \text{ d}^{-1}$; $k_2 = 0.053 \text{ d}^{-1}$ (fathead minnow, flow-through system, Muir et al. 1985; quoted, Adams et al. 1986)

$k_1 = 11 \text{ d}^{-1}$; $k_2 = 0.12 \text{ d}^{-1}$ (rainbow trout, flow-through system, Muir et al. 1985)

$k_1 = 17, 5.0 \text{ d}^{-1}$; $k_2 = 0.103, 0.142 \text{ d}^{-1}$ (rainbow trout exposed to concn of 20, 415 ng/L, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)

$k_1 = 142 \text{ d}^{-1}$; $k_2 = 0.053 \text{ d}^{-1}$ (fathead minnow exposed to concn of 9 ng/L, Muir et al. 1986; quoted, Opperhuizen & Sijm 1990)

$k_2 = 0.046 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986; quoted, Opperhuizen & Sijm 1990)

$k_1 = 984 \text{ d}^{-1}$; $k_2 = 1.4 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

$k_1 = 60 \text{ d}^{-1}$; $k_2 = 0.12 \text{ d}^{-1}$ (filter-feeder, Servos et al. 1992b)

$k_1 = 30 \text{ d}^{-1}$; $k_2 = 0.08 \text{ d}^{-1}$ (small fish, estimated from Muir et al. 1985 and Servos et al. 1989, Servos et al. 1992b)

$k_1 = 275 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 119 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994)

$k_2 = 0.0053 \text{ d}^{-1}$ with $t_{1/2} = 57$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: atmospheric lifetime of ~7–8 h for reaction with hydroxyl radicals (Atkinson 1987);

estimated reaction $k = 0.0015 \text{ h}^{-1}$ (Paterson et al. 1990);

photodegradation $t_{1/2} = 270$ h in a rotary photo-reactor adsorbed to clean silica gels by filtered $\lambda < 290$ nm of light (Koester & Hites 1992);

tropospheric lifetime $\tau = 9.6$ d, calculated based on gas-phase reaction with OH radicals (Atkinson 1991);

suggested $t_{1/2} = 3950$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000);

first-order photodegradation $k = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 5.8$ h when loaded on TiO_2 film under UV ($\lambda > 300$ nm) or solar light irradiation in the air (Choi et al. 2000).

Surface water: first order photolytic rate constant $k < (0.3 - 2.7) \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 7 - 16$ h exposed to sunlight in hexane solution (Dobbs & Grant 1979);

direct sunlight photolysis half-lives in aquatic bodies at latitude 40°N for various seasons: $t_{1/2} = 20.53$ in spring, $t_{1/2} = 17.85$ d in summer; $t_{1/2} = 31.26$ d in fall; $t_{1/2} = 50.45$ d in winter and $t_{1/2} = 853.22$ d averaged over full year (Choudhary & Webster 1986);

$k = 1.064 \times 10^{-6} \text{ s}^{-1}$ in water-acetonitrile (2:3, v/v) under direct sunlight (Choudhary & Webster 1985a, 1986);

photolysis $t_{1/2} = 183.95$ h in water-acetonitrile solution (2:3, v/v) at 313 nm and the calculated midday, mid-season direct photolysis half-lives near water bodies at 40°N latitude: $t_{1/2} = 21$ d in spring, $t_{1/2} = 18$ d in summer, $t_{1/2} = 31$ d in fall and $t_{1/2} = 50$ d in winter (Choudhary & Webster 1989);

$t_{1/2} = 4.0$ d in the water column of an experimental lake in northwestern Ontario (Servos et al. 1989);

transformation $k(\text{calc}) = 1.6 \times 10^{-3} \text{ h}^{-1}$ in simulated lake enclosure (Servos et al. 1992a);

photolysis $k = 1.6 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 440$ min in pure water, and $k = 1.0 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 680$ min in 60% acetonitrile/water aqueous solutions at 300 nm (Kim & O'Keefe 2000);

suggested $t_{1/2} = 79000$ h at 7°C for Baltic Proper environments (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: estimated reaction $k = (5.0 \times 10^{-3} - 1.0 \times 10^{-6}) \text{ h}^{-1}$ (Paterson et al. 1990);

$t_{1/2}(\text{calc}) = 10$ yr with a transformation rate constant $k = 7.9 \times 10^{-6} \text{ h}^{-1}$ (Servos et al. 1992a)

$t_{1/2} = 0.2 - 142$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 20-200$ yr in sediment for all homologues (estimated, Suzuki et al. 2000)

suggested $t_{1/2} = 130000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Soil: undergoes photoreduction on soil surfaces to lower chlorinated congeners (Kieatiwong et al. 1990);

estimated reaction $k = 7.0 \times 10^{-7} \text{ h}^{-1}$ (Paterson et al. 1990)

$t_{1/2} > 10$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 10-100$ yr in soil (estimated, Suzuki et al. 2000)

suggested $t_{1/2} = 130000$ h at 7°C for Baltic Proper environments (Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2} \sim 21$ d from rat (Norback et al. 1975; quoted, Birnbaum 1985);

elimination $t_{1/2} = 13.9$ d for fathead minnow (Muir et al. 1985, Adams et al. 1986);

elimination $t_{1/2} = 5-13$ d for both rainbow trout and fathead minnow (Muir et al. 1986);

mean biological $t_{1/2} \sim 15$ d in rainbow trout (Niimi 1986);

$t_{1/2} = 15$ d in rainbow trout (Niimi & Oliver 1986; quoted, Muir et al. 1986,1990);

$t_{1/2} = 57$ d in blue mussel for 99-d exposure experiment (Hektoen et al. 1994).

TABLE 8.1.1.26.1

Reported aqueous solubilities of octachlorodibenzo-*p*-dioxin at various temperatures

Webster et al. 1985		Friesen et al. 1985		Doucette & Andren 1988a	
generator column-HPLC/LSC		generator column-HPLC/LSC		generator column-GC/ECD	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20	4.0×10^{-7}	20	4.0×10^{-7}	40	3.11×10^{-7}
40	2.0×10^{-6}	40	2.0×10^{-6}	60	1.82×10^{-6}
				80	7.87×10^{-6}

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 74.5$
at $40-80^{\circ}\text{C}$

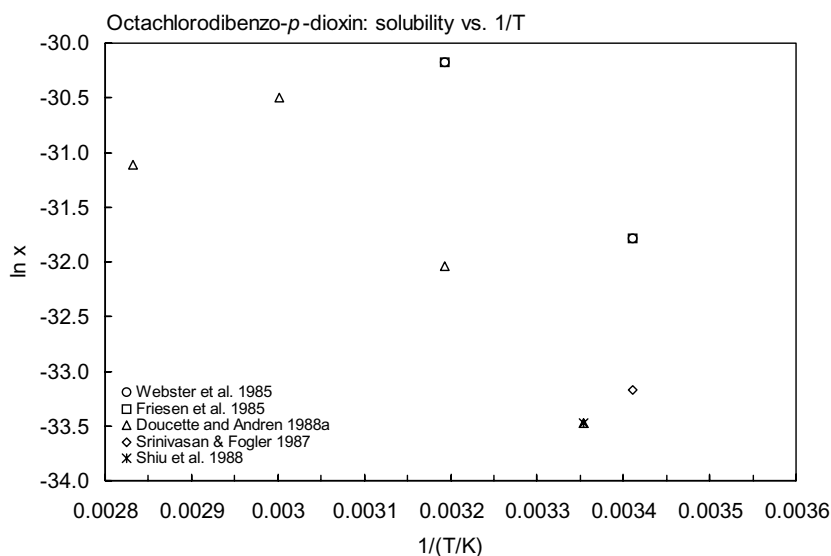


FIGURE 8.1.1.26.1 Logarithm of mole fraction solubility versus reciprocal temperature for octachlorodibenzo-*p*-dioxin.

TABLE 8.1.1.26.2
Reported vapor pressures of octachlorodibenzo-*p*-dioxin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Rordorf 1987, 1989		Rordorf 1990		Li et al. 2002	
gas saturation-GC		gas saturation-GC		Knudsen effusion	
<i>t</i> /°C	P/Pa	<i>t</i> /°C	P/Pa	<i>t</i> /°C	P/Pa
average					
25	1.1×10^{-10}	120.1	0.000280	175	0.0912
50	1.3×10^{-8}	124.9	0.000447	180	0.141
75	7.2×10^{-7}	129.9	0.000737	185	0.204
100	2.4×10^{-5}	134.9	0.00125	190	0.291
125	5.1×10^{-4}	139.9	0.00209	195	0.416
		144.8	0.00352	200	0.607
$\Delta H_v/(\text{kJ mol}^{-1}) = 86.7$		149.8	0.00581	205	0.838
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 151.13$		154.7	0.00949	210	1.20
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 61.4$		159.7	0.0153	215	1.67
$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 102$		165.0	0.0253	220	2.32
		170.0	0.0406		
		175.0	0.0654	eq. 1	P/Pa
		180.0	0.1023	A	32.825
		185.0	0.1585	B	15773
		189.8	0.2515		
		194.7	0.383		
		199.7	0.584		
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 149.822$			
		120 – 200 °C			

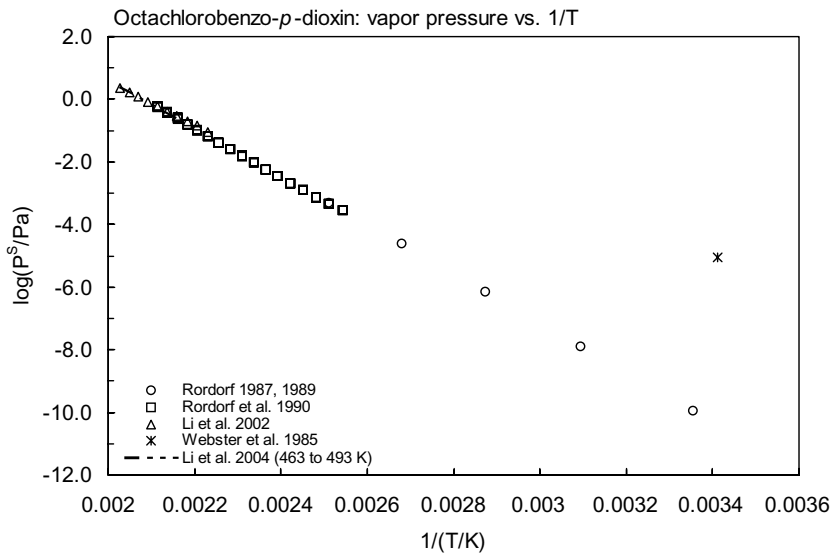


FIGURE 8.1.1.26.2 Logarithm of vapor pressure versus reciprocal temperature for octachlorodibenzo-*p*-dioxin.

8.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 8.2.1
Summary of physical properties of some chlorinated dioxins

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol	
							from ρ ^(a)	Le Bas
Dibenzo- <i>p</i> -dioxin	262-12-4	C ₁₂ H ₈ O ₂	184.191	120.5		0.116	143.82	177.0
1-Chloro-	39227-53-7	C ₁₂ H ₇ O ₂ Cl	218.636	105.5		0.162	157.41	197.9
2-Chloro-	39227-54-8	C ₁₂ H ₇ O ₂ Cl	218.636	89		0.236	154.85	197.9
2,3-Dichloro-	29446-15-9	C ₁₂ H ₆ O ₂ Cl ₂	253.081	164	358	0.0433	164.07	218.8
2,7-Dichloro-	33857-26-0	C ₁₂ H ₆ O ₂ Cl ₂	253.081	201	374.5	0.0188	165.88	218.8
2,8-Dichloro-	38964-22-6	C ₁₂ H ₆ O ₂ Cl ₂	253.081	151		0.0580	165.88	218.8
1,2,4-Trichloro-	39227-58-2	C ₁₂ H ₅ O ₂ Cl ₃	287.526	129	375	0.0954	179.66	239.7
1,3,7-Trichloro-	67026-17-5	C ₁₂ H ₅ O ₂ Cl ₃	287.526	148.5	398	0.0614	179.11	239.7
2,3,7-Trichloro-	33857-28-2	C ₁₂ H ₅ O ₂ Cl ₃	287.526	162–163	408.4	0.0448	175.10	239.7
1,2,3,4-Tetrachloro-	30746-58-8	C ₁₂ H ₄ O ₂ Cl ₄	321.971	189	419	0.0246	186.71	260.6
1,2,3,7-Tetrachloro-	67028-18-6	C ₁₂ H ₄ O ₂ Cl ₄	321.971	172	438.3	0.0361	186.52	260.6
1,2,7,8-Tetrachloro-	34816–53–0	C ₁₂ H ₄ O ₂ Cl ₄	321.971				186.88	260.6
1,3,6,8-Tetrachloro-	30746-58-8	C ₁₂ H ₄ O ₂ Cl ₄	321.971	219	438.3	0.0125	192.34	260.6
1,3,7,8-Tetrachloro-	50585-46-1	C ₁₂ H ₄ O ₂ Cl ₄	321.971	193.5–195	438.3	0.0218	188.33	260.6
1,3,7,9-Tetrachloro-	62470-53-5	C ₁₂ H ₄ O ₂ Cl ₄	321.971				192.34	260.6
2,3,7,8-Tetrachloro-	1746-01-6	C ₁₂ H ₄ O ₂ Cl ₄	321.971	295		0.00224	184.32	260.6
1,2,3,4,7-Pentachloro-	39227-61-7	C ₁₂ H ₃ O ₂ Cl ₅	356.416	195	464.7	0.0215	197.74	281.5
1,2,3,7,8-Pentachloro-	40321-76-4	C ₁₂ H ₃ O ₂ Cl ₅	356.416		464.7		195.74	281.5
1,2,4,7,8-Pentachloro-	58802-08-7	C ₁₂ H ₃ O ₂ Cl ₅	356.416	206	464.7	0.0168	199.91	281.5
1,2,3,4,7,8-Hexachloro-	39227-26-8	C ₁₂ H ₂ O ₂ Cl ₆	390.861	273	487.7	0.00369	206.96	302.4
1,2,3,6,7,8-Hexachloro-	57653-85-7	C ₁₂ H ₂ O ₂ Cl ₆	390.861	285	487.7	0.00281	207.16	302.4
1,2,3,7,8,9-Hexachloro-	19408-74-3	C ₁₂ H ₂ O ₂ Cl ₆	390.861	243–244	487.7	0.00718	207.16	302.4
1,2,4,6,7,9-Hexachloro-	39227-62-8	C ₁₂ H ₂ O ₂ Cl ₆	390.861	238–240	487.7	0.00795	215.50	302.4
1,2,3,4,6,7,8-Heptachloro-	35822-46-9	C ₁₂ HO ₂ Cl ₇	425.308	265	507.2	0.00442	218.38	323.3
1,2,3,4,7,8,9-Heptachloro-		C ₁₂ HO ₂ Cl ₇	425.308				222.55	323.3
Octachloro-	3268-87-9	C ₁₂ O ₂ Cl ₈	459.751	331	510	0.000995	229.60	344.2

*Assuming ΔS_{fus} = 56 J/mol K; (a) Govers et al. 1990 (at 25°C).

TABLE 8.2.2

Selected physical-chemical properties of some chlorinated dioxins at 25°C

Compound	Selected properties					log K _{OW}	Henry's law constant
	Vapor pressure		Solubility				H/(Pa·m ³ /mol)
	P ^S /Pa	P _L /Pa	S/(mg/m ³)	C ^S /(mmol/m ³)	C _L /(mmol/m ³)		calculated P/C
Dibenzo- <i>p</i> -dioxin	0.055	0.474	865	4.696	40.48	4.30	11.71
1-CDD	0.012	0.074	417	1.907	11.77	4.75	6.292
2-CDD	0.017	0.0730	295	1.350	5.717	5.00	12.60
2,3-DCDD	0.00039	0.00901	14.9	0.0589	1.360		6.624
2,7-DCDD	0.00012	0.00811	3.75	0.0148	0.788	6.38	8.098
2,8-DCDD	0.00014	0.00241	16.7	0.0660	1.138		2.122
1,2,4-T ₃ CDD	0.0001	0.00105	8.41	0.0293	0.306		3.419
1,2,3,4-T ₄ CDD	6.40 × 10 ⁻⁶	2.60 × 10 ⁻⁴	0.55	0.0017	0.0694	6.60	3.747
1,2,3,7-T ₄ CDD	1.00 × 10 ⁻⁶	2.77 × 10 ⁻⁵	0.42	0.0013	0.0361	6.90	0.766
1,3,6,8-T ₄ CDD	7.00 × 10 ⁻⁷	5.60 × 10 ⁻⁵	0.32	0.000994	0.0795	7.18	0.704
2,3,7,8-T ₄ CDD	2.00 × 10 ⁻⁷	8.93 × 10 ⁻⁵	0.0193	0.00006	0.0268	6.80	3.336
1,2,3,4,7-P ₅ CDD	8.80 × 10 ⁻⁸	4.09 × 10 ⁻⁶	0.118	0.000331	0.0154	7.40	0.266
1,2,3,4,7,8-H ₆ CDD	5.10 × 10 ⁻⁹	1.38 × 10 ⁻⁶	0.006	1.54 × 10 ⁻⁵	0.00416	7.80	0.332
1,2,3,4,6,7,8-H ₇ CDD	7.50 × 10 ⁻¹⁰	1.70 × 10 ⁻⁷	0.0024	5.64 × 10 ⁻⁶	0.00128	8.00	0.133
OCDD	1.10 × 10 ⁻¹⁰	1.11 × 10 ⁻⁷	0.000074	1.61 × 10 ⁻⁷	0.00016	8.20	0.683

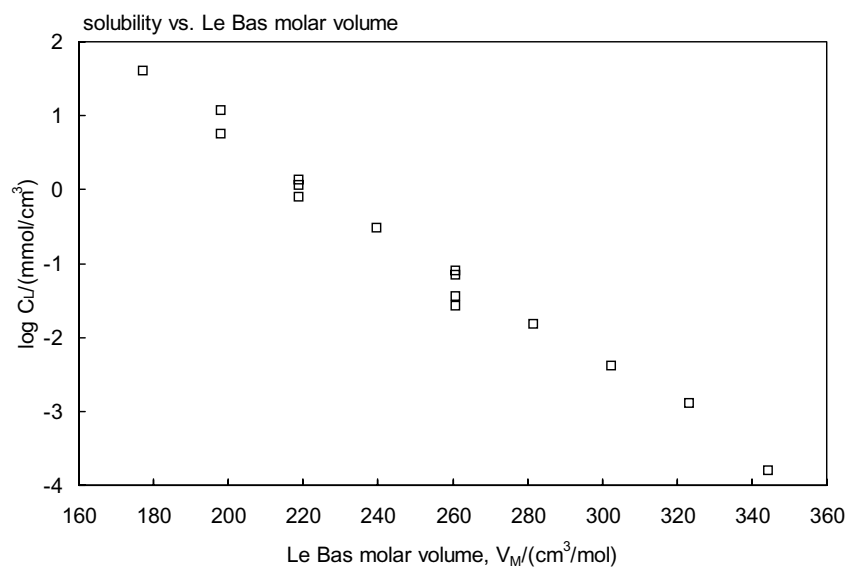
TABLE 8.2.3

Suggested half-life classes of polychlorinated dibenzo-*p*-dioxins in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Dibenzo- <i>p</i> -dioxin	3	3	6	7
2-CDD	4	4	7	8
2,7-DCDD	4	4	7	8
2,8-DCDD	4	4	7	8
1,2,4-T ₃ CDD	4	4	7	8
1,2,3,4-T ₄ CDD	4	5	8	9
2,3,7,8-T ₄ CDD	4	5	8	9
1,2,3,4,7-P ₅ CDD	5	5	8	9
1,2,3,4,7,8-H ₆ CDD	5	6	9	9
1,2,3,4,6,7,8-H ₇ CDD	5	6	9	9
OCDD	5	7	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55888 (~ 6 years)	> 30,000

FIGURE 8.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

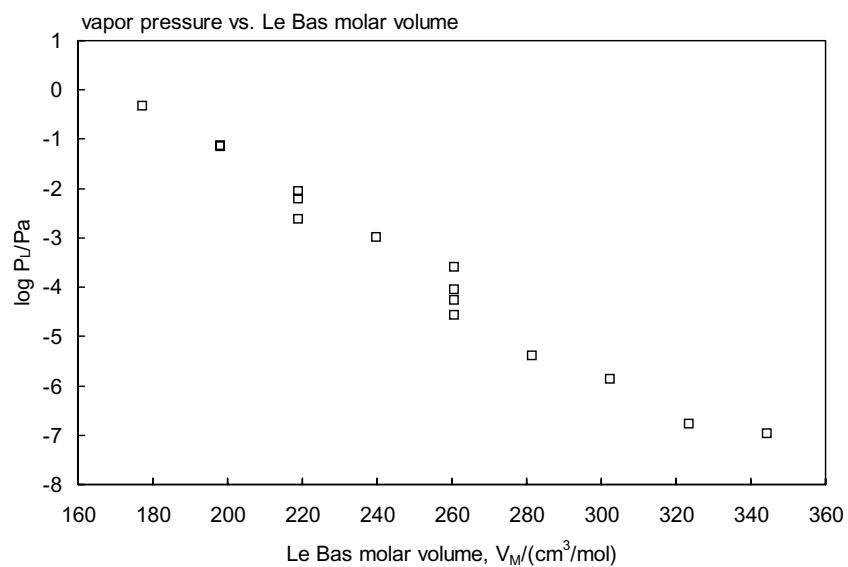


FIGURE 8.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

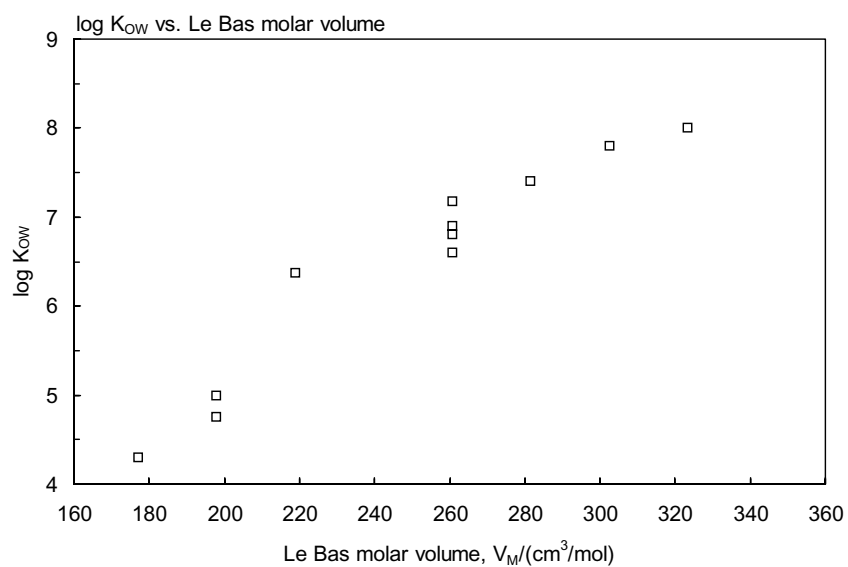


FIGURE 8.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

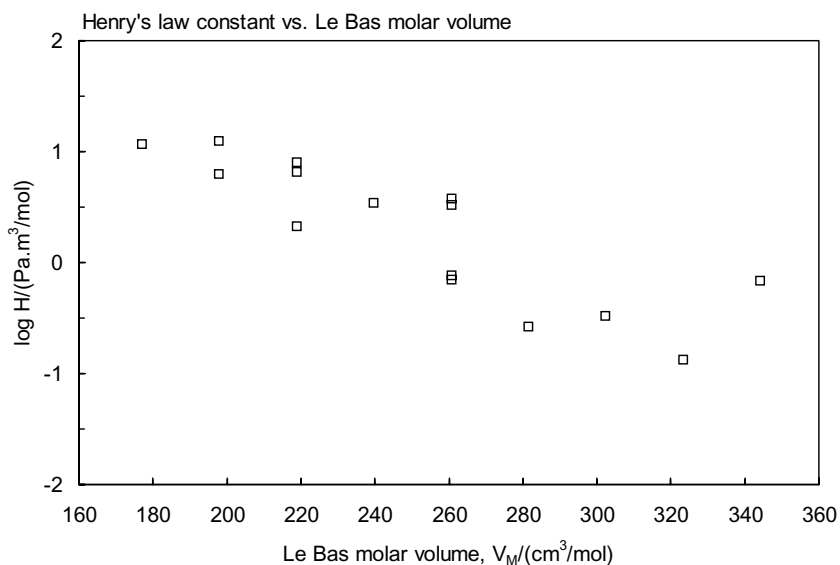


FIGURE 8.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated dibenzo-*p*-dioxins.

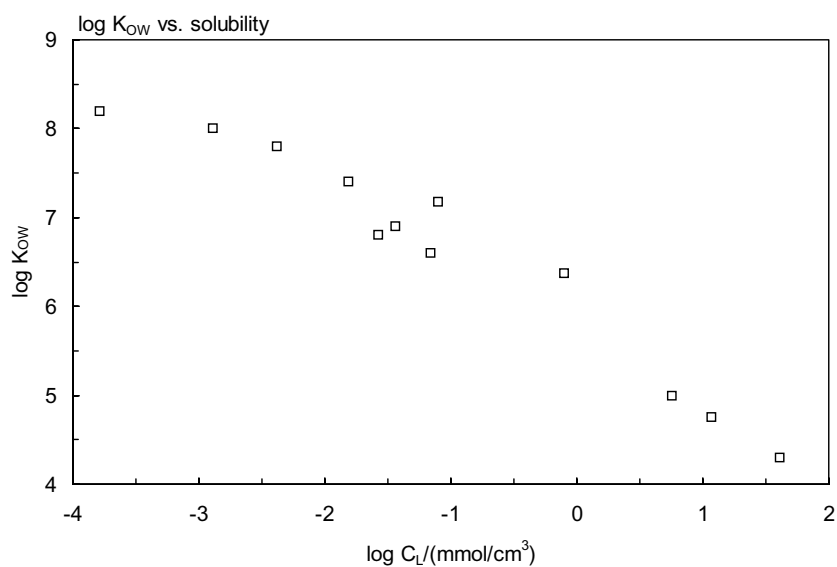


FIGURE 8.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated dibenzo-*p*-dioxins.

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9 Chlorinated Dibenzofurans

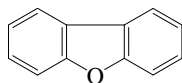
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9.1 LIST OF CHEMICALS AND DATA COMPILATIONS

9.1.1 DIBENZOFURAN AND CHLORINATED DIBENZOFURANS

9.1.1.1 Dibenzofuran



Common Name: Dibenzofuran

Synonym: diphenylene oxide

Chemical Name: dibenzofuran

CAS Registry No: 132-64-9

Molecular Formula: $C_{12}H_8O$, $C_6H_4OC_6H_4$

Molecular Weight: 168.191

Melting Point ($^{\circ}C$):

86.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

287 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0886 ($99^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

154.4 ($99^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

147.8 (Ruelle & Kesselring 1997)

176.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

65.4 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

85.63 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.6 (Rordorf 1987, 1989; quoted, Ruelle & Kesselring 1997)

18.6 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

54 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.249 (mp at $86.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3.11 (Lu et al. 1978)

10.03 (shake flask-HPLC/UV, Banerjee et al. 1980)

6.56 (selected average, Pearlman et al. 1984)

4.22* (generator column-GC, measured range $4-39.8^{\circ}C$, Doucette & Andren 1988a)

$S/(mol/L) = 8.32 \times 10^{-6} \exp(0.041 \cdot t/^{\circ}C)$; temp range $4-40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a); or

$\log x = -1558/(T/K) - 1.135$; temp range $4-40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

3.36 (calculated-TSA, Dickhut et al. 1994)

4.30 (computed-expert system SPARC, Kollig 1995)

$4.75^* \pm 0.22$ (generator column-HPLC/UV, Shiu et al. 1997)

4.69 ± 0.18 (shake flask-GC, Shiu et al. 1997)

2.43 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle Kesselring 1997)

17.21; 62.49 (supercooled liquid S_L , quoted lit. average; calculated-SOFA-Solubility parameters for Fate Analysis model, Govers & Krop 1998)

$\ln x = -1.6385 - 3842.2/(T/K)$; temp range $5-50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.276* (gas saturation, extrapolated-Antoine eq. from exptl. data, measured temp range, 30–70°C, Hansen & Eckert 1986)
- 0.506* (26°C, gas saturation exptl. data, measured range 49–74°C, Sato et al. 1986)
- 0.466 (gas saturation-GC, extrapolated-Antoine eq. derived from exptl. data, temp range 49–74°C, Sato et al. 1986)
- 0.35* (gas saturation-GC, measured range 25–125°C Rordorf 1986, 1989)
- 2.026 (extrapolated liquid value P_L , Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 5.8968 - 1851.27/(-82.64 + T/K)$; temp range 403–559 K (Antoine eq., Stephenson & Malanowski 1987)
- 0.40 (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
- $\log(P/\text{mmHg}) = 17.6646 - 3.1989 \times 10^3/(T/K) - 3.3346 \cdot \log(T/K) + 6.0686 \times 10^{-10} \cdot (T/K) + 4.4676 \times 10^{-7} \cdot (T/K)^2$; temp range 356–838 K (vapor pressure eq., Yaws et al. 1994)
- 0.360 (computed-expert system SPARC, Kollig 1995)
- 0.708; 0.123 (supercooled liquid P_L , quoted exptl. or exptl. average; calculated-SOFA model (Solubility parameters of Fate Analysis model), Govers & Krop 1998)
- $\log(P/\text{Pa}) = 13.17192 - 4083/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
- 0.429 (gas saturation-HPLC/fluorescence, de Seze et al. 2000)
- 0.398* (25.2°C, Knudsen effusion method, measured range 20.2–45°C Li et al. 2002)
- $\ln(P/\text{Pa}) = 33.54 - 10313/(T/K)$; temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2002 2004)
- $\ln(P/\text{Pa}) = (32.203 \pm 0.576) - (9880.4 \pm 176)/(T/K)$; temp range 295–318 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C):

- 14.16 (calculated-P/C with selected values)
- 14.20 (computed-expert system SPARC, Kollig 1995)
- 21.38, 13.80 (calculated-P/C, Govers & Krop 1998)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 4.12 (HPLC-RT correlation, Veith et al. 1979a)
- 4.12 (Hansch & Leo 1979)
- 4.17 (shake flask-HPLC/UV, Banerjee et al. 1980)
- 3.91, 4.12, 4.18; 3.96, 4.10, 4.17 (HPLC-RT, linear regressions; quadratic regressions, Sarna et al. 1984)
- 3.92 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
- 4.31 (generator column-GC/ECD, both phases, Doucette & Andren 1987)
- 3.86 (HPLC-RT correlation, Doucette & Andren 1988b)
- 4.21, 3.81 (shake flask-HPLC, TLC-RT correlation, De Voogt et al. 1990)
- 4.12 (recommended, Sangster 1993)
- 4.12 (recommended, Hansch et al. 1995)
- 4.27 (generator column-HPLC/UV, Shiu et al. 1997)
- 4.273* (shake flask-HPLC/UC, measured S_O and S_W , Shiu et al. 1997)
- 4.09 ± 0.19 , 4.12 ± 0.63 ; 4.12 (HPLC- k' correlation: ODS-65 column, Diol-35 column; quoted lit average value, Helweg et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 3.13 (fathead minnow, 28 d exposure, Veith et al. 1979b)
- 3.13, 2.80 (quoted exptl., calculated- K_{OW} , Mackay 1982)
- 3.13, 3.13 (quoted exptl., calculated-MCI χ , Sabljic 1987)

- 3.13 (calculated- K_{OW} , Isnard & Lambert 1989)
 3.68; 4.08 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.80 (computed- K_{OW} , Kollig 1995)
 4.15 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)
 3.45 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 3.84 (soil-pore-water partition coeff. for Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ corresponding to an atmospheric lifetime of about 8 h (Atkinson 1987a)

$k_{OH} = 3.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1987b)

$t_{1/2} = 1.9\text{--}19 \text{ h}$ based on estimated rate constant with OH radicals in air (Howard 1991)

$k_{OH} = 31 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ the tropospheric lifetime was calculated to be 0.5 d (Atkinson 1991)

$k_{OH} = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and with calculated tropospheric lifetime of 3.7 d; $k_{NO_3} < 7 \times 10^{-30} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $>7 \text{ yr}$ and $k_{O_3} < 8 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with O_3 with calculated tropospheric lifetime $>250 \text{ d}$ at room temp. (Kwok et al. 1994)

$k_{OH}(\text{exptl}) = 3.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ corresponding to a tropospheric lifetime of 3.7 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation: biodegradation $t_{1/2} \sim 168\text{--}672 \text{ h}$ and anaerobic $t_{1/2} = 672\text{--}2688 \text{ h}$, based on aerobic acclimated and unacclimated groundwater die-away test data (Lee et al. 1984; quoted, Ward et al. 1986; Howard et al. 1991); nonautoclaved groundwater samples at hazardous waste site with a concentration of approximate 0.09 mg/L are degraded by microbes at rates about 30% per week while the levels of the controls decreased only about half that rate (Lee et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the calculated atmospheric lifetime range from $\sim 60\text{--}120 \text{ h}$ (Atkinson 1987a);

$t_{1/2} = 1.9\text{--}19 \text{ h}$, based on estimated rate constants for reaction with OH radicals (Howard et al. 1991);

the tropospheric lifetime was calculated 0.5 d for the gas-phase reaction for OH radicals using a 12-h average daytime OH radical concn of 1.5×10^6 (Atkinson 1991);

calculated room temp. tropospheric lifetimes of 3.7 d for reaction with OH radical, $>7 \text{ yr}$ with NO_3 radical, and $>250 \text{ d}$ for reaction with O_3 (Kwok et al. 1994);

room temp. tropospheric lifetime was calculated to be 3.7 d for reaction with OH radical (Kwok et al. 1995).

Surface water: $t_{1/2} = 168\text{--}672 \text{ h}$, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).

Groundwater: $t_{1/2} = 205\text{--}835 \text{ h}$, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672 \text{ h}$, based on aerobic acclimated and unacclimated groundwater die-away test data (Howard et al. 1991).

Biota:

TABLE 9.1.1.1
Reported aqueous solubilities and octanol-water partition coefficients of dibenzofuran at various temperatures

Aqueous solubility				Octanol-water partition coefficient	
Shiu et al. 1997		Doucette & Andren 1988a		Shiu et al. 1997	
generator column-HPLC/UV		generator column-GC/ECD		generator column-HPLC/UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	log K _{OW}
5	1.914	3.9	1.652	5	4.405
15	3.004	25	4.222	15	4.346
25	4.75	39.8	6.963	25	4.273
35	7.56			35	4.190
45	11.8			45	4.116
		$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 29.8$			
		for 4–32°C			
shake flask-HPLC/UV				$\Delta H/(\text{kJ mol}^{-1}) = -12.4$	
25	4.69				
		$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 33.3$			
		5–45°C			

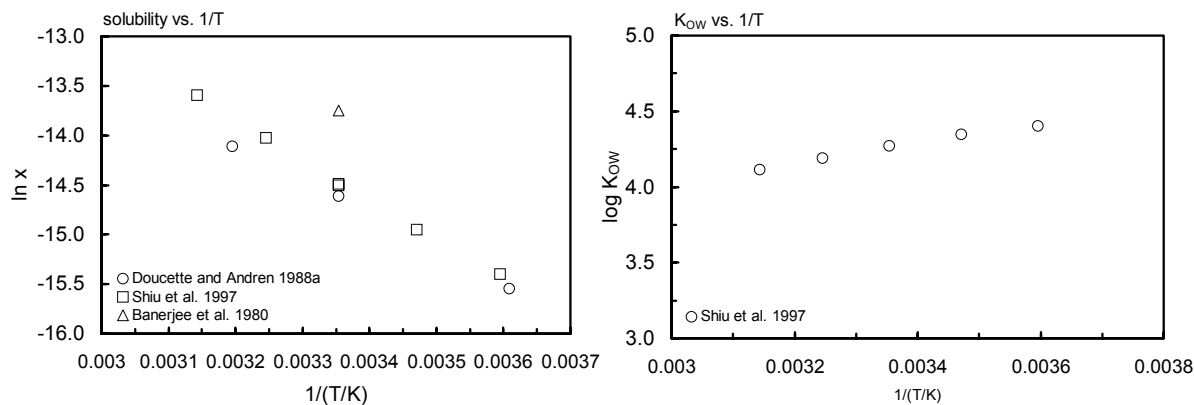


FIGURE 9.1.1.1 Logarithm of mole fraction solubility and K_{OW} versus reciprocal temperature for dibenzofuran.

TABLE 9.1.1.2

Reported vapor pressures of dibenzofuran at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Hanson & Eckert 1986		Sato et al. 1986		Rordorf 1989		Li et al. 2002	
gas saturation-IR		gas saturation-electrobalance		gas saturation-GC		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30	0.4874	25.85	0.506	25	0.35	20.2	0.284
35	0.7818	35.85	1.48	50	5.10	25.2	0.398
40	1.280	40.75	2.35	75	50.0	30	0.665
45	2.128	45.85	3.71	100	360	35	1.22
50	3.200	52.45	6.69	125	2100	40	1.94
55	4.679	55.65	8.8			45	3.04
60	7.246	59.75	12.5	$\Delta H_v/(\text{kJ mol}^{-1}) = 65.4$		eq. 1	P/Pa
65	12.78	60.35	13.5	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 85.630$			
70	19.71	64.45	18.3	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 19.6$			
		65.05	19.9	$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 54$			
$\log (P/\text{mPa}) = B - A/(T/K)$		66.15	21.5			B	9880.4
A	16.30	68.75	26.1				
B	4132	69.35	27.1				
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 79.1$		72.75	35.4				
		eq. 3	P/Pa				
		A	22.1098				
		B	4707.68				
		C	-92.332				

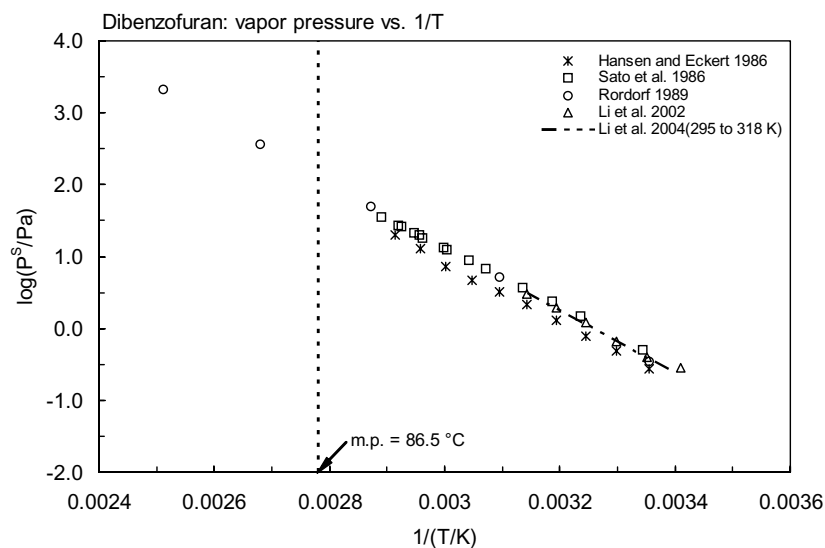
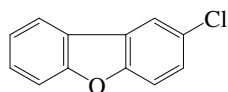


FIGURE 9.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for dibenzofuran.

9.1.1.2 2-Chlorodibenzofuran



Common Name: 2-Chlorodibenzofuran

Synonym: 2-MCDF

Chemical Name: 2-Chlorodibenzofuran

CAS Registry No: 51230-49-0

Molecular Formula: $C_{12}H_7ClO$, $C_6H_4OC_6H_3Cl$

Molecular Weight: 202.637

Melting Point ($^{\circ}C$):

101.5–102.5 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

338.2 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

197.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

75.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

95.28 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.4 (Rordorf 1987, 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

52 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

11.66 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

4.23, 11.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

9.6×10^{-3} , 0.190, 2.40, 22.0, 150 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

0.537 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 40.57 - 5556/(T/K) - 9.999 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

0.174; 0.537 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

9.12 (calculated-SOFA model, Govers & Krop 1998)

10.23; 9.12 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.37 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

5.15; 4.37 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.51 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

4.77; 4.51 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.38 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
3.96; 4.38 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (16-22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a mono-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 0.7–1.0 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (5.0-5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 2.9 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a mono-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 0.7–1.0 d (Atkinson 1991);

calculated tropospheric lifetime was 2.9 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

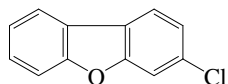
Ground water:

Sediment:

Soil:

Biota:

9.1.1.3 3-Chlorodibenzofuran



Common Name: 3-Chlorodibenzofuran

Synonym: 3-MCDF

Chemical Name: 3-Chlorodibenzofuran

CAS Registry No: 25074-67-3

Molecular Formula: $C_{12}H_7ClO$, $C_6H_4OC_6H_3Cl$

Molecular Weight: 202.637

Melting Point ($^{\circ}C$):

101–102 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

338.2 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

197.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

75.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

95.313 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

52 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

12.21 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

6.34; 12.21 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.970, 0.190, 2.40, 22.0, 150 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

0.490 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 40.57 - 5553/(T/K) - 9.999 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

0.174; 0.490 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

7.76 (calculated-SOFA model, Govers & Krop 1998)

10.23; 7.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.35 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

5.15; 4.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.53 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

4.77; 4.53 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

4.34 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

3.96; 4.34 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH} = (16-22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a mono-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 0.7–1.0 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991) $k_{OH}(\text{calc}) = (5.0-5.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 2.9 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a mono-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 0.7–1.0 d (Atkinson 1991);

calculated tropospheric lifetime of 2.9 d for with OH radical (Kwok et al. 1995).

Surface water:

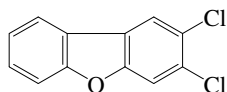
Ground water:

Sediment:

Soil:

Biota:

9.1.1.4 2,3-Dichlorodibenzofuran



Common Name: 2,3-Dichlorodibenzofuran

Synonym: 2,3-DCBF

Chemical Name: 2,3-dichlorodibenzofuran

CAS Registry No: 64126-86-9

Molecular Formula: $C_{12}H_8Cl_2O$

Molecular Weight: 237.082

Melting Point ($^{\circ}C$):

125.5–127 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

375 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

218.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

105.04 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

63 (Rordorf 1986, 1987, 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.50 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.716; 1.50 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.50×10^{-4} , 1.7×10^{-2} , 0.29, 3.20, 27.0 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

0.0282 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 39.20 - 5757/(T/K) - 9.466 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

0.1096; 0.0282 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

4.365 (calculated-SOFA model, Govers & Krop 1998)

4.79; 4.365 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.11 (calculated-SOFA model, Govers & Krop 1998)

5.43; 5.11 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{oa}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.82 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

5.04; 4.82 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

5.39 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

5.15; 5.39 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (6.6-16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.6-3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 0.7–1.0 d (Atkinson 1991);

room temp. tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical (Kwok et al. 1995).

Surface water:

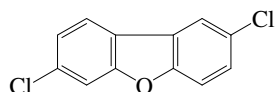
Ground water:

Sediment:

Soil:

Biota:

9.1.1.5 2,7-Dichlorodibenzofuran



Common Name: 2,7-Dichlorodibenzofuran

Synonym: 2,7-DCBF

Chemical Name: 2,7-dichlorodibenzofuran

CAS Registry No: 73992-98-6

Molecular Formula: $C_{12}H_8Cl_2O$

Molecular Weight: 237.082

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

218.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.32 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.785; 2.32 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0501 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 39.23 - 5755/(T/K) - 9.466 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

0.0123; 0.0501 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$):

5.01 (calculated-SOFA model, Govers & Krop 1998)

4.90; 5.01 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.02 (calculated-SOFA model, Govers & Krop 1998)

5.41; 5.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.79 (lipid wt base, calculated-SOFA model, Govers & Krop 1998)

5.03; 4.79 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{oc}$:

5.27 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

5.10; 5.27 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolysis $k = 0.23 \text{ min}^{-1}$ with $t_{1/2} = 3.0$ min in pure water and $k = 0.011 \text{ min}^{-1}$ with $t_{1/2} = 63$ min in 60 % acetonitrile/water solution in Corex centrifuge bottles at 300 nm photochemical reactor (Kim & O'Keefe 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (6.6\text{--}16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.6\text{--}3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 0.7–1.0 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical at room temp. (Kwok et al. 1995).

Surface water:

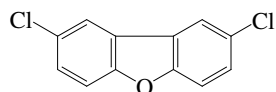
Ground water:

Sediment:

Soil:

Biota:

9.1.1.6 2,8-Dichlorodibenzofuran



Common Name: 2,8-Dichlorodibenzofuran

Synonym: 2,8-DCDF

Chemical Name: 2,8-dichlorodibenzofuran

CAS Registry No: 5409-83-6

Molecular Formula: $C_{12}H_6Cl_2O$

Molecular Weight: 237.082

Melting Point ($^{\circ}C$):

184–185 (Kuroki et al. 1984)

Boiling Point ($^{\circ}C$):

375 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

218.5 (calculated-Le Bas method at normal boiling point)

173.6 (Ruelle & Kesselring 1997)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

74.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

101.423 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.1 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

18.6 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

55 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0145* (generator column-GC, measured range 4.5 – $39.5^{\circ}C$, Doucette & Andren 1988a)

$S/(mol/L) = 1.24 \times 10^{-6} \exp(0.082 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range 4 – $40^{\circ}C$, Doucette & Andren 1988a); or

$\log x = -2344/(T/K) - 1.093$; temp range 4 – $40^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

0.024 (calculated-TSA, Dickhut et al. 1994)

0.0431 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

2.11 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\ln x = -2.515 - 5398.4/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

0.75; 2.11 (supercooled liquid S_L , GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9.6×10^{-4} (estimated, van den Berg & Olie 1985)

3.9×10^{-4} * (calculated-bp and ΔH_{fus} , Rordorf 1987, 1989)

0.0145; 0.0417 (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log (P/Pa) = 14.30669 - 5281.67/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. from literature data, Shiu & Ma 2000)

0.0115; 0.0417 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

1.06×10^{-3} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

0.0412 (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56 J/mol K$, Mader & Pankow 2003)

$\log (P_L/mmHg) = 39.21 - 5756/(T/K) - 9.466 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/\text{Pa}) = 32.943 - 12162/(T/\text{K})$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln(P/\text{Pa}) = (36.010 \pm 0.393) - (13262 \pm 144)/(T/\text{K})$; temp range 348–383 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

6.31; 4.57 (quoted lit.; calculated-SOFA model, Govers & Krop 1998)

4.79; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

5.56, 5.97, 6.16; 5.65, 5.95, 6.15 (HPLC-RT correlation, linear regressions; quadratic regressions, Sarna et al. 1984)

5.30 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)

5.44 (generator column-GC/ECD, Doucette & Andren 1987)

5.12 (HPLC-RT correlation, Doucette & Andren 1988b)

5.65 (recommended, Sangster 1993)

5.65 (recommended, Hansch et al. 1995)

5.42 (GC-RI correlation; Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

5.04 (guppy, Loonen et al. 1994a)

5.04; 4.81 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

5.04; 4.81 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

5.30 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

5.13; 5.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: when 5 mg/L in methanol was irradiated by sunlight simulator more than 95% disappears within 48 h while a similar experiment with highly purified methanol solution reveals only very slow photolysis within the same period of irradiation and results were same with 10 mg/L in methanol solution (Crosby & Moilanen 1973; quoted, Choudhary & Hutzinger 1982);

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (6.6\text{--}16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (2.6\text{--}3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 1.0–2.3 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radicals (Kwok et al. 1995).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: mean biological $t_{1/2} \sim 11$ d in rainbow trout (Niimi 1986).

TABLE 9.1.6.1

Reported aqueous solubilities and vapor pressures of 2,8-dichlorodibenzofuran at various temperatures

Aqueous solubility		Vapor pressure	
Doucette & Andren 1988a		Rordorf 1989	
generator column-GC/ECD		vapor pressure correlation	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
4.5	0.00384	25	3.9×10^{-4}
25	0.0145	50	9.1×10^{-3}
39.5	0.0339	75	0.14
		100	1.40
		125	11.0
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$		$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 74.2$	
4–32 $^{\circ}\text{C}$		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 101.423$	
$S/(\text{mol/L}) = a \cdot \exp[b \cdot (t/^{\circ}\text{C})]$		$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 25.1$	
a		$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{K}^{-1}) = 55$	
b			
	1.24×10^{-8}		
	0.062		

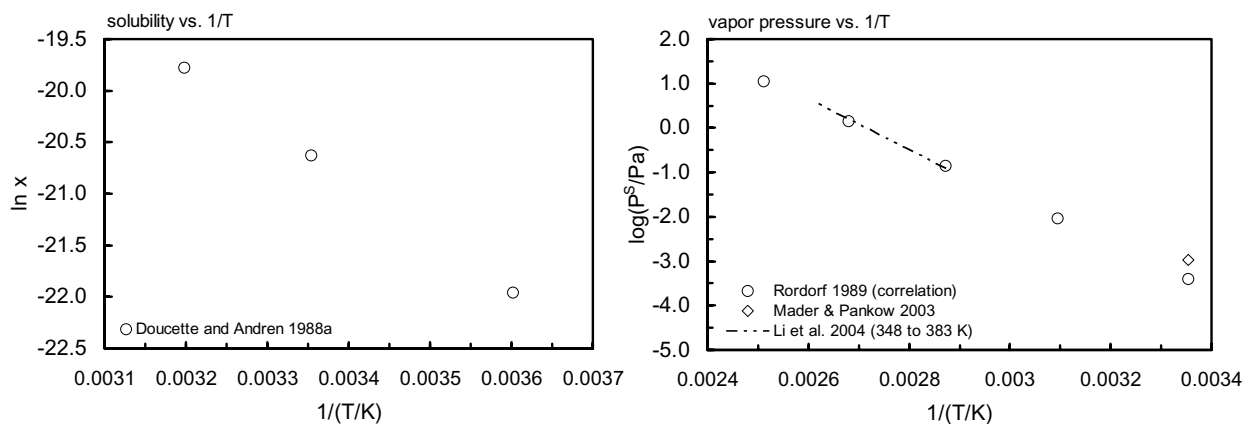
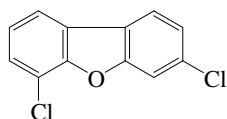


FIGURE 9.1.6.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for 2,8-dichlorodibenzofuran.

9.1.1.7 3,6-Dichlorodibenzofuran



Common Name: 3,6-Dichlorodibenzofuran

Synonym: 3,6-DCDF

Chemical Name: 3,6-dichlorodibenzofuran

CAS Registry No: 94570-83-9

Molecular Formula: $C_{12}H_6Cl_2O$

Molecular Weight: 237.082

Melting Point ($^{\circ}C$):

188 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

357 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

218.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.7 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

110.87 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

38.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

83 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0252 (mp at $188^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.76 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.684; 1.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.0×10^{-4} , 6.3×10^{-3} , 0.12, 1.60, 15 (25, 50, 75, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1985a,b, 1987, 1989)

0.0355 (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

0.0123; 0.0355 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log(P_L/mmHg) = 39.18 - 5755/(T/K) - 9.466 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

4.57 (calculated-SOFA model, Govers & Krop 1998)

4.68; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.08 (calculated-SOFA model, Govers & Krop 1998)

5.44; 5.08 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.81 (lipid wt. basis, calculated-SOFA model, Govers & Krop 1998)

5.05; 4.81 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

5.35 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

5.18; 5.35 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (6.6-16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a di-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.0–2.3 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (2.6-3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 4.0–5.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: lifetime was calculated based on the gas-phase reaction rate constant for a di-chlorinated PCDF with OH radicals to be 1.0–2.3 d (Atkinson 1991);

tropospheric lifetime was calculated to be 4.0–5.5 d for dichloro-CDFs, for the reaction with OH radical (Kwok et al. 1995).

Surface water:

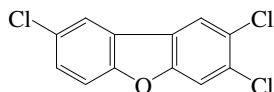
Ground water:

Sediment:

Soil:

Biota: mean biological $t_{1/2} = 24 \text{ d}$ in rainbow trout (Niimi & Oliver 1986)

9.1.1.8 2,3,8-Trichlorodibenzofuran



Common Name: 2,3,8-Trichlorodibenzofuran

Synonym: 2,3,8-TCDF

Chemical Name: 2,3,8-trichlorodibenzofuran

CAS Registry No: 57117-32-5

Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$

Molecular Weight: 271.527

Melting Point ($^{\circ}C$):

189–191 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

408.4 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

239.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

111.823 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

67 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.291 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.113, 0.291 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.0×10^{-5} , 9.9×10^{-4} , 2.0×10^{-2} , 0.26, 2.50 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

4.27×10^{-3} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

9.12×10^{-4} , 4.27×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

2.48×10^{-4} (solid P_S , gas saturation-GC/MS, Mader & Pankow 2003)

0.0108 (supercooled liquid P_L , calculated from P_S assuming $\Delta S_{fus} = 56\ J/mol\ K$, Mader & Pankow 2003)

$\log(P_L/mmHg) = 37.66 - 5911/(T/K) - 8.932 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.24 (calculated-SOFA model, Govers & Krop 1998)

2.57; 3.24 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.76 (calculated-SOFA model, Govers & Krop 1998)

5.75; 5.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.94 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.20; 4.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.30 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.26; 6.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (3.4-12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tri-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.3–4.5 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.5-2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 5.5–9.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991);

calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

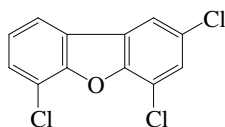
Ground water:

Sediment:

Soil:

Biota:

9.1.1.9 2,4,6-Trichlorodibenzofuran



Common Name: 2,4,6-Trichlorodibenzofuran

Synonym: 2,4,6-PCDF

Chemical Name: 2,4,6-trichlorodibenzofuran

CAS Registry No: 58802-14-6

Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$

Molecular Weight: 271.527

Melting Point ($^{\circ}C$):

116–117 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

408.4 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

239.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

116.061 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

79 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.461 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.175; 0.461 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

5.33×10^{-4} (estimated, Van den Berg & Olie 1985)

8.2×10^{-5} , 3.1×10^{-3} , 6.8×10^{-2} , 1.0, 10.0 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

4.27×10^{-3} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

1.32×10^{-3} , 4.27×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

9.22×10^{-4} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

7.50×10^{-3} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56\ J/mol\ K$, Mader & Pankow 2003)

$\log(P_L/mmHg) = 37.77 - 5908/(T/K) - 8.932 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

$\ln(P/Pa) = 37.264 - 13912/(T/K)$, temp range 298–398 K (regression eq. of Rordorf 1989 data, Li et al. 2004)

$\ln(P/Pa) = (35.837 \pm 0.729) - (13090 \pm 259)/(T/K)$; temp range 338–373 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.40 (calculated-SOFA model, Govers & Krop 1998)

2.82; 2.40 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.64 (calculated-SOFA model, Govers & Krop 1998)

5.69; 5.64 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.99 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.18; 4.99 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 6.12 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 6.09; 6.12 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (3.4 - 4.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (3.4 - 12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 1.3–4.5 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a tri-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.5 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 4.0–5.5 d for a tri-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991); calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical for a tri-chlorinated dibenzofuran (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

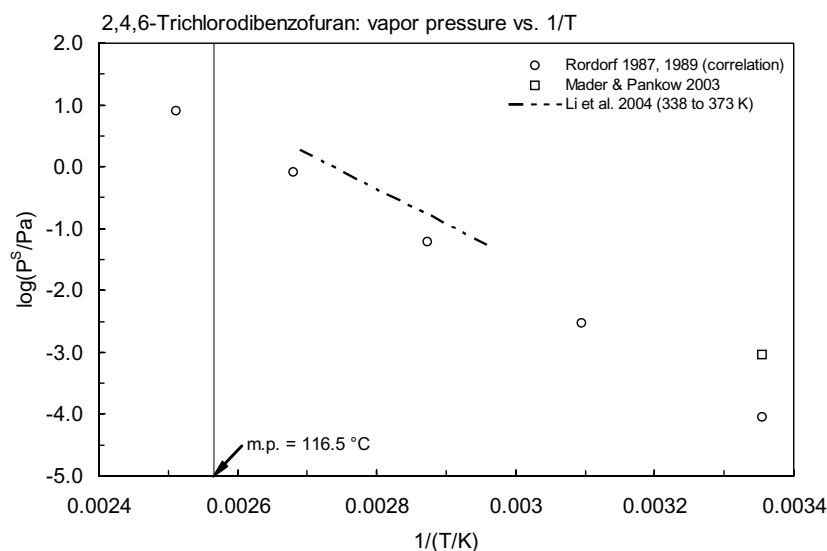
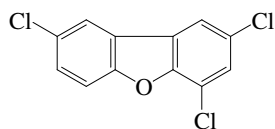


FIGURE 9.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trichlorodibenzofuran.

9.1.1.10 2,4,8-Trichlorodibenzofuran



Common Name: 2,4,8-Trichlorodibenzofuran

Synonym: 2,4,8-TCDF

Chemical Name: 2,4,8-trichlorodibenzofuran

CAS Registry No: 54589-71-8

Molecular Formula: $C_{12}H_5Cl_3O$, $C_6H_3ClOC_6H_2Cl_2$

Molecular Weight: 271.527

Melting Point ($^{\circ}C$):

155–156 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

392.5 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

239.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.7 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

112.3 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

32.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

76 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0542 (mp at $154^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.494 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.157; 0.494 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9.1×10^{-5} * (gas saturation-GC, Rordorf 1989)

5.75×10^{-3} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 37.78 - 5809/(T/K) - 8.932 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.38×10^{-3} , 5.75×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.09 (calculated-SOFA model, Govers & Krop 1998)

2.88; 3.09 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.64 (calculated-SOFA model, Govers & Krop 1998)

5.69; 5.64 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.94 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.18; 4.94 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Sorption Partition Coefficient, log K_{OC} :

6.14 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

6.06; 6.14 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (3.4-12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tri-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.3–4.5 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (1.5-2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 5.5–9.5 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated for a tri-chlorinated dibenzofuran based on the gas-phase reaction with OH radicals to be 1.3–4.5 d (Atkinson 1991);

calculated tropospheric lifetime was 5.5–9.5 d for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 9.1.10.1
Reported vapor pressures of 2,4,8-tetrachlorodibenzofuran at various temperatures

Rordorf 1987, 1989	
gas saturation-GC	
$t/^{\circ}\text{C}$	P/Pa
25	9.1×10^{-5}
50	3.0×10^{-3}
75	6.1×10^{-2}
100	0.82
125	8.0
$\Delta H_v/(\text{kJ mol}^{-1}) = 78.7$	
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 112.3$	
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 32.6$	
$\Delta S_{\text{fus}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 76$	

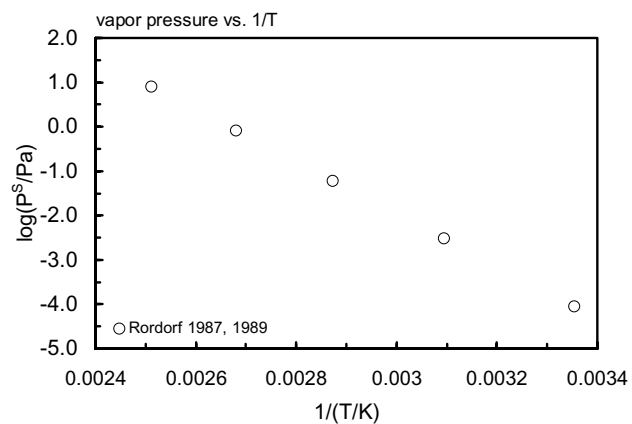
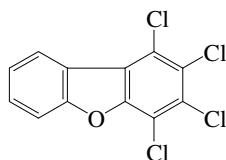


FIGURE 9.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,8-trichlorodibenzofuran.

9.1.1.11 1,2,3,4-Tetrachlorodibenzofuran



Common Name: 1,2,3,4-Tetrachlorodibenzofuran

Synonym: 1,2,3,4-TCDF

Chemical Name: 1,2,3,4-tetrachlorodibenzofuran

CAS Registry No: 24478-72-6

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

168.5–169 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.4 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

122.826 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

83 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0717 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0306; 0.0717 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.1×10^{-6} , 1.9×10^{-4} , 5.1×10^{-3} , 8.7×10^{-2} , 1.0 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

6.76×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 36.02 - 6019/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.17×10^{-4} , 6.76×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.75 (calculated-SOFA model, Govers & Krop 1998)

1.74; 2.75 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.17 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)

6.34 (calculated-SOFA model, Govers & Krop 1998)

6.07; 6.34 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.92 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.22; 4.92 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.12 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.18; 7.12 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctance solution, and solid phase photolysis half-life, $t_{1/2} = 95$ h with PCDF dispersed as solid films (Buser 1988)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.4\text{--}8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8\text{--}1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 154, 134 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 > 1.8, > 1.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}, 220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_5 CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCF_s for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

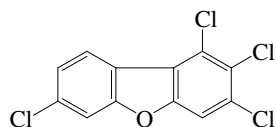
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: half-lives in gold fish: $t_{1/2} < 0.4$ d for PBO treated and $t_{1/2} > 0.5$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.12 1,2,3,7-Tetrachlorodibenzofuran



Common Name: 1,2,3,7-Tetrachlorodibenzofuran

Synonym: 1,2,3,7-TCDF

Chemical Name: 1,2,3,7-tetrachlorodibenzofuran

CAS Registry No: 83704-22-7

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

167.5–168 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.4 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

122.879 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

83 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0805 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0306; 0.0805 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.2×10^{-6} , 1.9×10^{-4} , 5.2×10^{-3} , 8.9×10^{-2} , 1.1 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.08×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

1.41×10^{-4} , 7.08×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log(P_L/mmHg) = 36.07 - 6015/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

2.57 (calculated-SOFA model, Govers & Krop 1998)

1.78; 2.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.31 (calculated-SOFA model, Govers & Krop 1998)

6.04; 6.31 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.41 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)

4.93 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.23; 4.93 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

7.07 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

7.10; 7.07 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase photolysis $t_{1/2} = 95$ h with PCDF dispersed as solid films (Buser 1988)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (4.9 - 6.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.4 - 8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 1.9\text{--}11$ d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8 - 1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 7.7\text{--}18$ d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 142 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.007 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}$, $220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCF_s for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

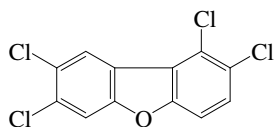
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} = 96$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.13 1,2,7,8-Tetrachlorodibenzofuran



Common Name: 1,2,7,8-Tetrachlorodibenzofuran

Synonym:

Chemical Name: 1,2,7,8-tetrachlorodibenzofuran

CAS Registry No: 58802-20-3

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

210–211 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

81.5 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

120.604 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

76 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0496 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0273; 0.0496 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.67×10^{-4} (estimated, Van den Berg et al. 1985)

1.30×10^{-4} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

2.4×10^{-6} , 1.0×10^{-4} , 2.610^{-3} , 4.2×10^{-2} , 0.49 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

3.55×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 35.97 - 6020/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.047×10^{-4} , 3.35×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.09 (calculated-SOFA model, Govers & Krop 1998)

1.70; 2.09 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.23 (shake flask-slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989)

6.41 (calculated-SOFA model, Govers & Krop 1998)

5.964 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)

6.10; 6.41 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.97 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.22; 4.97 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.20 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.24; 7.20 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase photolysis half-life, $t_{1/2} = 35$ h with PCDF dispersed as solid films (Buser 1988);

$k = 0.014 \text{ min}^{-1}$ with $t_{1/2} = 50$ min in pure water and $k = 0.0041 \text{ min}^{-1}$ with $t_{1/2} = 170$ min in 60 % acetonitrile/water solution in Corex centrifuge bottles at 300 nm photochemical reactor; $k = 0.08 \text{ h}^{-1}$ with $t_{1/2} = 8.3$ h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.4\text{--}8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8\text{--}1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 162, 130 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.14, >1.0 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}$, $220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

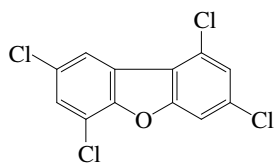
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} = 4.9$ d for PBO treated goldfish, and $t_{1/2} < 0.7$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.14 1,3,6,8-Tetrachlorodibenzofuran



Common Name: 1,3,6,8-Tetrachlorodibenzofuran

Synonym:

Chemical Name: 1,3,6,8-tetrachlorodibenzofuran

CAS Registry No: 71998-72-6

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

177–178 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

122.36 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

81 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.212 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0625; 0.212 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.6×10^{-6} , 1.6×10^{-4} , 4.3×10^{-3} , 7.4×10^{-2} , 0.88 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

1.17×10^{-3} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 36.34 - 6020/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

2.95×10^{-4} , 1.17×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.62 (calculated-SOFA model, Govers & Krop 1998)

2.04; 1.62 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.37 (shake flask/slow stirring-GC/MS, fly-ash extract, Sijm et al. 1989)

6.06 (calculated-SOFA model, Govers & Krop 1998)

5.92; 6.06 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or log K_B :

- 5.0 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
5.23; 5.0 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

- 6.71 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
6.76; 6.71 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.4-8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8-1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCFs for the gas-phase reaction with OH radicals (Kwok et al. 1995).

Surface water:

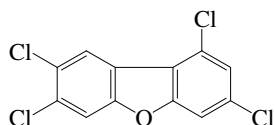
Ground water:

Sediment: degradation $t_{1/2} = 20-200 \text{ yr}$ in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota:

9.1.1.15 1,3,7,8-Tetrachlorodibenzofuran



Common Name: 1,3,7,8-Tetrachlorodibenzofuran

Synonym: 1,3,7,8-TCDF

Chemical Name: 1,3,7,9-tetrachlorodibenzofuran

CAS Registry No: 57117-35-8

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 306

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.116 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0463; 0.116 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and the reported temperature dependence equations):

6.03×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

2.00×10^{-4} , 6.03×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

3.51×10^{-5} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

$\log(P_L/mmHg) = 36.20 - 6020/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.55 (calculated-SOFA model, Govers & Krop 1998)

1.91; 1.55 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.39 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)

6.20 (calculated-SOFA model, Govers & Krop 1998)

5.98; 6.20 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.83 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)

5.01 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.23; 5.01 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

6.90 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

6.95; 6.90 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (4.9 - 6.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991) $k_{OH} = (1.4 - 8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 1.9\text{--}11 \text{ d}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991) $k_{OH}(\text{calc}) = (0.8 - 1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 7.7\text{--}18 \text{ d}$ for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2): $k_1 = 164, 293 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, > 1.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993) $k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}$, $220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for TCDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$, the tropospheric lifetime of a tetra-CDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DFs for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

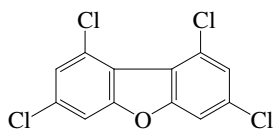
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} > 7 \text{ d}$ for PBO treated goldfish and $t_{1/2} < 0.5 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.16 1,3,7,9-Tetrachlorodibenzofuran



Common Name: 1,3,7,9-Tetrachlorodibenzofuran

Synonym: 1,3,7,9-TCDF

Chemical Name: 1,3,7,9-tetrachlorodibenzofuran

CAS Registry No: 64560-17-4

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

206.5–207.5 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

438.3 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.3 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

121.988 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

80 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.104 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.0422; 0.104 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.5×10^{-6} , 1.1×10^{-4} , 2.7×10^{-3} , 4.5×10^{-2} , 0.51 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

4.37×10^{-4} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

1.78×10^{-4} , 4.36×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log(P_L/mmHg) = 36.15 - 6018/(T/K) - 8.399 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.26 (calculated-SOFA model, Govers & Krop 1998)

1.86; 1.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.39 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)

6.22 (calculated-SOFA model, Govers & Krop 1998)

6.00; 6.22 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.83 (gold fish treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)

5.06 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.23; 5.06 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

6.91 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

7.00; 6.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.4\text{--}8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a tetra-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 1.9–11 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.8\text{--}1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and the calculated tropospheric lifetime was 7.7–18 d at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 164, 293 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, > 1.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}, 220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime of 7.7–18 d for tetrachloro-DCF_s for the gas-phase reaction with OH radical (Kwok et al. 1995).

Surface water:

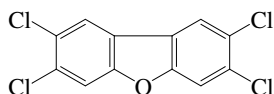
Ground water:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ in sediment for all homologues (Suzuki et al. 2000)

Soil:

Biota: $t_{1/2} > 7 \text{ d}$ for PBO treated gold fish and $t_{1/2} < 0.5 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.17 2,3,7,8-Tetrachlorodibenzofuran



Common Name: 2,3,7,8-Tetrachlorodibenzofuran

Synonym: 2,3,7,8-TCDF

Chemical Name: 2,3,7,8-Tetrachlorodibenzofuran

CAS Registry No: 51207-31-9

Molecular Formula: $C_{12}H_4Cl_4O$, $C_6H_2Cl_2OC_6H_2Cl_2$

Molecular Weight: 305.978

Melting Point ($^{\circ}C$):

227 (Lide 2003)

Boiling Point ($^{\circ}C$):

438.3 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

260.3 (calculated-Le Bas method at normal boiling point)

199.4 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

80.3 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

119.699 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

36.6 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

73.2 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.0104 (calculated-assuming $\Delta S_{fus} = 56 J/mol K$ and $mp = 227^{\circ}C$)

0.00256 (calculated- ΔS_{fus} and mp , Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.19×10^{-4} ($22.7^{\circ}C$, generator column-HPLC/LSC, Friesen et al. 1990)

3.51×10^{-3} (calculated-QSAR, Fiedler & Schramm 1990)

4.20×10^{-4} ; 5.32×10^{-4} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.0413; 0.0413 (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.655 - 1915/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

0.0243; 0.0413 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.0×10^{-6} (quoted, Van den Berg & Olie 1985)

2.0×10^{-6} , 8.5×10^{-5} , 2.1×10^{-3} , 3.3×10^{-2} , 0.38 (25 , 50 , 75 , 100 , $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

1.23×10^{-4} (GC-RT correlation, supercooled liquid P_L , Eitzer & Hites 1988, 1991; quoted, Della Site 1997)

1.13×10^{-4} (GC-RT correlation, supercooled liquid P_L , Eitzer & Hites 1989; quoted, Della Site 1997)

2.00×10^{-4} (supercooled liquid P_L , Falconer & Bidleman 1994; quoted, Kaupp & McLachlan 1999)

1.23×10^{-6} , 1.13×10^{-6} (calculated from reported P_L , solid vapor pressures, Della Site 1997)

7.50×10^{-4} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)

1.62×10^{-4} ; 3.72×10^{-4} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

7.39×10^{-4} ; 1.89×10^{-6} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.48 - 5425/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.66 - 3513/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

- 1.678×10^{-5} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)
 1.718×10^{-3} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56$ J/mol K, Mader & Pankow 2003)
 $\log (P_L/\text{mmHg}) = 35.91 - 6019/(T/K) - 8.399 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 8.91×10^{-5} , 3.72×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 1.50 (calculated for tetrachloro-PCDFs, Eitzer & Hites 1989)
 1.70 (gas stripping-GC, 21°C , Friesen et al. 1993)
 1.17; 2.69 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 8.01 - 1598/(T/K)$ (Passivirta et al. 1999)
 1.66; 2.69 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 5.82 (HPLC-RT correlation, Burkhard & Kuehl 1986)
 6.53 (shake flask/slow stirring-GC/MS, from mixture of fly ash extract, Sijm et al. 1989)
 6.19 (correlated, Ma et al. 1990)
 7.10 (calculated-QSAR, Fiedler & Schramm 1990)
 7.70 (calculated, Broman et al. 1991)
 5.83 (HPLC-RT correlation, Jackson et al. 1993)
 6.53 (recommended, Hansch et al. 1995)
 6.46 (calculated-SOFA model, Govers & Krop 1998)
 6.46, 6.58 (quoted, calculated-solubility $\log S_L$ and regression from lit. $\log K_{ow}$, Passivirta et al. 1999)
 6.225 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 6.13; 6.46 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations:

- 9.42 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
 10.02; 9.44 (generator column-GC/ECD; calculated, Harner et al. 2000)
 10.90 (7°C , GC retention time correlation, Harner et al. 2000)
 $\log K_{OA} = -4.92 + 4450/(T/K)$; temp range $10\text{--}50^\circ\text{C}$ (Harner et al. 2000)

Bioconcentration Factor, $\log \text{BCF}$:

- 4.82 (guppy, Opperhuizen et al. 1986)
 3.78, 3.39 (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988)
 3.64, 3.41 (rainbow trout, quoted, Opperhuizen & Sijm 1990)
 3.82 (guppy, quoted, Opperhuizen & Sijm 1990)
 4.19; 4.12 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.19; 4.33; 5.02 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.93 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.23, 6.53 (fish with 5% lipid: wet weight basis, lipid weight basis, Geyer et al. 2000)
 6.54, 5.75 (fish muscle $\log \text{BCF}_L$ calculated from water, sediment, Wu et al. 2001)
 5.22; 4.93 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{oc}$:

- 5.20 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 7.50 (calculated, Broman et al. 1991)
 6.62 (calculated- K_{ow} , Kollig 1993)
 5.18; 5.34 (sediment in lake mesocosm, Muir et al. 1992)
 7.08; 7.29 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.32; 7.29 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: sunlight induced photolysis $t_{1/2} = 220$ min in isooctane solution, and solid phase $t_{1/2} = 120$ h with PCDF dispersed as solid films (Buser 1988);

photolytic $t_{1/2} = 9.8$ h in extract of fly-ash and in tetradecane solution for native congener and $t_{1/2} = 3.0$ h for ^{13}C -labelled congener (Tysklind & Rappe 1991).

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}(\text{calc}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1987b)

$k_{\text{O}_3} = 1.32 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$ oxidative degradation rate constant for water dissolved PCDF by ozone under alkaline conditions at pH 10 and 20°C (Palauscek & Scholz 1987);

$k_{\text{OH}}(\text{calc}) = (2.4 - 3.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = (1.4 - 8.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 1.9\text{--}11$ d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a tetra-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = (0.8 - 1.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 7.7\text{--}18$ d for a tetra-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 400 \text{ d}^{-1}$; $k_2 = 0.062 \text{ d}^{-1}$ (guppy, exposed to fly-ash extract, Opperhuizen et al. 1986)

$k_1 = 1228, 6853 \text{ d}^{-1}$; $k_2 = 0.28, 2.60 \text{ d}^{-1}$ (rainbow trout, exposed to: 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988)

$k_1 = 56, 453 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, 0.22 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 171 \text{ L kg}^{-1} \text{ d}^{-1}, 220 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_3CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0058 \text{ d}^{-1}$ with a biological $t_{1/2} = 58$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 603 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.292 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994a)

$k_2 = 0.0263 \text{ d}^{-1}$ with $t_{1/2} = 26$ d (newly contaminated oysters, Gardinali et al. 2004)

$k_2 = 0.0194 \text{ d}^{-1}$ with $t_{1/2} = 36$ d (chronically contaminated oysters, Gardinali et al. 2004)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a tetra-PCDF for the gas-phase reaction with OH radical was calculated to be 1.9–11 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be 7.7–18 d for the gas-phase reaction with OH radical (Kwok et al. 1995);

$t_{1/2} = 320$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 90$ min in isooctane solution in summer sunlight (Palauscek & Scholz 1987);

suggested $t_{1/2} = 6400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: $t_{1/2} = 61$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 20\text{--}200$ yr in sediment for all homologues (Suzuki et al. 2000)

$t_{1/2} = 550\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr in soil (Suzuki et al. 2000)

$t_{1/2} = 550\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: Elimination $t_{1/2} = 2$ d from rat (Birnbaum et al. 1980; quoted, Birnbaum 1985);

$t_{1/2} = 8$ d from monkey (Birnbaum et al. 1981; quoted, Birnbaum 1985);

$t_{1/2} = 2\text{--}4$ d from mouse (Decad et al. 1981b; quoted, Birnbaum 1985);

$t_{1/2} = 40$ d from guinea pig (Decad et al. 1981a; Ioannou et al. 1983; quoted, Birnbaum 1985);

elimination half-lives: in guinea pigs, 20 d; rats, < 2 d; monkeys, 8 d; and mice, 2–4 d (quoted,

Van den Berg & Olie 1985);

$t_{1/2} < 336$ d in carp (Kuehl et al. 1987);

elimination $t_{1/2} = 3.0$ d, 0.27 d (rainbow trout, exposed to 0.41 ng/L, 3.93 ng/L for 28 d, Mehrle et al. 1988);

elimination $t_{1/2} = 0.8$ d for lactating cows (Olling et al. 1991);

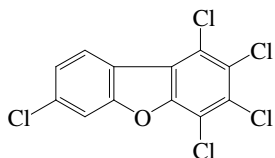
$t_{1/2} > 7$ d for PBO treated goldfish, $t_{1/2} = 3.1$ d for control fish in 120-h exposure studies (Sijm et al. 1993)

elimination $t_{1/2} = 111$ d from soft-shell clam (Brown 1994).

biological $t_{1/2} = 58$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

Depuration $t_{1/2} = 26$ d for newly contaminated oysters, and $t_{1/2} = 36$ d for chronically contaminated oysters (Gardinali et al. 2004)

9.1.1.18 1,2,3,4,7-Pentachlorodibenzofuran



Common Name: 1,2,3,4,7-Pentachlorodibenzofuran

Synonym: 1,2,3,4,7-PCDF

Chemical Name: 1,2,3,4,7-pentachlorodibenzofuron

CAS Registry No: 83704-48-7

Molecular Formula: $C_{12}H_3Cl_5O$, $C_6Cl_4OC_6H_3Cl$

Molecular Weight: 340.418

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

281.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0179 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.00745; 0.0179 (GC-RT correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.43×10^{-5} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

2.09×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

$\log(P_L/mmHg) = 34.22 - 6088/(T/K) - 7.865 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.905×10^{-5} , 1.202×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$):

2.24 (calculated-SOFA model, Govers & Krop 1998)

1.35; 2.24 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.53 (shake flask/slow stirring-GC/MS, mixture of fly-ash extract, Sijm et al. 1989)

6.89 (calculated-SOFA model, Govers & Krop 1998)

6.45; 6.89 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.80 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)

5.13; 4.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

7.89 (sediment/water, calculated-SOFA model, Govers & Krop 1998)

8.06; 7.89 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference: $k_{OH}(\text{calc}) = (3.6 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991) $k_{OH} = (1.0 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 3.6\text{--}15 \text{ d}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991) $k_{OH}(\text{calc}) = (0.5 - 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 15\text{--}29 \text{ d}$ for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2): $k_1 = 68 \text{ L kg}^{-1} \text{ d}^{-1}$ (goldfish after 120-h exposure: control fish, Sijm et al. 1993) $k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993) $k_2 > 0.5$, $< 1.7 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991)
calculated tropospheric lifetime to be 15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995)

Surface water:

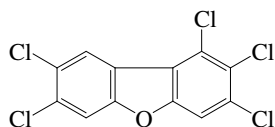
Ground water:

Sediment:

Soil:

Biota: $t_{1/2} < 1.4 \text{ d}$ for PBO treated goldfish and $t_{1/2} < 0.4 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.19 1,2,3,7,8-Pentachlorodibenzofuran



Common Name: 1,2,3,7,8-Pentachlorodibenzofuran

Synonym:

Chemical Name:

CAS Registry No: 57117-41-6

Molecular Formula: $C_{12}H_3Cl_5O$, $C_6HCl_3OC_6H_2Cl_2$

Molecular Weight: 340.418

Melting Point ($^{\circ}C$):

225–227 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

464.7 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

281.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.6 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

128.978 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

42.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

85 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0108 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.794 - 2223/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

0.0679; 0.0108 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.27×10^{-5} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

2.3×10^{-7} , 1.5×10^{-5} , 4.0×10^{-4} , 8.0×10^{-3} , 0.11 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

6.17×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

2.40×10^{-4} ; 2.35×10^{-7} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.67 - 5750/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.23 - 3529/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.084×10^{-6} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)

1.084×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56$ J/mol K, Mader & Pankow 2003)

$\log (P_L/mmHg) = 34.15 - 6081/(T/K) - 7.865 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

1.70×10^{-3} , 6.17×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ or as indicated and reported temperature dependence equations):

1.91 (calculated-SOFA model, Govers & Krop 1998)

$\log (H/(Pa \cdot m^3/mol)) = 7.44 - 1306/(T/K)$ (Passivirta et al. 1999)

1.35; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.79 (shake flask/slow stirring-GC/MS, Sijm et al. 1989)
 6.99 (calculated-SOFA model, Govers & Krop 1998)
 7.07 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
 6.47; 6.99 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 11.4 (7°C, GC retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 3.38 (guppy, Opperhuizen et al. 1986)
 3.84, 3.61 (gold fish: treated with metabolic inhibitor PBO, control fish, 120-h exposure, Sijm et al. 1993)
 4.84 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.12; 4.84 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.60 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 8.03 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 8.11; 8.03 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution, $t_{1/2} = 10.0$ h for native congener (Tysklind & Rappe 1991)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.0 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 3.6–15 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.5 - 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 98, 252 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}, 174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_5 CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0126 \text{ d}^{-1}$ with a biological $t_{1/2} = 24$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be 15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995);

suggested $t_{1/2} = 660$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2} = 13200$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Ground water:

Sediment: $t_{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

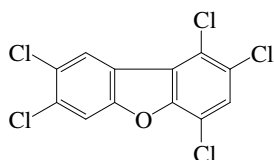
Soil: $t_{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: elimination $t_{1/2} = 3.3$ –3.5 d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);

$t_{1/2} > 7$ d for PBO treated goldfish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2} = 24$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.20 1,2,4,7,8-Pentachlorodibenzofuran



Common Name: 1,2,4,7,8-Pentachlorodibenzofuran

Synonym: 1,2,4,7,8-PeCDF

Chemical Name: 1,2,4,7,8-pentachlorodibenzofuran

CAS Registry No: 83704-51-2

Molecular Formula: $C_{12}H_3Cl_5O$, $C_6HCl_3OC_6H_2Cl_2$

Molecular Weight: 340.418

Melting Point ($^{\circ}C$):

236–238 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

464.7 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

281.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

128.442 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

42.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

89 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00179 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

0.00618; 0.00179 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.0×10^{-7} , 1.1×10^{-5} , 3.4×10^{-4} , 6.7×10^{-3} , 0.091 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

8.92×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

2.34×10^{-5} , 8.91×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log(P_L/mmHg) = 34.28 - 6082/(T/K) - 7.865 \cdot \log(T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.62 (calculated-SOFA model, Govers & Krop 1998)

1.35; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.26 (shake flask/slow stirring-GC/MS, mixture of fly ash extract, Sijm et al. 1989)

6.87 (calculated-SOFA model, Govers & Krop 1998)

6.40; 6.87 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF or log K_B :

- 3.02 (gold fish: treated with metabolic inhibitor PBO, 120-h exposure, Sijm et al. 1993)
 4.85 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.15; 4.85 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

- 7.86 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.96; 7.86 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 48.5$ d on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (1.8 - 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.0 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 3.6–15 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.5 - 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 15–29 d for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 63, 77 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1, > 1.3 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}, 174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P_5 CDF homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated tropospheric lifetime $\tau = 15\text{--}29$ d for the gas-phase reaction with OH radical at room temp. (Kwok et al. 1995);

suggested $t_{1/2} = 660$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: suggested $t_{1/2} = 13200$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000)

Ground water:

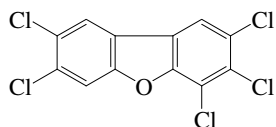
Sediment: suggested $t_{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{1/2} = 450000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: elimination $t_{1/2} = 3.3\text{--}3.5$ d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);

$t_{1/2} > 7$ d for metabolic inhibitor PBO treated gold fish and $t_{1/2} < 1.5$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.21 2,3,4,7,8-Pentachlorodibenzofuran



Common Name: 2,3,4,7,8-Pentachlorodibenzofuran

Synonym: 2,3,4,7,8-PCDF

Chemical Name: 2,3,4,7,8-pentachlorodibenzofuran

CAS Registry No: 57117-31-4

Molecular Formula: $C_{12}H_3Cl_5O$, $C_6H_2Cl_2OC_6HCl_3$

Molecular Weight: 340.418

Melting Point ($^{\circ}C$):

196–196.5 (Kuroki et al. 1984, Rordorf 1989)

Boiling Point ($^{\circ}C$):

464.7 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

281.2 (calculated-Le Bas method at normal boiling point)

212.3 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.6 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

130.43 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

42.4 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

90 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.0208 (calculated-assuming $\Delta S_{fus} = 56\ J/mol\ K$ and $mp = 196.5^{\circ}C$)

0.00196 (calculated- ΔS_{fus} and mp , Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.000515 (calculated-QSAR, Fiedler & Schramm 1990)

0.000236 ($22.7^{\circ}C$, generator column-GC/MS, Friesen et al. 1990)

0.00015 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.0115; 7.11×10^{-3} (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 1.076 - 2218/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

0.00481; 0.00711 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.17×10^{-5} (supercooled liquid P_L -GC-RT correlation, Eitzer & Hites 1988, 1991)

2.43×10^{-5} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

3.5×10^{-7} , 2.1×10^{-5} , 6.7×10^{-4} , 1.4×10^{-2} , 0.19 (25 , 50 , 75 , 100 , $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

1.74×10^{-5} (supercooled liquid P_L , Falconer & Bidleman 1994; quoted, Kaupp & McLachlan 1999)

1.53×10^{-4} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)

1.95×10^{-5} ; 5.50×10^{-5} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

1.91×10^{-4} ; 3.74×10^{-7} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.62 - 5677/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.90 - 3462/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

- 6.53×10^{-6} (solid P_s , gas saturation-GC/MS, Mader & Pankow 2003)
 3.20×10^{-4} (supercooled liquid P_L , calculated from P_s assuming $\Delta S_{fus} = 56$ J/mol K, Mader & Pankow 2003)
 $\log (P_L/\text{mmHg}) = 33.99 - 6084/(T/K) - 7.865 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 1.15×10^{-5} , 5.50×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations):

- 0.505 (calculated-P/C with selected values)
 0.575; 2.57 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log (H/(\text{Pa m}^3/\text{mol})) = 6.82 - 1244/(T/K)$ (Passivirta et al. 1999)
 1.29; 2.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 6.92 (shake flask/slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989)
 7.82 (calculated-QSAR, Fiedler & Schramm 1990)
 7.60 (calculated, Broman et al. 1991)
 6.92 (recommended, Hansch et al. 1995)
 7.11 (calculated-SOFA model, Govers & Krop 1998)
 7.11, 6.90 (quoted, calculated-solubility $\log S_L$ and regression from lit. $\log K_{ow}$, Passivirta et al. 1999)
 6.757 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 6.56; 7.11 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 10.09 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
 11.52 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

- 3.70 (guppy, Opperhuizen et al. 1986; quoted, Opperhuizen & Sijm 1990)
 5.14; 4.92 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 5.14; 5.15; 5.38 (guppies, 21-d exposure, lipid weight basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 5.14; 4.79 (lipid wt basis, quoted exptl.; quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 5.62; 5.92, 6.92 (fish 5% lipid: wet wt basis; fish 10% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
 6.42, 5.88 (fish muscle $\log BCF_L$ calculated from water, sediment, Wu et al. 2001)
 5.08; 4.79 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Bioaccumulation Factor, BAF:

- 1.44, 1.33 (rainbow trout, concn in food: 0.82, 9.01 ng/g, Muir et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.59 (organic carbon, calculated-QSAR, Fiedler & Schramm 1990)
 7.40 (calculated, Broman et al. 1991)
 6.60, 6.92 (calculated- K_{ow} , Kollig 1993)
 8.20 (calculated-SOFA model, sediment/water, Govers & Krop 1998)
 8.30; 8.20 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

- Photolysis: photolytic degradation $t_{1/2} = 3.5$ h of PCDD in extract of fly-ash in tetradecane solution for native congener and $t_{1/2} = 3.1$ h for ^{13}C -labelled congener (Tysklind & Rappe 1991)
 $t_{1/2} = 55.0$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (1.7 - 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (1.0 - 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 3.6\text{--}15 \text{ d}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ for a penta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

$k_{OH}(\text{calc}) = (0.5 - 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime $\tau = 15\text{--}29 \text{ d}$ for a penta-chlorinated dibenzofuran at room temp. (Kwok et al. 1995)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0027 \text{ d}^{-1}$ (carp, calculated from data reported by Kuehl et al. 1987, Sijm et al. 1990)

$k_1 = 400 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.079 \text{ d}^{-1}$ (guppy, Opperhuizen et al. 1986)

$k_2 = 0.0064 \text{ d}^{-1}$ (liver of female rat, Van den Berg et al. 1989)

$k_2 = -2.1 \times 10^{-2}$, $1.5 \times 10^{-2} \text{ d}^{-1}$ (rainbow trout, 2 to 21 d exposure: metabolic inhibitor PBO-treated, control, Sijm et al. 1990)

$k_2 = 10.1 \times 10^{-3} \text{ d}^{-1}$ and $k_2 = 8.10 \times 10^{-3} \text{ d}^{-1}$; $k_2 = 12.6 \times 10^{-3} \text{ d}^{-1}$ and $k_2 = 11.4 \times 10^{-3} \text{ d}^{-1}$ (rainbow trout, 0–140 d and 0–180 d exposure at 0.82 ng/g PCDF concn.; 0–140 d and 0–180 d exposure at 9.01 ng/g PCDF concn., Muir et al. 1990)

$k_1 = 105$, $561 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.11$, $< 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0081 \text{ d}^{-1}$ with a biological $t_{1/2} = 36 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 1012 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.044 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$, the tropospheric lifetime of a penta-PCDF for the gas-phase reaction with OH radical was calculated to be 3.6–15 d (Atkinson 1991); calculated room temp. tropospheric lifetime to be 15–29 d for the gas-phase reaction with OH radical (Kwok et al. 1995);

$t_{1/2} = 660 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolytic $t_{1/2} = 3.5 \text{ h}$ in the extract from fly-ash in tetradecane solution, for native congener and $t_{1/2} = 3.1 \text{ h}$ for ^{13}C labelled congener (Tysklind & Rappe 1991)

$t_{1/2} = 13200 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{1/2} = 60 \text{ yr}$ (Geyer et al. 2000)

degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ in sediment for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 550\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50 \text{ yr}$ (estimated, Suzuki et al. 2000);

$t_{1/2} = 550\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: elimination $t_{1/2} = 108 \text{ d}$ in the liver of female rats (Van den Berg et al. 1989);

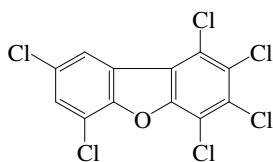
$t_{1/2} = 69 \text{ d}$ in rainbow trout at the 0.82 ng/g exposure concentration from 0–140 d data, $t_{1/2} = 61 \text{ d}$ at 9.0 ng/g exposure concentration from 0–180 d data; $t_{1/2} = 65 \text{ d}$ in whole body rainbow trout with 31-d dietary exposure (Muir et al. 1990);

elimination $t_{1/2} = 48.5 \text{ d}$ for lactating cows (Olling et al. 1991);

$t_{1/2} = 6.1 \text{ d}$ for PBO treated goldfish and $t_{1/2} > 7 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2} = 49 \text{ d}$ in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.22 1,2,3,4,6,8-Hexachlorodibenzofuran



Common Name: 1,2,3,4,6,8-Hexachlorodibenzofuran

Synonym: 1,2,3,4,6,8-HxCDF

Chemical Name: 1,2,3,4,6,8-Hexachlorodibenzofuran

CAS Registry No: 69698-60-8

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6H_2Cl_2OC_6Cl_4$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

233.5–234 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.049 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1989; quod, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

95 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F :

0.000332 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

6.08×10^{-3} (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.839 - 2520/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

2.48×10^{-3} , 5.08×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.9×10^{-8} , 2.1×10^{-6} , 8.1×10^{-5} , 1.9×10^{-3} , 0.031 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.67×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

1.74×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

9.39×10^{-5} ; 4.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.84 - 6057/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.88 - 3540/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

5.13×10^{-6} , 1.74×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log (P_L/mmHg) = 32.06 - 6015/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.023 (calculated-SOFA model, Govers & Krop 1998)

$\log (H/(Pa \cdot m^3/mol)) = 7.04 - 1020/(T/K)$ (Passivirta et al. 1999)

1.26; 1.012 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.31 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.58 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$ s, Passivirta et al. 1999)
 6.78; 7.31 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

- 4.66 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 4.96; 4.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 8.47 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 8.72; 8.47 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 59.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 168 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_6\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

suggested $t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_{1/2} = 28\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000);

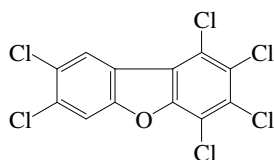
suggested $t_{1/2} = 450\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 450\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Biota: $t_{1/2} > 7$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993)

9.1.1.23 1,2,3,4,7,8-Hexachlorodibenzofuran



Common Name: 1,2,3,4,7,8-Hexachlorodibenzofuran

Synonym: 1,2,3,4,7,8-HxCDF

Chemical Name: 1,2,3,4,7,8-Hexachlorodibenzofuran

CAS Registry No: 70658-26-9

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6H_2Cl_2OC_6Cl_4$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

225.5–226.5 (Kuroki et al. 1984; Rordorf 1989)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.5 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.397 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1989; quod, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

96 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F :

0.0107 (calculated-assuming $\Delta S_{fus} = 56\ J/mol\ K$ and $mp = 226^{\circ}C$)

0.000402 (calculated- ΔS_{fus} and mp , Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

8.25×10^{-6} ($22.7^{\circ}C$, generator column-GC/MS, Friesen et al. 1990)

7.30×10^{-6} (computed-expert system SPARC, Kollig 1995)

8.2×10^{-6} , 1.13×10^{-6} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

8.01×10^{-4} ; 2.65×10^{-3} (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.913 - 2516/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.64×10^{-3} , 2.65×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

8.093×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988; quoted, Della Site 1997)

3.2×10^{-8} , 2.4×10^{-6} , 9.3×10^{-5} , 2.2×10^{-3} , 0.036 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.85×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989; quoted, Della Site 1997)

8.90×10^{-8} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

3.09×10^{-6} (supercooled liquid P_L , Falconer & Bidleman 1994;)

8.67×10^{-8} (computed-expert system SPARC, Kollig 1995)

8.41×10^{-8} , 3.68×10^{-8} (P_s solid vapor pressure calculated from reported P_L , Della Site 1997)

6.05×10^{-5} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)
 5.62×10^{-6} ; 1.38×10^{-5} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 2.87×10^{-8} ; 7.13×10^{-5} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F , Passivirta et al. 1999)
 $\log (P_s/Pa) = 12.85 - 6077/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/Pa) = 7.81 - 3564/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P_L/\text{mmHg}) = 32.14 - 6106/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 3.24×10^{-6} , 1.38×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

1.454 (calculated-P/C with selected values)
 4.26 (computed-expert system SPARC, Kollig 1995)
 2.63; 1.91 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 6.90 - 1048/(T/K)$ (Passivirta et al. 1999)
 1.26; 1.905 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.70 (calculated, Broman et al. 1991)
 7.86 (computed-expert system SPARC, Kollig 1995)
 7.53 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 7.54 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{ow}$, Passivirta et al. 1999)
 7.184 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 6.92; 7.53 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

10.64 (Finizio et al. 1997; quoted, Kaupp & McLachlan 1999)
 11.98 (7°C , GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

4.91; 4.40 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.91; 4.99; 5.04 (guppies, 21-d exposure, lipid weight basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.57 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.90, 5.26 (fish muscle $\log BCF_L$ calculated from water, sediment, Wu et al. 2001)
 4.88; 4.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

7.40 (calculated, Broman et al. 1991)
 7.54 (computed-expert system SPARC, Kollig 1995)
 8.83; 8.80 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 8.95; 8.80 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic $t_{1/2} = 5.5$ h of the PCDD in extract of fly ash in tetradecane solution for native congener (Tysklind & Rappe 1991).

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3}(\text{aq.}) = 7.28 \times 10^4 \text{ L} \cdot \text{g}^{-1} \cdot \text{min}^{-1}$, oxidative degradation rate constant of water dissolved PDCF by ozone under alkaline conditions at pH 10 and 20°C (Palaushek & Scholz 1987)

$k_{\text{OH}} = (0.7\text{--}2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for a hexa-chlorinated dibenzofuran, tropospheric lifetime was calculated to be 5.9–22 d using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule cm}^{-3}$ (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 100, 439 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.31, < 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P₅CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0126 \text{ d}^{-1}$ with a biological $t_{1/2} = 24 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 879 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.087 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 28\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200 \text{ yr}$ for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 600\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50 \text{ yr}$ (estimated, Suzuki et al. 2000);

$t_{1/2} = 600\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

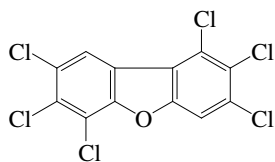
Biota: $t_{1/2} \sim 336 \text{ d}$ in carp (Kuehl et al. 1987);

elimination $t_{1/2} = 48.5 \text{ d}$ from lactating cows (Olling et al. 1991);

$t_{1/2} = 2.2 \text{ d}$ for PBO treated goldfish and $t_{1/2} > 7 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2} = 24 \text{ d}$ in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.24 1,2,3,6,7,8-Hexachlorodibenzofuran



Common Name: 1,2,3,6,7,8-Hexachlorodibenzofuran

Synonym:

Chemical Name: 1,2,3,6,7,8-hexachlorodibenzofuran

CAS Registry No: 57117-44-9

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

232–234 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.1 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.083 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

95 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.000358 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00226 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.125 - 2515/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.56×10^{-3} , 2.26×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

7.33×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

2.9×10^{-8} , 2.1×10^{-6} , 8.2×10^{-5} , 2.0×10^{-3} , 0.031 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1985a,b, 1987, 1989)

1.20×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

6.91×10^{-5} ; 2.47×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.87 - 6101/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.91 - 3954/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P_L/mmHg) = 32.12 - 6108/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

3.09×10^{-6} , 1.20×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.91 (calculated-SOFA model, Govers & Krop 1998)

$\log (H/(Pa \cdot m^3/mol)) = 7.79 - 1439/(T/K)$, (Passivirta et al. 1999)

1.26; 1.91 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.60 (calculated, Broman et al. 1991)
 7.57 (calculated-SOFA model, Govers & Krop 1998)
 7.96 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
 7.196 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 6.93; 7.57 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.0 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.95; 4.49 (guppies, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.95, 5.15; 5.24 (guppies, 21-d exposure, lipid weight basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.58 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.51 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)
 4.87; 4.58 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 7.40 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 8.85 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 8.97; 8.85 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic $t_{1/2} = 5.9$ h in extract of fly-ash and in tetradecane solution for native congener (Tysklind & Rappe 1991);

$t_{1/2} = 74.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (1.3 - 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 103, 460 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.26, < 0.1 \text{ d}^{-1}$ (goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $P_5\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0138 \text{ d}^{-1}$ with a biological $t_{1/2} = 22$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 1310 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.078 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Ground water:

Sediment: $t_{1/2} = 700000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

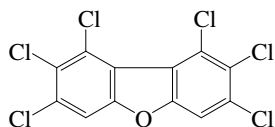
Soil: $t_{1/2} = 700000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: elimination $t_{1/2} = 73$ –156 d in the liver of female Sprague Dawley rats (Van den Berg et al. 1989);

$t_{1/2} = 2.7$ d for PBO treated goldfish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993)

biological $t_{1/2} = 22$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994).

9.1.1.25 1,2,3,7,8,9-Hexachlorodibenzofuran



Common Name: 1,2,3,7,8,9-Hexachlorodibenzofuran

Synonym: 1,2,3,7,8,9-HxCDF

Chemical Name: 1,2,3,7,8,9-hexachlorodibenzofuran

CAS Registry No: 72918-21-9

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

246–249 (Rordorf 1989)

230 (calculated, Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

96 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.00036 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.000859 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.892 - 2526/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.06×10^{-3} , 8.59×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.99×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988, 1991)

4.31×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

3.88×10^{-5} (corrected, supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)

2.24×10^{-6} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

4.01×10^{-5} ; 1.44×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.91 - 6185/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.90 - 3625/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P_L/mmHg) = 31.92 - 6114/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

2.09×10^{-6} , 2.24×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.955 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa \cdot m^3/mol)] = 7.01 - 1136/(T/K)$ (Passivirta et al. 1999)

1.29; 0.955 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.00 (calculated, Broman et al. 1991)

7.76 (calculated-SOFA model, Govers & Krop 1998)

- 7.57 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
 7.125 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 7.07; 7.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

- 12.17 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.71 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 5.04 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)
 4.77; 4.71 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 9.08 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 9.19; 9.08 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution: $t_{1/2} = 2.2$ h for native congener and $t_{1/2} = 3.6$ h for ^{13}C -labelled congener (Tysklind & Rappe 1991);
 $t_{1/2} = 78.8$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = (1.3 - 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.01651 \text{ d}^{-1}$ with a biological $t_{1/2} = 18$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 1101 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.103 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

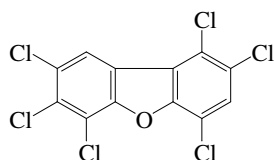
Ground water:

Sediment: $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: biological $t_{1/2} = 18$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.26 1,2,4,6,7,8-Hexachlorodibenzofuran



Common Name: 1,2,4,6,7,8-Hexachlorodibenzofuran

Synonym: 1,2,4,6,7,8-HxCDF

Chemical Name: 1,2,4,6,7,8-hexachlorodibenzofuran

CAS Registry No: 67562-40-7

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

221–222 (Kuroki et al. 1986; Rordorf 1989; Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

137.593 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

97 (Rordorf 1989; Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.000483 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

0.00451 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.944 - 2512/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

2.26×10^{-3} , 4.51×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.5×10^{-8} , 2.6×10^{-6} , 1.0×10^{-4} , 2.4×10^{-3} , 0.040 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

1.35×10^{-5} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

9.39×10^{-5} ; 4.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.81 - 6006/(T/K)$, (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.74 - 3497/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

4.47×10^{-6} , 2.35×10^{-5} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log (P_L/mmHg) = 32.31 - 6108/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

1.072 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa\ m^3/mol)] = 6.80 - 985/(T/K)$, (Passivirta et al. 1999)

1.26; 1.072 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.38 (calculated-SOFA model, Govers & Krop 1998)
- 7.51 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 6.83; 7.38 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.66 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 4.94; 4.66 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 8.58 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 8.78; 8.58 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 58.2$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 345, 293 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.10, > 2.4 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 170 \text{ L kg}^{-1} \text{ d}^{-1}$, $369 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_6\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_1 = 1101 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.103 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

suggested $t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: suggested $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

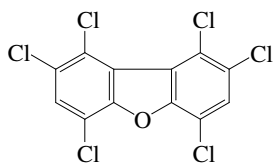
Ground water:

Sediment: suggested $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: $t_{1/2} > 7$ d for PBO treated goldfish and $t_{1/2} < 0.3$ d for control fish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.27 1,2,4,6,8,9-Hexachlorodibenzofuran



Common Name: 1,2,4,6,8,9-Hexachlorodibenzofuran

Synonym: 1,2,3,4,8,9-HxCDF

Chemical Name: 1,2,4,6,8,9-hexachlorodibenzofuran

CAS Registry No: 69698-59-5

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

246–248 (Kuroki et al. 1984; Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

487.7 (Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

225.2 (Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

136.462 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

93 (Rordorf 1989; Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.000245 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

0.00305 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.892 - 2526/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.92×10^{-3} , 3.05×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.4×10^{-8} , 1.7×10^{-6} , 6.4×10^{-5} , 1.5×10^{-3} , 0.024 (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

9.22×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

3.55×10^{-6} supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

7.96×10^{-5} ; 1.95×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.89 - 6137/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.08 - 3629/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

3.89×10^{-6} , 3.55×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log (P_L/mmHg) = 32.22 - 6105/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.417 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa \cdot m^3/mol)] = 7.40 - 1117/(T/K)$ (Passivirta et al. 1999)

1.26; 0.417 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 7.43 (calculated-SOFA model, Govers & Krop 1998)
- 7.65 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 6.87; 7.43 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.84 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 4.91; 4.84 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 8.58 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 8.86; 8.58 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 82.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 170 \text{ L kg}^{-1} \text{ d}^{-1}$, $369 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_6\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 > 2.0 \text{ d}^{-1}$ (120-h exposure: metabolic inhibitor PBO-treated goldfish, Sijm et al. 1993)

$k_1 = 1101 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.103 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

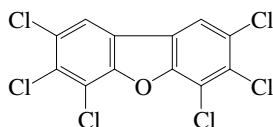
Ground water:

Sediment: $t_{1/2} = 150000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: suggested $t_{1/2} = 150000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

Biota: $t_{1/2} < 0.3$ d for PBO treated goldfish in 120-h exposure studies (Sijm et al. 1993).

9.1.1.28 2,3,4,6,7,8-Hexachlorodibenzofuran



Common Name: 2,3,4,6,7,8-Hexachlorodibenzofuran

Synonym: 2,3,4,6,7,8-HCDF

Chemical Name: 2,3,4,6,7,8-hexachlorodibenzofuran

CAS Registry No: 60851-34-5

Molecular Formula: $C_{12}H_2Cl_6O$, $C_6HCl_3OC_6HCl_3$

Molecular Weight: 374.863

Melting Point ($^{\circ}C$):

239–240 (Rordorf 1989)

Boiling Point ($^{\circ}C$):

487.7 (calculated, Rordorf 1989)

Density (g/cm^3):

Molar Volume (cm^3/mol):

302.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.7 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

136.794 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

48.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

94 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at 25 $^{\circ}C$, F:

0.000276 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00156 (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.787 - 2527/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

1.24×10^{-3} , 1.56×10^{-3} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations):

4.99×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988, 1991)

5.82×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

3.88×10^{-5} (corrected, supercooled liquid P_L , in Eitzer & Hites 1988, Eitzer & Hites 1998)

2.6×10^{-8} , 1.9×10^{-6} , 7.3×10^{-5} , 1.7×10^{-3} , 0.028 (25, 50, 75, 100, 125 $^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.59×10^{-6} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

5.54×10^{-5} ; 1.53×10^{-8} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.91 - 6175/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.00 - 3651/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P_L/mmHg) = 31.99 - 6108/(T/K) - 7.332 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

2.45×10^{-6} , 7.59×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant (Pa $\cdot m^3/mol$ or as indicated and reported temperature dependence equations):

1.78 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa \cdot m^3/mol)] = 7.21 - 1124/(T/K)$ (Passivirta et al. 1999)

1.26; 1.78 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, log K_{OW} :

- 7.0 (calculated, Broman et al. 1991)
- 7.65 (calculated-SOFA model, Govers & Krop 1998)
- 7.62 (estimated-solubility S_L and regression eq. using lit. K_{OW} values, Passivirta et al. 1999)
- 6.937 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.01; 7.65 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated:

- 12.10 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, log BCF or log K_B :

- 4.88 (goldfish, 120-h exposure studies, Sijm et al. 1993)
- 4.99; 4.94; 5.02 (guppies, 21-d exposure, lipid weight basis: measured- C_{fish}/C_W ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
- 4.59 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
- 5.51 (fish muscle log BCF_L calculated from water, Wu et al. 2001)
- 4.81; 4.59 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, log K_{OC} :

- 6.80 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 8.96 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
- 9.10; 8.96 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

- Photolysis: photolytic half-life in extract of fly-ash and in tetradecane solution: $t_{1/2} = 2.8$ h for native congener (Tysklind & Rappe 1991);
- $t_{1/2} = 70.7$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

- $k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)
- $k_{OH} = (0.7 - 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 5.9–22 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hexa-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

- $k_1 = 267 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 < 0.1 \text{ d}^{-1}$ (goldfish after 120-h exposure: control fish, Sijm et al. 1993)
- $k_2 = 0.36$ (metabolic inhibitor PBO-treated goldfish, 120-h exposure studies, Sijm et al. 1993)
- $k_1 = 110 \text{ L kg}^{-1} \text{ d}^{-1}$, $174 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P₅CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)
- $k_2 = 0.0119 \text{ d}^{-1}$ with a biological $t_{1/2} = 25$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

Half-Lives in the Environment:

- Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hexa-chlorinated PCDF with OH radicals to be 5.9–22 d (Atkinson 1991);

$t_{1/2} = 1400$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

- Surface water: $t_{1/2} = 28000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

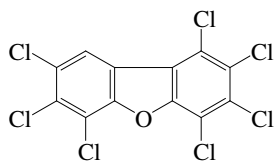
Ground water:

- Sediment: $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

- Soil: $t_{1/2} = 500000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000)

- Biota: $t_{1/2} = 1.9$ d for PBO treated goldfish and $t_{1/2} > 7$ d for control fish in 120-h exposure studies (Sijm et al. 1993). biological $t_{1/2} = 25$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.29 1,2,3,4,6,7,8-Heptachlorodibenzofuran



Common Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran

Synonym: 1,2,3,4,6,7,8-HCDF

Chemical Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran

CAS Registry No: 67562-39-4

Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$

Molecular Weight: 409.308

Melting Point ($^{\circ}C$):

236–237 (Kuroki et al. 1984; Rordorf 1989; Della Site 1997)

Boiling Point ($^{\circ}C$):

507.2 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

323.0 (calculated-Le Bas method at normal boiling point)

238.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

87.8 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

144.642 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

53.9 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

106 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.000122 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.35×10^{-6} ($22.7^{\circ}C$, generator column-GC/MS, Friesen et al. 1990)

1.08×10^{-5} (calculated-QSAR, Fiedler & Schramm 1990)

9.50×10^{-7} (computed-expert system SPARC, Kollig 1995)

1.26×10^{-7} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.63×10^{-4} ; 7.11×10^{-4} (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.917 - 2812/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

4.92×10^{-4} , 7.11×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.24×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988, 1991; quoted, Della Site 1997)

1.93×10^{-6} (supercooled liquid P_L GC-RT correlation, Eitzer & Hites 1989; quoted, Della Site 1997)

4.7×10^{-9} , 4.3×10^{-7} , 2.0×10^{-5} , 5.8×10^{-4} , 1.1×10^{-2} (25 , 50 , 75 , 100 , $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

5.10×10^{-8} (gas saturation method, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)

8.70×10^{-9} (computed-expert system SPARC, Kollig 1995)

1.83×10^{-8} , 1.58×10^{-8} (P_s solid vapor pressure calculated from reported P_L , Della Site 1997)

1.84×10^{-5} (corrected supercooled liquid P_L in Eitzer & Hites 1988, Eitzer & Hites 1998)

1.4×10^{-6} ; 2.51×10^{-6} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

5.54×10^{-5} ; 6.76×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.98 - 6302/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/Pa) = 7.45 - 3486/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P_L/mmHg) = 30.03 - 6090/(T/K) - 6.798 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)
 9.33×10^{-7} , 2.51×10^{-6} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($Pa \text{ m}^3/\text{mol}$ at 25°C):

3.80 (computed-expert system SPARC, Kollig 1995)
 3.47; 1.41 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(Pa \text{ m}^3/\text{mol})] = 6.53 - 674/(T/K)$ (Passivirta et al. 1999)
 1.41; 1.41 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.92 (shake flask/slow stirring-GC/MS, from fly-ash extract, Sijm et al. 1989a)
 9.25 (calculated-QSAR, Friedler & Schramm 1990)
 7.90 (quoted, Loonen et al. 1991)
 8.10 (calculated, Broman et al. 1991)
 7.92 (recommended, Hansch et al. 1995)
 8.52 (computed-expert system SPARC, Kollig 1995)
 8.01 (calculated-SOFA model, Govers & Krop 1998)
 8.07 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{ow}$, Passivirta et al. 1999)
 7.477 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 7.37; 8.00 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

12.06 (7°C , GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

4.46; 4.08 (guppy, 21-d exposure, lipid wt: system I - absence of sediment; system II - with presence of sediment, Loonen et al. 1994a)
 4.46; 4.60; 4.63 (guppy, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 4.46; 4.26 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 6.62; 6.92 (wet wt basis, fish 5% lipid, 10% lipid, Geyer et al. 2000)
 5.89, 6.03 (fish muscle $\log BCF_L$ calculated from water, sediment, Wu et al. 2001)
 4.51; 4.26 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

6.37 (organic carbon, calculated-QSAR, Friedler & Schramm 1990)
 6.00 (organic carbon, calculated, Broman et al. 1991)
 7.90 (calculated, Broman et al. 1991)
 8.20 (computed- K_{ow} , Kollig 1995)
 9.07; 9.48 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 9.64; 9.48 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic degradation $t_{1/2} = 9.8 \text{ h}$ with extract of fly-ash and in tetradecane solution for native congener and $t_{1/2} = 3.7 \text{ h}$ for ^{13}C -labelled congener (Tysklind & Rappe 1991).

$t_{1/2} = 84.5 \text{ h}$ on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3}(aq.) = 1.08 \times 10^5 \text{ L g}^{-1} \text{ min}^{-1}$, oxidative degradation rate constant of water dissolved PCDF by ozone under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{OH}(calc) = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.5 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 17\text{--}31 \text{ d}$, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 42, 61 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.43, 0.1 \text{ d}^{-1}$ (metabolic inhibitor PBO-treated goldfish, control fish, 120-h exposure studies, Sijm et al. 1993)

$k_1 = 42 \text{ L kg}^{-1} \text{ d}^{-1}$, $61 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for P₅CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

$k_2 = 0.0084 \text{ d}^{-1}$ with a biological $t_{1/2} = 36 \text{ d}$ (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 524 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.127 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF with OH radicals to be 17–31 d (Atkinson 1991);

$t_{1/2} = 3200 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 64\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{1/2} = 36 \text{ yr}$ (Geyer et al. 2000)

degradation $t_{1/2} = 2\text{--}200 \text{ yr}$ for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 350\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50 \text{ yr}$ (estimated, Suzuki et al. 2000);

$t_{1/2} = 350\,000 \text{ h}$ at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

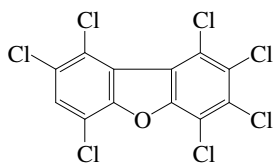
Biota: depuration $t_{1/2} > 336 \text{ d}$ for carp in Lake Superior water (Kuehl et al. 1987);

elimination $t_{1/2} = 33.9 \text{ d}$ from lactating cow (Olling et al. 1991);

$t_{1/2} = 1.6 \text{ d}$ for PBO treated goldfish and $t_{1/2} = 6.8 \text{ d}$ for control fish in 120-h exposure studies (Sijm et al. 1993).

biological $t_{1/2} = 37 \text{ d}$ in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

9.1.1.30 1,2,3,4,6,8,9-Heptachlorodibenzofuran



Common Name: 1,2,3,4,6,8,9-Heptachlorodibenzofuran

Synonym: 1,2,3,4,6,8,9-HpCDF

Chemical Name: 1,2,3,4,6,8,9-Heptachlorodibenzofuran

CAS Registry No: 69698-58-4

Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$

Molecular Weight: 409.308

Melting Point ($^{\circ}C$):

211–212 (Kuroki et al. 1984; Rordorf 1989; Della Site 1997)

Boiling Point ($^{\circ}C$):

507.2 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

323.0 (calculated-Le Bas method)

238.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

89.2 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

145.64 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

53.9 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

111 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.00021 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

5.65×10^{-4} (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 1.200 - 2861/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

4.19×10^{-4} , 5.65×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

7.7×10^{-9} , 7.2×10^{-7} , 3.6×10^{-5} , 1.0×10^{-3} , 2.0×10^{-2} (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1989)

7.24×10^{-7} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

1.55×10^{-5} ; 3.57×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 13.03 - 6394/(T/K)$, (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.23 - 3581/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

8.13×10^{-7} , 7.24×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

$\log (P_L/mmHg) = 29.94 - 6089/(T/K) - 6.798 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

5.13 (calculated-SOFA model, Govers & Krop 1998)

$\log [H/(Pa \cdot m^3/mol)] = 6.03 - 756/(T/K)$, (Passivirta et al. 1999)

1.45; 5.13 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 8.02 (calculated-SOFA model, Govers & Krop 1998)
 7.91 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$, Passivirta et al. 1999)
 7.43; 8.02 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

- 4.42 (lipid wt basis, calculated-SOFA model, Govers & Krop 1998)
 4.46; 4.42 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 9.45 (sediment/water, calculated-SOFA model, Govers & Krop 1998)
 9.72; 9.45 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 85.6$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003)

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.5 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 17–31 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 42 \text{ L kg}^{-1} \text{ d}^{-1}$, $61 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for $H_7\text{CDD}$ homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF with OH radical to be 17–31 d (Atkinson 1991);

suggested $t_{1/2} = 3200$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: suggested $t_{1/2} = 64\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 2\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000);

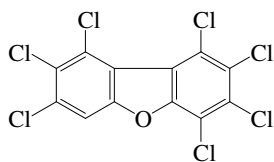
suggested $t_{1/2} = 350\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr (estimated, Suzuki et al. 2000);

suggested $t_{1/2} = 350\,000$ h at 7°C in Baltic Proper environment (Sinkkonen & Passivirta 2000).

Biota:

9.1.1.31 1,2,3,4,7,8,9-Heptachlorodibenzofuran



Common Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran

Synonym: 1,2,3,4,7,8,9-HCDF

Chemical Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran

CAS Registry No: 55673-89-7

Molecular Formula: $C_{12}HCl_7O$, $C_6HCl_3OC_6Cl_4$

Molecular Weight: 409.308

Melting Point ($^{\circ}C$):

221–223 (Kuroki et al. 1984)

Boiling Point ($^{\circ}C$):

507.2 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

323.0 (calculated-Le Bas method at normal boiling point)

248.1 (Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.6 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

145.221 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

53.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

109 (Rordorf 1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.000179 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.30×10^{-6} (computed-expert system SPARC, Kollig 1995)

2.58×10^{-4} (supercooled liquid S_L , calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 1.100 - 2819/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

2.83×10^{-4} , 2.58×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.2×10^{-9} , 5.8×10^{-7} , 2.8×10^{-5} , 8.0×10^{-4} , 1.5×10^{-2} (25, 50, 75, 100, $125^{\circ}C$, predicted-vapor pressure correlation method, Rordorf 1987, 1989)

1.305×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1988, 1991)

1.011×10^{-6} (supercooled liquid P_L , GC-RT correlation, Eitzer & Hites 1989)

1.27×10^{-9} (computed-expert system SPARC, Kollig 1995)

1.48×10^{-8} , 1.14×10^{-8} (solid vapor pressures calculated from reported P_L , Della Site 1997)

6.61×10^{-7} (supercooled liquid P_L , calculated-SOFA model, Govers & Krop 1998)

7.87×10^{-6} ; 1.41×10^{-9} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 13.12 - 6547/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 7.23 - 3581/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\log (P_L/mmHg) = 29.69 - 6089/(T/K) - 6.798 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

5.75×10^{-7} , 6.60×10^{-7} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations):

- 3.85 (computed-expert system SPARC, Kollig 1995)
- 1.0 (calculated-SOFA model, Govers & Krop 1998)
- $\log [H/(\text{Pa m}^3/\text{mol})] = 6.32 - 912/(T/K)$ (Passivirta et al. 1999)
- 1.58; 1.0 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 6.90 (calculated, Broman et al. 1991)
- 8.50 (computed-expert system SPARC, Kollig 1995)
- 8.23 (calculated-SOFA model, Govers & Krop 1998)
- 7.99 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$, Passivirta et al. 1999)
- 7.616 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
- 7.60; 8.23 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25 °C or as indicated:

- 12.34 (7°C, GC-retention time correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

- 4.32 (calculated-SOFA model, Govers & Krop 1998)
- 5.59 (fish muscle $\log BCF_L$ calculated from water, Wu et al. 2001)
- 4.30; 4.32 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.00 (organic carbon, calculated, Broman et al. 1991)
- 6.70 (calculated, Broman et al. 1991)
- 8.23 (computed- K_{OW} , Kollig 1995)
- 9.78; 9.76 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
- 9.92; 9.76 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolysis $t_{1/2} = 3.3$ h in the extract from fly ash in tetradecane, for ^{13}C labelled congener (Tysklind & Rappe 1991)

$t_{1/2} = 84.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 0.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{OH} = (0.5 - 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime of 17–31 d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for a hepta-chlorinated dibenzofuran at room temp. (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 42 \text{ L kg}^{-1} \text{ d}^{-1}$, $61 \text{ L kg}^{-1} \text{ d}^{-1}$ (average k_1 for H_7CDD homolog group, goldfish after 120-h exposure: metabolic inhibitor PBO-treated, control fish, Sijm et al. 1993)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for a hepta-chlorinated PCDF, with OH radicals to be 17–31 d (Atkinson 1991);

$t_{1/2} = 3200$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: $t_{1/2} = 64\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: degradation $t_{1/2} = 20\text{--}200$ y for all homologues (estimated, Suzuki et al. 2000);

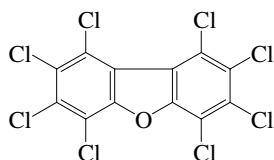
$t_{1/2} = 300\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr (estimated, Suzuki et al. 2000);

$t_{1/2} = 300\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota:

9.1.1.32 Octachlorodibenzofuran



Common Name: Octachlorodibenzofuran

Synonym: OCDF

Chemical Name: octachlorodibenzofuran

CAS Registry No: 39001-02-0

Molecular Formula: $C_6Cl_4OC_6Cl_4$

Molecular Weight: 443.753

Melting Point ($^{\circ}C$):

258–260 (Rordorf 1986,1989)

259 (Ruelle & Kesselring 1997, Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

510 (calculated, Rordorf 1986)

537 (calculated, Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

343.9 (calculated-Le Bas method at normal boiling point)

251.0 (Ruelle & Kesselring 1997, quoted, Passivirta et al. 1999)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

90 (Rordorf 1989)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

149.43 (Rordorf 1989)

284.38 (Dickhut et al. 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

57.5 (Rordorf 1989; quoted, Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

108 (Rordorf 1986,1989; quoted, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.00518 (calculated-assuming $\Delta S_{fus} = 56$ J/mol K and mp = $258^{\circ}C$)

0.000037 (calculated- ΔS_{fus} and mp, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.16×10^{-6} * (extrapolated, generator column-GC, measured range 39.8 – $80^{\circ}C$, Doucette & Andren 1988a)

$S/(mol/L) = 2.77 \times 10^{-14} \exp(0.081 \cdot t/^{\circ}C)$ (generator column-GC/ECD, temp range 40 – $80^{\circ}C$, Doucette & Andren 1988a)

$\log x = -3264/(T/K) - 2.376$, temp range 40 – $80^{\circ}C$ (generator column-GC/ECD, Doucette & Andren 1988a)

1.54×10^{-6} (calculated-QSAR, Fiedler & Schramm 1990)

1.37×10^{-7} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

2.33×10^{-4} ; 1.02×10^{-4} (supercooled liquid S_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)

$\log [S_L/(mol/L)] = 0.5720 - 3008/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

$\ln x = -5.0496 - 7455.1/(T/K)$; temp range 5 – $50^{\circ}C$ (regression eq. of literature data, Shiu & Ma 2000)

1.22×10^{-4} , 1.02×10^{-4} (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5.00×10^{-10} * (gas saturation, Rordorf 1985, 1989)

2.60×10^{-7} (supercooled liquid P_L , GC-RC correlation, Eitzer & Hites 1989)

0.000221* (105.6 °C, average value, gas saturation-GC, measured range 105.6–261.2 °C, Rordorf 1990)
 5.00×10^{-10} (gas saturation, estimated from extrapolated vapor pressure vs. halogen substitution no. plot, Rordorf et al. 1990)
 1.26×10^{-9} (solid vapor pressure calculated from reported P_L , Delle Site 1997)
 7.08×10^{-7} ; 1.82×10^{-7} (supercooled liquid P_L , quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 1.30×10^{-6} ; 4.83×10^{-11} (supercooled liquid P_L from GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 13.42 - 7073/(T/K)$ (solid, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 7.77 - 4068/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P/\text{Pa}) = 16.88937 - 7808.74/(T/K)$; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
 0.107* (165 °C, Knudsen effusion, measured range 165–195°C, Li et al. 2002)
 $\log (P_L/\text{mmHg}) = 27.96 - 6148/(T/K) - 6.267 \cdot \log (T/K)$ (supercooled liquid P_L , Kirchoff/Rankin eq., GC-RI correlation, Mader & Pankow 2003)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations):

0.10 (estimated, Clark & Mackay 1991)
 1.31; 0.776 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 7.20 - 1060/(T/K)$ (Passivirta et al. 1999)
 2.14; 0.776 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

13.06, 13.22, 13.78; 12.54, 13.37, 13.93 (HPLC-RT correlation, linear regressions; quadratic regressions, Sarna et al. 1984)
 8.78 (re-evaluated HPLC-RT data, Burkhard & Kuehl 1986)
 7.97 (generator column-GC/ECD, Doucette & Andren 1987, 1988b)
 7.90 (HPLC-RT correlation, Doucette & Andren 1988b)
 7.97 (recommended, Hansch et al. 1995)
 8.78; 8.60 (quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 8.62 (calculated-solubility $\log S_L$ and regression from lit. $\log K_{OW}$, Passivirta et al. 1999)
 7.992 (calculated-QSPR by PM3 Hamiltonian descriptors and partial least-square analysis, Chen et al. 2001)
 8.03; 8.60 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated:

12.84 (7°C, GC-retention time indices correlation, Harner et al. 2000)

Bioconcentration Factor, $\log BCF$:

1.613, 0.70 (human fat, calculated-different K_{OWS} , wet weight basis, Geyer et al. 1987)
 1.71, 0.778 (human fat, calculated-different K_{OWS} , lipid basis, Geyer et al. 1987)
 2.77; 3.89 (guppy, wet weight based; lipid weight based, Gobas & Schrap 1990)
 3.90; 4.10; 4.11 (guppies, 21-d exposure, lipid wt basis: measured- C_{fish}/C_w ; calculated; rate constant ratio k_1/k_2 from non-linear regression analysis, Loonen et al. 1994b)
 3.90; 3.88 (lipid wt basis, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 7.48; 7.78 (wet wt basis: fish with 5% lipid, with 10% lipid, Geyer et al. 2000)
 7.61, 7.63 (fish muscle $\log BCF_L$ calculated from water, sediment, Wu et al. 2001)
 3.85; 3.88 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Sorption Partition Coefficient, $\log K_{OC}$:

6.75 (calculated-QSAR, Fiedler & Schramm 1990)
 6.00 (organic carbon, calculated, Broman et al. 1991)
 7.40 (calculated, Broman et al. 1991)
 7.40 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
 8.13, 8.48 (calculated- K_{OW} , Kollig 1993)
 10.49; 10.30 (sediment/water, quoted exptl.; calculated-SOFA model, Govers & Krop 1998)
 10.39; 10.30 (GC-RI correlation; calculated-SOFA method, Wang & Wong 2003)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolytic $t_{1/2} = 2.1$ h from extract of fly ash in tetradecane solution for native congener (Tysklind & Rappe 1991);

photolysis $k = 2.7 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 260$ min in pure water and $t_{1/2} = 6.3 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 110$ min in 60% acetonitrile/water at 300 nm photochemical reactor; $k = 0.11 \text{ h}^{-1}$ with $t_{1/2} = 6.5$ h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000).

$t_{1/2} = 100.5$ h on spruce needle surfaces under sunlight irradiation (Niu et al. 2003).

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

k (oxidative degradation rate constant of water dissolved OCDF by ozone) is $1.05 \times 10^4 \text{ L g}^{-1} \text{ min}^{-1}$ under alkaline conditions at pH 10 and 20°C (Palauschek & Scholz 1987)

$k_{\text{OH}}(\text{calc}) = 0.39 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

$k_{\text{OH}} = 0.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 39$ d, using a 12-h average daytime OH radical concn of $1.5 \times 10^6 \text{ molecule/cm}^3$ for OCDF at room temp. (Atkinson 1991)

photodegradation $t_{1/2} = 9$ h for OCDF adsorbed to clean silica gels in a rotary photo-reactor by filtered < 290 nm of light (Koester & Hites 1992)

Biodegradation:

Biotransformation: metabolism half-time 10^7 h (guppy, Clark & Mackay 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.012 \text{ d}^{-1}$ (rainbow trout, Niimi & Oliver 1986)

$k_1 = 824 \text{ d}^{-1}$; $k_2 = 1.40 \text{ d}^{-1}$ (guppy, Gobas & Schrap 1990)

$k_2 = 0.0101 \text{ d}^{-1}$ with a biological $t_{1/2} = 30$ d (blue mussel, 99-d exposure, Hektoen et al. 1994)

$k_1 = 217 \text{ L kg}^{-1} \text{ d}^{-1}$; $k_2 = 0.174 \text{ d}^{-1}$ (guppy, 21-d exposure, wet wt base, Loonen et al. 1994b)

Half-Lives in the Environment:

Air: tropospheric lifetime was calculated based on the gas-phase reaction rate constant for OCDF with OH radicals to be 39 d (Atkinson 1991);

$t_{1/2} = 9600$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Surface water: photolysis $k = 2.7 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 260$ min in pure water and $k = 6.3 \times 10^{-3} \text{ min}^{-1}$ with $t_{1/2} = 110$ min in 60% acetonitrile/water at 300 nm photochemical reactor; $k = 0.11 \text{ h}^{-1}$ with a $t_{1/2} = 6.5$ h in pure water in sunlight at 42°N latitude in middle of July (Kim & O'Keefe 2000);

$t_{1/2} = 192000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Groundwater:

Sediment: very persistent $t_{1/2} = 29$ yr (Geyer et al. 2000)

degradation $t_{1/2} = 20\text{--}200$ yr for all homologues (estimated, Suzuki et al. 2000);

$t_{1/2} = 250\,000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Soil: degradation $t_{1/2} = 5\text{--}50$ yr (estimated, Suzuki et al. 2000);

$t_{1/2} = 250000$ h at 7°C in Baltic Proper environment (estimated, Sinkkonen & Passivirta 2000).

Biota: mean biological $t_{1/2} = 7$ d in rainbow trout (Niimi 1986)

$t_{1/2} = 7$ to 12 d in rainbow trout (Niimi & Oliver 1986)

biological $t_{1/2} = 30$ d in blue mussel, 99-d exposure experiment (Hektoen et al. 1994)

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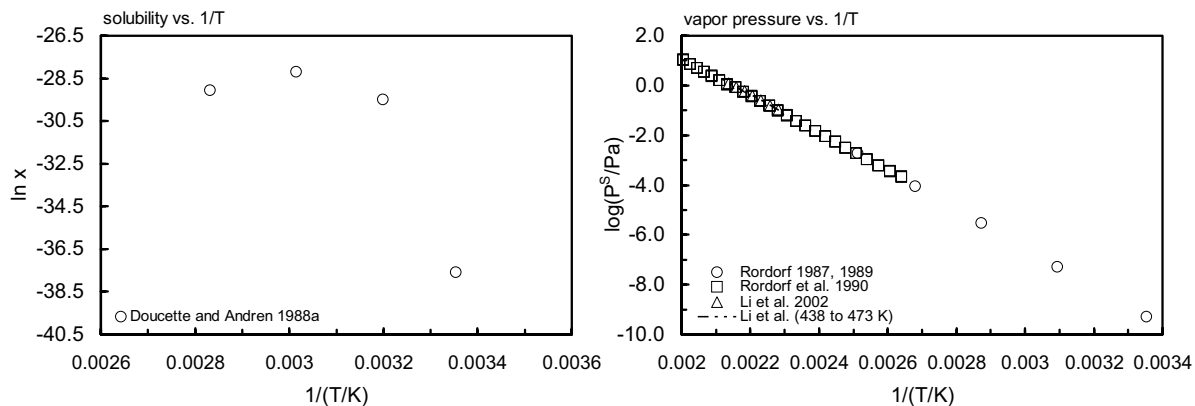


FIGURE 9.1.32.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for octachlorodibenzofuran.

9.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 9.2.1
Summary of physical properties of some chlorinated furans

Compound	CAS no.	Molecular formula	Chlorine no. n	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume V _M cm ³ /mol
Dibenzofuran	132-64-9	C ₁₂ H ₈ O	0	168.191	86.5	287	0.249	176.1
2-Chloro-	51230-49-0	C ₁₂ H ₇ OCl	1	202.637	101.5–102.5	338.2	0.175	197.6
3-Chloro-	25074-67-3	C ₁₂ H ₇ OCl	1	202.637	101–102	338.2	0.178	197.6
2,3-Dichloro-	64126-86-9	C ₁₂ H ₆ OCl ₂	2	237.082	125.5–127	375.0	0.102	218.5
2,7-Dichloro-	73992-98-6	C ₁₂ H ₆ OCl ₂	2	237.082				218.5
2,8-Dichloro-	5409-83-6	C ₁₂ H ₆ OCl ₂	2	237.082	184–185	375	0.0272	218.5
3,6-Dichloro-	94570-83-9	C ₁₂ H ₆ OCl ₂	2	237.082	188	375	0.0252	218.5
2,3,8-Trichloro-	57117-32-5	C ₁₂ H ₅ OCl ₃	3	271.527	189–191	408.4	0.0240	239.4
2,4,6-Trichloro-	58802-14-5	C ₁₂ H ₅ OCl ₃	3	271.527	116–117	408.4	0.126	239.4
2,4,8-Trichloro-	54589-71-8	C ₁₂ H ₅ OCl ₃	3	271.527	154	392.5	0.0542	239.4
1,2,3,4-Tetrachloro-	24478-72-6	C ₁₂ H ₄ OCl ₄	4	305.978	168.5–169	438.3	0.0389	260.3
1,2,3,7-Tetrachloro-	83704-22-7	C ₁₂ H ₄ OCl ₄	4	305.978	167.5–168	438.3	0.0398	260.3
1,2,7,8-Tetrachloro-	58802-20-3	C ₁₂ H ₄ OCl ₄	4	305.978	210–211	438.3	0.0151	260.3
1,3,6,8-Tetrachloro-	71998-72-6	C ₁₂ H ₄ OCl ₄	4	305.978	177–178	438.3	0.0319	260.3
1,3,7,8-Tetrachloro-	57117-35-8	C ₁₂ H ₄ OCl ₄	4	305.978				260.3
1,3,7,9-Tetrachloro-	64650-17-4	C ₁₂ H ₄ OCl ₄	4	305.978	206.5–207.5	438.3	0.0168	260.3
2,3,7,8-Tetrachloro-	51207-31-9	C ₁₂ H ₄ OCl ₄	4	305.978	227	438.3	0.0104	260.3
1,2,3,4,7-Pentachloro-	83704-48-7	C ₁₂ H ₃ OCl ₅	5	340.418				281.2
1,2,3,7,8-Pentachloro-	57117-41-6	C ₁₂ H ₃ OCl ₅	5	340.418	225–227	464.7	0.0107	281.2
1,2,4,7,8-Pentachloro-	83704-51-2	C ₁₂ H ₃ OCl ₅	5	340.418	236–238	464.7	0.00832	281.2
2,3,4,7,8-Pentachloro-	57117-31-4	C ₁₂ H ₃ OCl ₅	5	340.418	196–196.5	464.7	0.0209	281.2
1,2,3,4,6,8-Hexachloro-	69698-60-8	C ₁₂ H ₂ OCl ₆	6	374.863	233.5–234	487.7	0.00895	302.1
1,2,3,4,7,8-Hexachloro-	70658-26-9	C ₁₂ H ₂ OCl ₆	6	374.863	226	487.7	0.107	302.1
1,2,3,4,7,9-Hexachloro-	91538-84-0	C ₁₂ H ₂ OCl ₆	6	374.863	216–217	487.7	0.0132	302.1
1,2,3,6,7,8-Hexachloro-	57117-44-9	C ₁₂ H ₂ OCl ₆	6	374.863	232–234	487.7	0.00910	302.1
1,2,3,7,8,9-Hexachloro-	72918-21-9	C ₁₂ H ₂ OCl ₆	6	374.863	246–249	487.7	0.00656	302.1
1,2,4,6,7,8-Hexachloro-	67562-40-7	C ₁₂ H ₂ OCl ₆	6	374.863	221–222	487.7	0.0118	302.1
1,2,4,6,8,9-Hexachloro-	68698-59-5	C ₁₂ H ₂ OCl ₆	6	374.863	246–248	487.7	0.00664	302.1

Continued

TABLE 9.2.1 (continued)

Compound	CAS no.	Molecular formula	Chlorine no. n	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Le Bas molar volume V_M cm ³ /mol
2,3,4,6,7,8-Hexachloro-	60851-34-5	C ₁₂ H ₂ OCl ₆	6	374.863	239-240	487.7	0.00786	302.1
1,2,3,4,6,7,8-Heptachloro-	67462-39-4	C ₁₂ HOCl ₇	7	409.308	236-237	507.2	0.00841	323.0
1,2,3,4,6,8,9-Heptachloro-	69698-58-4	C ₁₂ HOCl ₇	7	409.308	211-212	507.2	0.0148	323.0
1,2,3,4,7,8,9-Heptachloro-	55673-89-7	C ₁₂ HOCl ₇	7	409.308	221-223	507.2	0.0117	323.0
Octachlorodibenzofuran	39001-02-0	C ₁₂ OCl ₈	8	443.753	258	537	0.00518	343.9

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

TABLE 9.2.2

Selected physical-chemical properties of some chlorinated furans at 25°C

Compound	Selected properties					log K _{OW}	Henry's law const. H/(Pa·m ³ /mol)
	Vapor pressure		Solubility				
	P ^S /Pa	P _L /Pa	S/(mg/m ³)	C ^S /(mmol/m ³)	C _L /(mmol/m ³)		calculated P/C
Dibenzofuran	0.400	1.606	4750	28.240	114.42	4.27	14.16
2,8-DCDF	0.00039	1.46×10 ⁻²	14.5	0.0612	2.246	5.44	6.377
3,6-DCDF	2.00×10 ⁻⁴	7.94×10 ⁻³					
2,3,8-T ₃ CDF	2.48×10 ⁻⁴	1.03×10 ⁻²					
2,4,6-T ₃ CDF	9.22×10 ⁻⁴	7.29×10 ⁻³					
2,4,8-T ₃ CDF	9.1×10 ⁻⁵	1.68×10 ⁻³					
1,3,7,8-T ₄ CDF	3.51×10 ⁻⁵					6.39	
2,3,7,8-T ₄ CDF	2.00×10 ⁻⁶	1.92×10 ⁻⁴	0.419	1.37×10 ⁻³	0.132	6.53	1.461
2,3,4,7,8-P ₅ CDF	3.50×10 ⁻⁷	1.68×10 ⁻⁵	0.236	6.93×10 ⁻⁴	0.0332	6.5	0.505
1,2,3,4,7,8-H ₆ CDF	3.20×10 ⁻⁸	2.99×10 ⁻⁶	0.00825	2.20×10 ⁻⁵	2.06×10 ⁻³	7.0	1.454
1,2,3,4,6,7,8-H ₇ CDF	4.70×10 ⁻⁹	5.59×10 ⁻⁷	0.00135	3.30×10 ⁻⁶	3.92×10 ⁻⁴	7.4	1.425
OCDF	5.0×10 ⁻¹⁰	9.65×10 ⁻⁸	0.00116	2.61×10 ⁻⁶	5.05×10 ⁻⁵	8.0	0.191

TABLE 9.2.3

Suggested half-life classes of polychlorinated dibenzofurans in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Dibenzofuran	3	4	6	7
2,8-Dichloro-	4	5	7	8
2,3,7,8-Tetrachloro-	4	5	8	9
2,3,4,7,8-Pentachloro-	5	5	8	9
1,2,3,4,6,7,8-Heptachloro-	5	6	8	9
Octachlorodibenzofuran	5	7	9	9

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

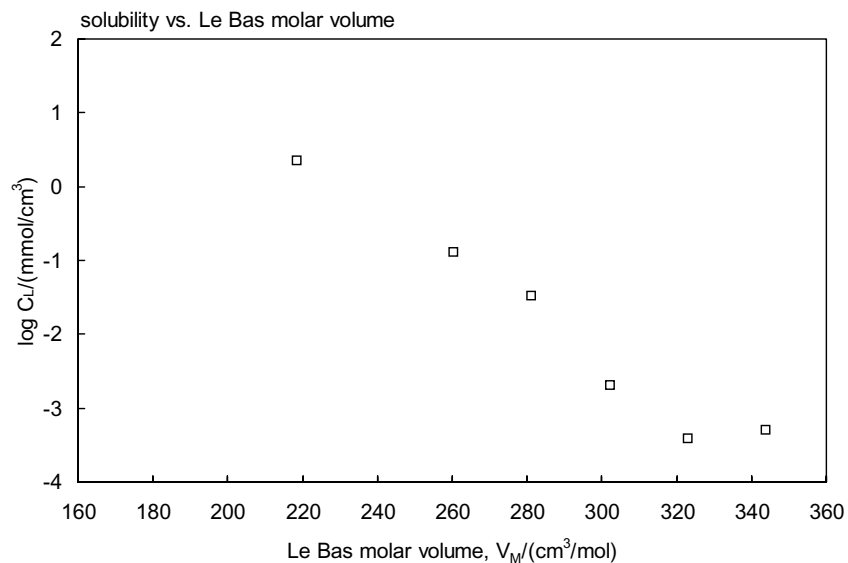


FIGURE 9.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzofurans.

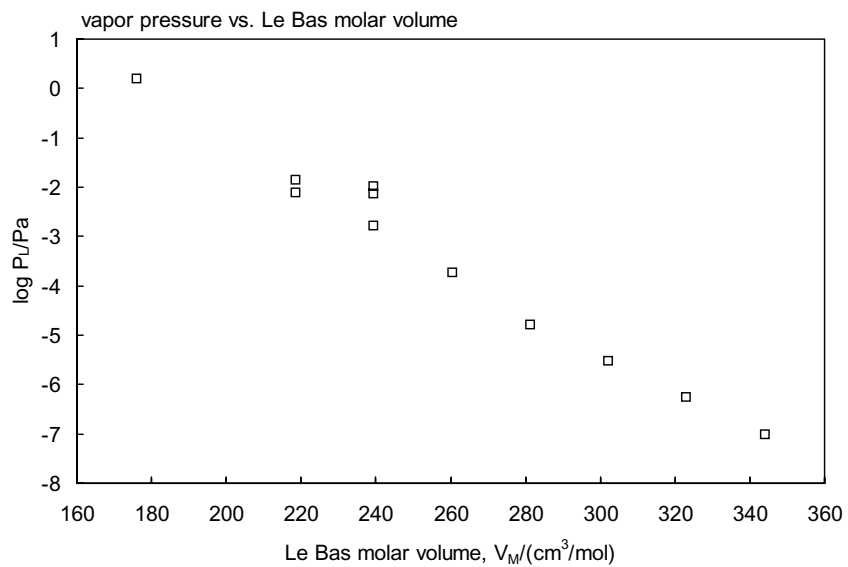


FIGURE 9.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polychlorinated dibenzofurans.

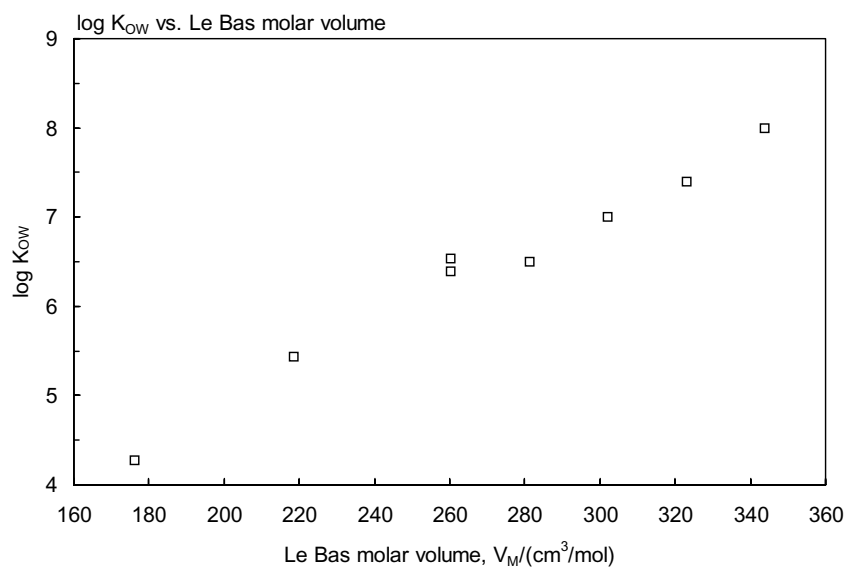


FIGURE 9.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polychlorinated dibenzofurans.

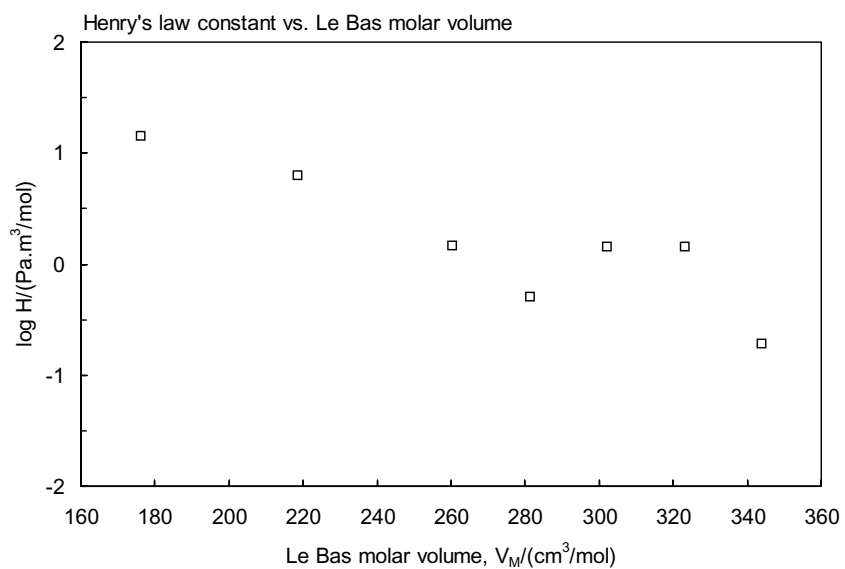


FIGURE 9.2.4 Henry's law constant versus Le Bas molar volume for polychlorinated dibenzofurans.

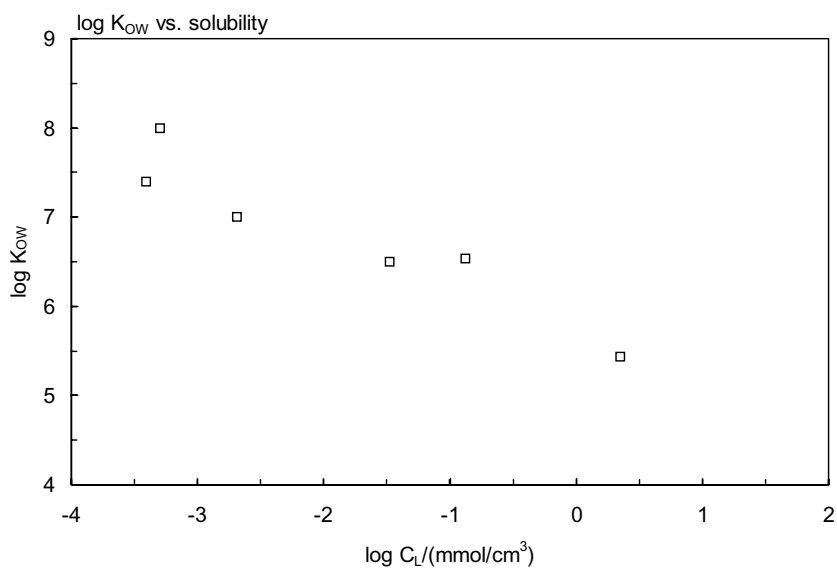


FIGURE 9.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polychlorinated dibenzofurans.

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10 Ethers

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10.1 LIST OF CHEMICALS AND DATA COMPILATIONS

10.1.1 ALIPHATIC ETHERS

10.1.1.1 Dimethyl ether (Methyl ether)



Common Name: Dimethyl ether

Synonym: methyl ether, oxapropane, oxybismethane

Chemical Name: dimethyl ether, methyl ether,

CAS Registry No: 115-10-6

Molecular Formula: C_2H_6O , CH_3OCH_3

Molecular Weight: 46.068

Melting Point ($^{\circ}C$):

–138.5 (Stull 1947; Stephenson & Malanowski 1987)

–141.5 (Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

–24.75 (Ambrose et al. 1976)

–23.60 (Stephenson & Malanowski 1987)

–24.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6689 (Riddick et al. 1986)

0.6612 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

68.87 ($20^{\circ}C$, calculated-density)

60.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.941 (Riddick et al. 1986; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

71000 (Seidell 1941; Lange 1971)

35.3% ($24^{\circ}C$, selected, Riddick et al. 1986)

65200 (literature data compilation, Yaws et al. 1990)

47480 (calculated- V_M , Wang et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

100847* ($-24.91^{\circ}C$, static method-manometer, measured range -78.22 to $-24.91^{\circ}C$, Kennedy et al. 1941)

678090* (calculated-Antoine eq. regression, temp range -115.7 to $-23.7^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 5409.8/(T/K)] + 7.585479$; temp range -115.7 to $125.2^{\circ}C$ (Antoine eq., Weast 1972–73)

593300 (Ambrose et al. 1976, Riddick et al. 1986)

$\log(P/kPa) = 6.0823 - 882.52/\{(T/K) + 31.90\}$ (Antoine eq., Ambrose et al. 1976)

$\log(P/mmHg) = 6.97603 - 889.3645/(241.96 + t/^{\circ}C)$; temp range -71 to $-25^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/kPa) = 5.44136 - 1025.56/(256.05 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

575530, 593340 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.44136 - 1025.56/(-17.1 + T/K)$; temp range 183–265 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.30358 - 982.46/(-20.894 + T/K)$, temp range not specified (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.36332 - 995.747/(-19.864 + T/K)$; temp range 180–249 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.09354 - 880.813/(-33.007 + T/\text{K})$; temp range 241–303 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.28318 - 987.484/(-16.813 + T/\text{K})$; temp range 293–360 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.48877 - 1971.127/(122.787 + T/\text{K})$; temp range 349–400 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

374000* (10°C, vapor-liquid equilibrium, measured range 203.15–395 K, Noles & Zollweg 1992)

$\log (P/\text{mmHg}) = 20.2699 - 1.5914 \times 10^3/(T/\text{K}) - 4.653 \cdot \log (T/\text{K}) - 1.3178 \times 10^{-10} \cdot (T/\text{K}) + 2.5623 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 132–400 K (vapor pressure eq., Yaws et al. 1994)

510000* (20.5°C, vapor-liquid equilibrium, measured range 0.51–120.12°C, Jónasson et al. 1995)

589100 (25.02°C, vapor-liquid equilibrium, measured range 283.12–313.22 K, Bobbo et al. 2000)

596210* (25.022°C, static-pressure sensor, measured range 233–399 K, data fitted to Wagner type eq., Wu et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

101.0 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

49.5, 105.7 (calculated-group contribution, calculated-bond contribution method, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.10 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1987)

0.10 (recommended, Sangster 1989)

0.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

1.37 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O(3P)} = 5.7 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(3P)$ at room temp. (Gaffney & Levine 1979)

$k_{OH}^* = 3.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.9 K, measured range 298–505 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH}(\text{calc}) = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{NO_3} \leq 3.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (flash photolysis-visible absorption, Wallington et al. 1986; quoted, Sabljic & Güsten 1990; Atkinson 1991)

$k_{OH}^* = 2.95 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–442 K (Tully & Droege 1987)

$k_{NO_3} = 2.92 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Sabljic & Güsten 1990)

$k_{OH}(\text{exptl}) = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (24.9 \pm 2.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988b)

$k_{OH} = 2.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{OH}^* = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (2.35 \pm 0.24) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (3.19 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}^* = 2.95 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–650 K (laser photolysis-laser induced fluorescence technique, Arif et al. 1997)

$k_{\text{OH}}^* = 2.86 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 263–351 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); calculated lifetimes of 4.1 d and 180 d for reactions with OH radical, NO_3 radical, respectively (Atkinson .2000)

TABLE 10.1.1.1.1

Reported vapor pressures of dimethyl ether at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\log P = A - B/(T/K) + C \cdot \log (T/K) - D \cdot (T/K)$	(5)						
1.							
Kennedy et al. 1941	Stull 1947	Jónasson et al. 1995	Wu et al. 2004				
static method-manometer	summary of literature data	static-pressure gauge	quartz pressure sensors				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
−78.22	4684	−115.7	133.3	0.51	270000	233.128	54610
−70.66	8121	−101.1	666.6	3.07	300000	238.126	68490
−65.25	11706	−93.3	1333	4.97	330000	243.157	85570
−60.03	16315	−85.2	2666	15.01	430000	248.152	105590
−55.14	21910	−76.2	5333	20.50	510000	253.152	129.42
−49.90	29585	−70.4	7999	27.11	630000	258.160	157530
−45.10	38334	−62.7	13332	33.39	750000	263.160	190440
−40.02	49810	−50.0	26664	44.39	990000	268.161	228480
−35.10	63401	−37.8	53329	50.25	1160000	273.153	272170
−27.67	89362	−23.7	101325	63.94	1590000	278.145	321870
−24.91	100847			76.67	2080000	283.160	378660
		mp/°C	−138.5	89.25	2680000	288.174	444570
mp/°C	−141.5			103.77	3500000	293.161	515530
bp/°C	−24.82			120.12	4720000	298.172	596210
		Noles & Zollweg 1992				303.160	687370
		vapor-liquid equilibrium				305.160	726260
eq. 5	P/mmHg	t/°C	P/Pa			308.158	787070
A	23.686185	10	37400			313.156	897590
B	1691.8056	50	114900			316.154	968550
C	−6.04560	90	273800			318.158	1018910
D	0.00195754	99.95	328400			323.149	1152350
temp range 195–284.34 K		109.85	357000			328.149	1298230
		121.85	488200			333.157	1457500
						more to	
						400.378	5355800
						data fitted to Wagner eq.	

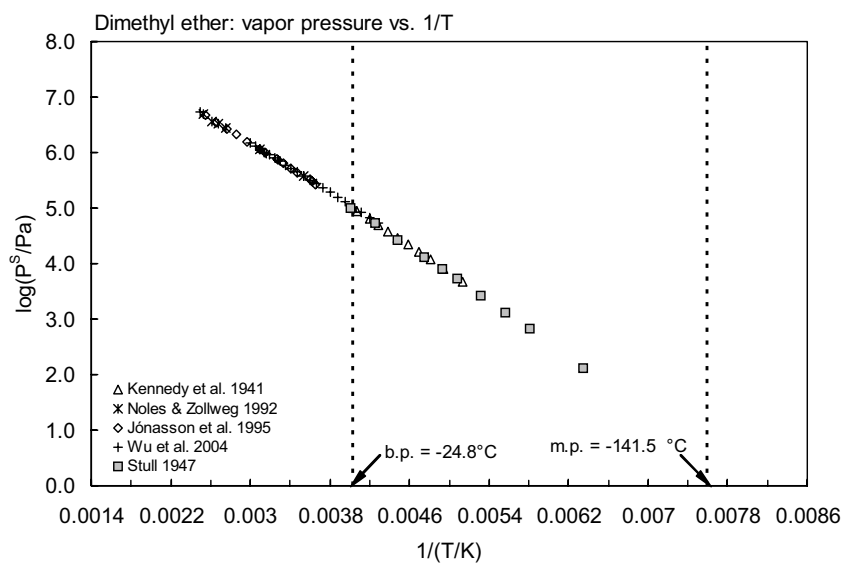
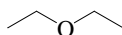


FIGURE 10.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl ether.

10.1.1.2 Diethyl ether (Ethyl ether)



Common Name: Diethyl ether

Synonym: ether, ethyl ether, ethoxyethane, ethyl oxide, 3-oxapentane, 1,1'-oxybisethane, sulfuric ether

Chemical Name: ether, diethyl ether, ethoxyethane, ethyl oxide, 3-oxapentane, 1,1'-oxybisethane

CAS Registry No: 60-29-7

Molecular Formula: $C_4H_{10}O$, $CH_3CH_2OCH_2CH_3$

Molecular Weight: 74.121

Melting Point ($^{\circ}C$):

-116.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

34.5 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7136. 0.7078 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

103.9 ($20^{\circ}C$, calculated-density)

106.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.439 (quoted, Riddick et al. 1986)

7.19 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

60270* (thermostatic volumetric method, measured range -3.83 to $30^{\circ}C$, Hill 1923)

60400* (volumetric method, measured range 10 – $30^{\circ}C$, Kablukov & Malischeva 1925)

60300* (volumetric method, measured range 10 – $25^{\circ}C$, Bennett & Phillip 1928)

69000 (Seidell 1941; Lange 1971)

60400 (selected, Riddick et al. 1986)

60900 (literature data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

58335* ($19.871^{\circ}C$, manometer, measured range -60.799 – $19.871^{\circ}C$, Taylor & Smith)

74690* (calculated-Antoine eq. regression, temp range -74 to $35.6^{\circ}C$, Stull 1947)

323835* ($71.11^{\circ}C$, static method-Bourdon, measured range 71.11 – $187.78^{\circ}C$, Kobe et al. 1956)

$\log (P/mmHg) = [-0.2185 \times 6946.2/(T/K)] + 7.56659$; temp range -74.3 to $183.3^{\circ}C$ (Antoine eq., Weast 1972–73)

58920 ($20^{\circ}C$, Verschueren 1983)

63340* ($21.82^{\circ}C$, ebulliometry, measured range 250 – $467 K$, Ambrose et al. 1972; quoted, Boublik et al. 1984)

$\log (P/kPa) = 6.05115 - 1062.409/[(T/K) - 44.967]$; temp range 250 – $329 K$ (ebulliometry, Antoine eq., Ambrose et al. 1972)

71620 (Ambrose et al. 1976)

71240, 71610 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.04972 - 1066.052/(220.003 + t/^{\circ}C)$; temp range -70.0 to $19.87^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 6.0492 - 1061.391/(228.06 + t/^{\circ}C)$; temp range -23.1 to $55.434^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose et al. 1972, Boublik et al. 1984)

$\log (P/mmHg) = 6.92032 - 1064.07/(228.8 + t/^{\circ}C)$; temp range -61 to $20^{\circ}C$ (Antoine eq., Dean 1985, 1992)

71620 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.05115 - 1062.409/(228.183 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
71620, 71604 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.02962 - 1051.432/(-44.967 + T/\text{K})$; temp range 286–329 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.05115 - 1062.409/(-44.967 + T/\text{K})$; temp range 250–329 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.30714 - 1236.75/(-20.11 + T/\text{K})$; temp range 307–457 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.05933 - 1067.576/(-44.217 + T/\text{K})$; temp range 305–360 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.37811 - 1276.822/(-14.869 + T/\text{K})$; temp range 417–467 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 41.7519 - 2.741 \times 10^3/(T/\text{K}) - 12.27 \cdot \log (T/\text{K}) - 3.1948 \times 10^{-10} \cdot (T/\text{K}) + 5.9802 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 157–467 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence):

130 (calculated- $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

90.0 (calculated-group contribution method, Hine & Mookerjee 1975)

237 (calculated-bond contribution method, Hine & Mookerjee 1975)

87.9 (calculated-P/C using Riddick et al. 1986 data)

86.8 (23°C , batch air stripping-IR, Nielsen et al. 1994)

95.05 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 5.953 - 2158/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.83 (20°C , shake flask-CR, Collander 1951)

1.03 (Hansch et al. 1968)

0.89 (shake flask-GC, both phases, Hansch et al. 1975)

0.77 (shake flask, Log P Database, Hansch & Leo 1987)

0.89 (recommended, Sangster 1989)

0.89 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C :

2.19 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}(\text{calc}) = 1.43 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.34 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^* = 13.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–442 K (Tully & Droege 1987)

$k_{\text{OH}}(\text{exptl}) = 1.34 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 1.06 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^* = (13.6 \pm 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988b)

$k_{\text{OH}} = 1.36 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{\text{OH}} = 1.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (relative rate method, Bennett & Keer 1989)

$k_{\text{OH}}^* = 1.33 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}} = (11.3 \pm 0.10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{\text{OH}} = (12.8 \pm 0.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from the air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetimes of 11 h and 17 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

TABLE 10.1.1.2.1
Reported aqueous solubilities of diethyl ether at various temperatures

Hill 1923		Kablukov & Malischeva 1925		Bennett & Phillip 1928	
volumetric method		volumetric method		volumetric method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
-3.83	127520	10	90100	10	91000
0	116680	15	78700	15	79500
10	90400	20	68800	20	68700
15	79130	25	60400	25	60300
20	68960	30	53400		
25	60270				
30	53400				

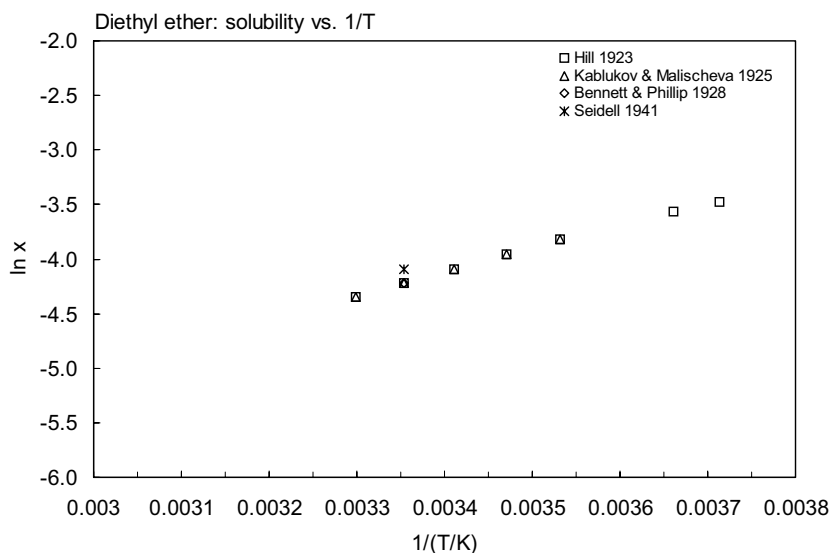


FIGURE 10.1.1.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for diethyl ether.

TABLE 10.1.1.2.2

Reported vapor pressures of diethyl ether at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Taylor & Smith 1922		Stull 1947		Kobe et al. 1956		Ambrose et al. 1972	
manometer		summary of literature data		static method-Bourdon gauge		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-60.799	527	-20.4	133.3	71.11	323835	-23.104	7430
-55.748	791	-3.0	666.6	76.67	372065	-19.889	8933
-50.873	1169	5.5	1333	82.22	427186	-16.744	10619
-45.998	1683	14.3	2666	87.78	496087	-13.492	12664
-41.125	2370	24.5	5333	93.33	564988	-10.135	15090
-36.231	3302	31.0	7999	98.89	647669	-6.929	17753
-31.329	4537	39.8	13332	104.44	730351	-2.762	21778
-26.421	6107	52.7	26664	110.00	826812	0.828	25813
-21.502	8174	68.0	53329	115.56	923273	4.912	31134
-16.578	10755	82.9	101325	121.11	1040405	8.914	37179
-11.637	13971	mp/°C	25.3	126.67	1157537	13.137	44534
-6.698	17966			132.22	1288449	17.785	53941
0.009	24815			137.78	1426251	21.821	63.343
4.975	31161			143.33	1584723	26.115	74719
9.937	38746			148.89	1743195	30.764	88.801
14.093	47749			154.44	1929288	34.321	100931
19.871	58335			160.00	2122151	35.064	103618
				165.56	2287513	39.222	119720
				171.11	2542447	42.978	135889
				176.67	2797381	47.470	157395
				182.22	3059204	51.765	180321
				187.78	3341699	55.434	201878
						eq. 3	P/kPa
						A	6.05115
						B	1062.409
						C	-44.967

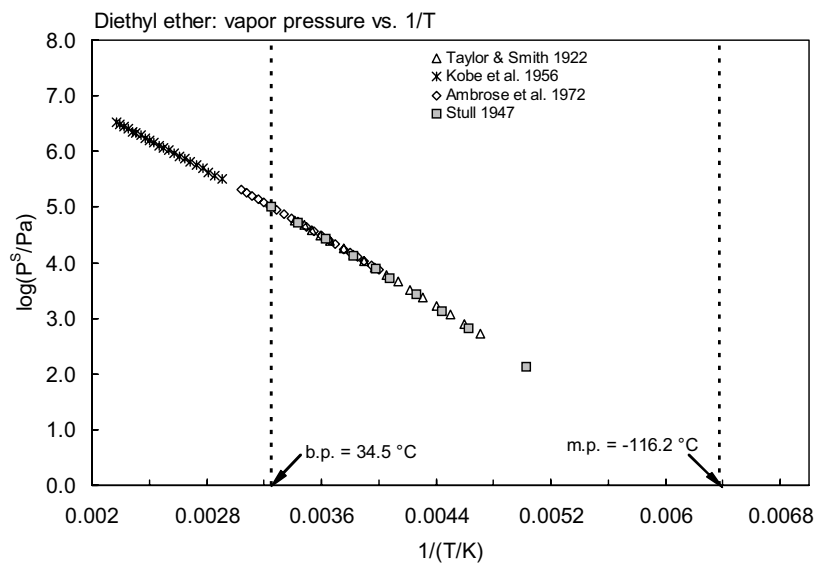


FIGURE 10.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for diethyl ether.

10.1.1.3 Methyl *t*-butyl ether (MTBE)

Common Name: Methyl *t*-butyl ether

Synonym: MTBE, 3-oxa-3,3-dimethylbutane, 2-methoxy-2-methyl-propane

Chemical Name: methyl *tert*-butyl ether

CAS Registry No: 1634-04-4

Molecular Formula: C₅H₁₂O, CH₃-O-C(CH₃)₃

Molecular Weight: 88.148

Melting Point (°C):

−108.6 (Lide 2003)

Boiling Point (°C):

55.0 (Lide 2003)

Density (g/cm³ at 20°C):

0.7578 (Bennett & Phillip 1928)

0.7404 (Windholz 1983; Budavari 1989)

Molar Volume (cm³/mol):

119.1 (20°C, calculated-density)

127.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

7.60 (exptl., Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

51600* (thermostatic volumetric method, measured range 0–25°C, Bennett & Phillip 1928)

48000 (Windholz 1983; Budavari 1989)

52100 (literature data compilation, Yaws et al. 1990)

42000* (19.8°C, shake flask-GC/TC, measured range 0–48.6°C, Stephenson 1992)

62100, 35500 (5, 20°C, shake flask-GC, Fischer et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

31156* (23.243°C, comparative ebulliometry, measured range 288–351 K, Ambrose et al. 1976)

log (P/kPa) = 6.09379 – 1173.036/{(T/K) + 41.366}; temp range 288–351 K (Antoine equation, comparative ebulliometry, Ambrose et al. 1976)

32660 (Windholz 1983; Budavari 1989)

33545 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P₁/kPa) = 6.09111 – 1171.54/(−41.542 + T/K); temp range 287–351 K (Antoine eq., Stephenson & Malanowski 1987)

37417* (27.806°C, static method, measured range 301–411 K, Krähenbühl & Gmehling 1994)

log (P/kPa) = 6.070343 – 1158.923/(T/K) – 43.20; temp range 301–411 K (Antoine eq., static method, Krähenbühl & Gmehling 1994)

log (P/mmHg) = 4.7409 – 1.9493 × 10³/(T/K) + 3.077 · log (T/K) – 1.4463 × 10^{−2} · (T/K) + 1.0039 × 10^{−5} · (T/K)²; temp range 165–497 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section):

59.46 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

142.6, 305 (calculated-group contribution, calculated-bond contribution method, Hine & Mookerjee 1975)

53.54*, 121 (25, 30°C, static headspace-GC, Robbins et al. 1993)

63.2 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

137.6* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)

$\ln K_{AW} = 6.6475 - 2901.4/(T/K)$; temp range 15–40°C (SPME-GC, Bierwagen & Keller 2001)

41.2 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 9.070 - 3178/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

72.4* (equilibrium concentration ratio-GC, measured range 3–25°C, Fischer et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.06 (Hansch et al. 1968; Kier & Hall 1976)

1.30 (calculated-fragment const., Hansch & Leo 1979)

0.94 (shake flask-GC, Funasaki et al. 1985)

0.94 (recommended, Sangster 1989)

0.94 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}(\text{calc}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{exptl}) = 2.64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (3.09 \pm 0.15) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 3.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 2.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 2.83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = (2.44 - 3.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295–298 K (Atkinson 1989)

$k_{OH}^* = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 293 K, measured range 293–750 K (laser photolysis-laser induced fluorescence technique, Arif et al. 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetimes of 3.9 d and 72 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

TABLE 10.1.1.3.1**Reported aqueous solubilities of methyl *tert*-butyl ether (MTBE) at various temperatures**

Bennett & Phillip 1928		Stephenson 1992		Fischer et al. 2004	
volumetric method		shake flask-GC/TC		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	91200	0	83000	5	62100
10	73000	9.7	51000	20	35500
15	65500	19.8	42000		
20	58300	29.6	31000		
25	51600	39.3	25000		
		48.6	19000		

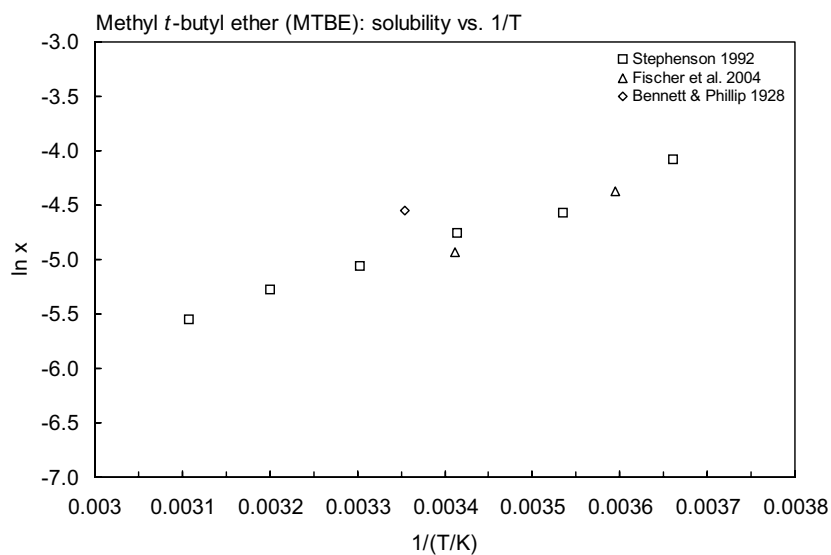
**FIGURE 10.1.1.3.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

TABLE 10.1.1.3.2

Reported vapor pressures of methyl *tert*-butyl ether (MTBE) at various temperatures

Ambrose et al. 1976				Krähenbühl & Gmehling 1994			
comparative ebulliometry				static method*			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
14.847	21805	73.873	180280	300.956	37417	342.570	158286
18.83	25843	77.828	201818	304.397	42944	342.592	158403
23.243	31156	25	33530	307.896	49188	342.652	158669
27.518	37194			312.707	58733		
32.143	44576	log P = A – B/(C + t/°C)		318.586	72841	*complete list see ref.	
37.16	53942		P/mmHg	323.663	86748		
41.525	63351	A	6.09379	323.666	86855		
44.835	71313	B	1173.036	328.498	102046		
51.182	88805	C	–41.366	328.528	102133		
55.028	100933	bp	328.30 K	333.387	119445		
55.826	103610			333.386	119444		
60.318	119700	coefficients of		338.224	138873		
64.376	135835	also given in text		338.229	138893		
69.193	157164			338.232	138905		

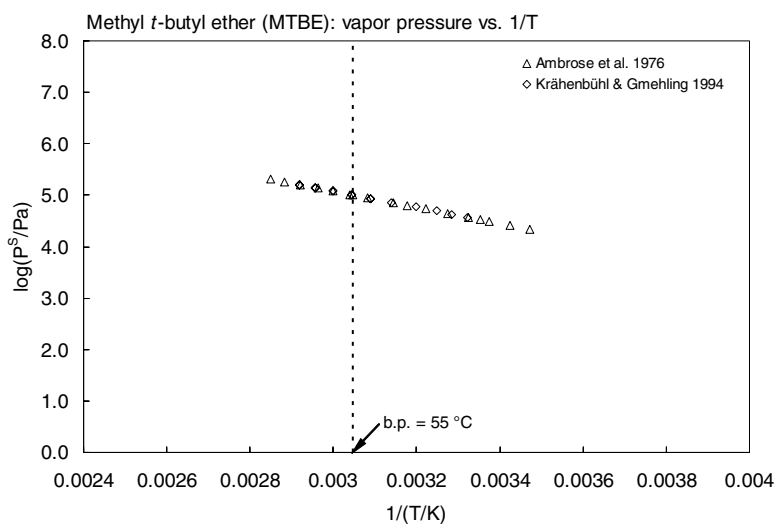
FIGURE 10.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

TABLE 10.1.1.3.3
Reported Henry's law constants of methyl *tert*-butyl ether (MTBE) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Robbins 1993		Bierwagen & Keller 2001		Fischer et al. 2004	
static headspace-GC		SPME-GC		equilibrium concn ratio-GC	
<i>t</i> /°C	H/(Pa m ³ /mol)	<i>t</i> /°C	H/(Pa m ³ /mol)	<i>t</i> /°C	H/(Pa m ³ /mol)
25	53.5	15	93.2	3	20.9
30	120.6	25	137.6	5	25.9
40	223.9	30	179.2	10	27.5
45	367.8	40	222.0	15	42.4
50	413.4			20	54.6
				25	72.4
eq. 1	H/(atm m ³ /mol)	eq. 1a	K _{AW}		
A	18.4	A	6.6475		
B	7666	B	3178		

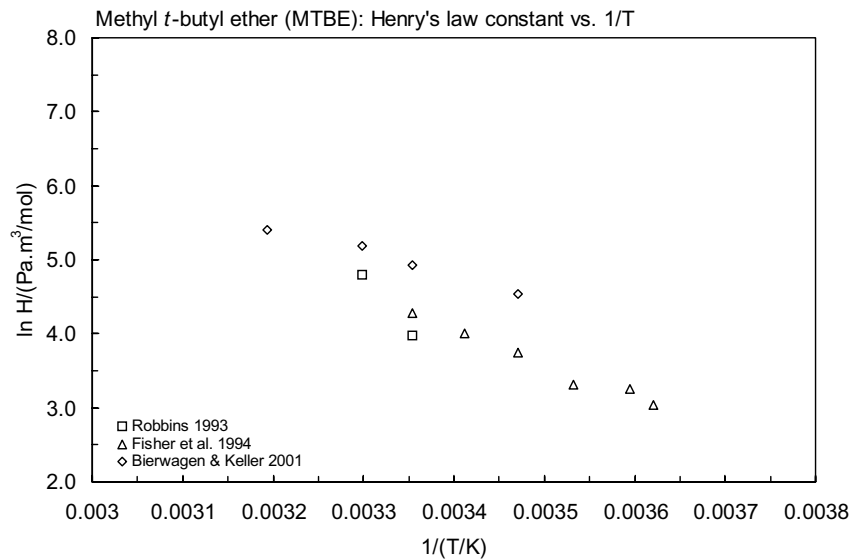
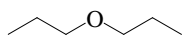


FIGURE 10.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

10.1.1.4 Di-*n*-propyl ether

Common Name: Di-*n*-propyl ether

Synonym: 4-oxaheptane, 1,1'-oxibispropane, 1-propoxypropane, propyl ether

Chemical Name: di-*n*-propyl ether, propyl ether, 4-oxaheptane

CAS Registry No: 111-43-3

Molecular Formula: C₆H₁₄O, (*n*-C₃H₇)₂O

Molecular Weight: 102.174

Melting Point (°C):

−114.8 (Lide 2003)

Boiling Point (°C):

90.08 (Riddick et al. 1986; Lide 2003)

Density (g/cm³ at 20°C):

0.7466, 0.7419 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

136.9 (20°C, calculated-density)

151.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.78 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

4900* (thermostatic volumetric method, measured range 0–25°C, Bennett & Phillip 1928)

2500* (synthetic method, measured range 0–25°C, Bennett & Phillip 1928)

3000 (Seidell 1941; Lange 1971)

2508 (selected, Hine & Mookerjee 1975)

4900 (selected, Riddick et al. 1986)

3820 (literature data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9072* (calculated-Antoine eq. regression, temp range −43.3 to 89.5°C, Stull 1947)

16358* (39.703°C, comparative ebulliometry, measured range 39.703–98.183°C, Meyer & Hotz 1973)

log (P/mmHg) = [−0.2185 × 8229.6/(T/K)] + 7.863332; temp range −43.3 to 89.5°C (Antoine eq., Weast 1972–73)

9041* (26.59°C, ebulliometry, measured range 26.59–88.65°C, Cidlinski & Polak 1969; quoted, Boublik et al. 1984)

log (P/cmHg) = 5.894812 − 1227.468/(215.7007 + t/°C); temp range 39.7–98.2°C (comparative ebulliometry, Meyer & Hotz 1973)

7621* (23.174°C, ebulliometry, measured range 292.974–387.883 K, Ambrose et al. 1976)

log (P/kPa) = 6.03075 − 1233.148/[(T/K) + 56.708]; temp range 293–388 K (Antoine eq., ebulliometry, Ambrose et al. 1976)

8378, 8320 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.06887 − 1254.429/(218.781 + t/°C); temp range 26.59–88.65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.01902 − 1227.068/(215.654 + t/°C); temp range 39.7–86.18°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 6.9476 − 1256.5/(219.0 + t/°C); temp range 26–89°C (Antoine eq., Dean 1985, 1992)

8334 (selected, Riddick et al. 1986)

log (P/kPa) = 6.03075 − 1133.748/(216.442 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

8334 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.019715 - 1227.468/(-57.449 + T/\text{K})$; temp range 312–371 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.0361 - 1236.828/(-56.358 + T/\text{K})$; temp range 292–389 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.50879 - 1579.466/(-12.142 + T/\text{K})$; temp range 385–467 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 8.20381 - 3494.323/(209.259 + T/\text{K})$; temp range 465–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 44.0232 - 3.282 \times 10^3/(T/\text{K}) - 12.792 \cdot \log (T/\text{K}) + 1.2682 \times 10^{-10} \cdot (T/\text{K}) + 4.8776 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 150–531 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

350.1 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

175.5, 594.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

223.3 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.03 (shake flask, Hansch et al. 1968; Leo et al. 1971)

2.03 (recommended, Sangster 1989)

2.03 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C:

2.97 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (relative rate, Lloyd et al. 1976)

$k_{OH}(\text{calc}) = 2.05 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{calc}) = 1.57 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (18.0 \pm 2.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 ± 2 K (relative rate method, Bennett & Kerr 1989)

$k_{OH}^* = 1.72 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = (19.9 \pm 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (20.3 \pm 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air) for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.1.4.1

Reported aqueous solubilities of di-*n*-propyl ether at various temperatures

Bennett & Phillip 1928			
volumetric method		synthetic method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	10500	0	5800
10	7100	10	4100
15	6100	15	3800
20	5400	20	3000
25	4900	25	2500

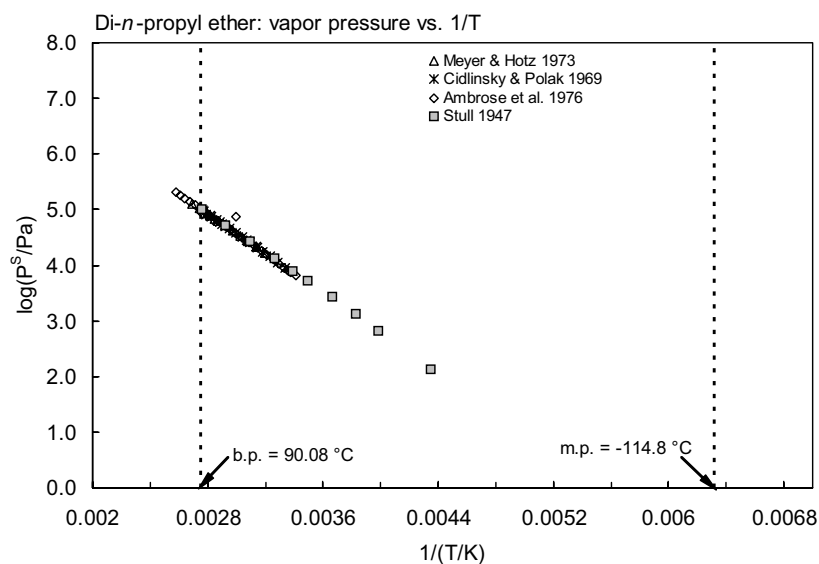
FIGURE 10.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-propyl ether.

TABLE 10.1.1.4.2

Reported vapor pressures of di-*n*-propyl ether at various temperatures and the coefficients for the vapor pressure equations

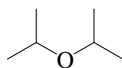
log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		
log P = A = [1 – T _B /T]	(5)	where log A = (a + bT + CT ²)	

Stull 1947		Meyer & Hotz 1973		Cidlinsky & Polak 1969		Ambrose et al. 1976	
summary of literature data		comparative ebulliometry		Boublik et al. 1984		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–43.3	133.3	39.703	16358	26.59	9041	19.824	6442
–22.3	666.6	45.857	21223	31.42	11344	23.174	7621
–11.8	1333	51.773	26.953	36.48	14271	26.887	9130
0	2666	57.749	33962	40.83	17252	30.501	10829
13.2	5333	63.263	41649	45.08	20.662	34.27	12873
21.6	7999	69.298	51617	46	21463	38.124	15283
33	13332	75.199	63121	50.47	25724	41.833	17938

TABLE 10.1.1.4.2 (Continued)

Stull 1947		Meyer & Hotz 1973		Cidlinsky & Polak 1969		Ambrose et al. 1976	
summary of literature data		comparative ebulliometry		Boublik et al. 1984		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
50.3	26664	77.936	69101	52.94	28338	46.698	21992
69.5	53329	81.601	77811	55.89	31760	50.87	26026
89.5	101325	84.221	84548	60.7	38035	55.827	31341
		91.016	104174	65.98	46095	60.296	37380
mp/°C	−112	98.183	128564	68.76	50822	65.228	44739
				71.44	55747	70.661	54144
		bp/°C	340.096	73.77	60355	75.383	63545
				76.27	65592	60.404	74921
		constants for Antoine eq.		80.49	76152	85.849	89008
		eq. 2	P/cmHg	82.13	79460	90.007	101105
		A	5.894812	85.77	83202	95.743	119879
		B	1227.468	87.34	93648	100.145	136045
		C	215.707	88.65	97250	105.407	157559
		temp range: 39.7–58.2°C				110.436	180476
				eq. 2	P/kPa	114.733	202031
		constants for Cox eq.		A	6.06887	25	8334
		eq. 5	P/atm	B	1254.429		
		a	0.866715	C	216.781	eq. 2	P/kPa
		−b × 10 ³	0.812825	bp/°C	89.952	A	6.03075
		b × 10 ⁶	0.809693			B	1233.748
		T _B /K	364.2462			C	−56.708
						coefficients of Chebyshev eq. also given in text	

10.1.1.5 Di-isopropyl ether



Common Name: Di-isopropyl ether

Synonym: diisopropoxyde, isopropyl ether, 2-isopropoxypropane, 2,2'-oxybispropane, 3-oxa-2,4-dimethylpentane, IPE, DIPE

Chemical Name: diisopropyl ether, isopropyl ether, 2-isopropoxypropane, 2,2'-oxybispropane, 3-oxa-2,4-dimethylpentane

CAS Registry No: 108-20-3

Molecular Formula: $C_6H_{14}O$, $[(CH_3)_2CH]_2O$

Molecular Weight: 102.174

Melting Point ($^{\circ}C$):

−85.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

68.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7360 (Bennett & Phillip 1928)

0.7239, 0.7185 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

140.0 ($20^{\circ}C$, calculated-density)

151.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.033 (quoted, Riddick et al. 1986)

12.05 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2040 (selected, Hine & Mookerjee 1975)

9000 ($20^{\circ}C$, Verschueren 1983)

12000 ($20^{\circ}C$, selected, Riddick et al. 1986)

11200 (literature data compilation, Yaws et al. 1990)

7900*, 5400 ($20^{\circ}C$, $31^{\circ}C$, shake flask-GC/TC, measured range 0 – $61^{\circ}C$. Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

21410* (calculated-Antoine eq. regression, temp range -57 to $67.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.09712 - 1257.6/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

20093* (temp range 0 – $60^{\circ}C$, Nicolini & Laffitte 1949)

21532* ($26.8^{\circ}C$, ebulliometry, measured range 13.5 – $70.6^{\circ}C$, Flom et al. 1951)

20194* ($25.29^{\circ}C$, ebulliometry, measured range 23.5 – $67.21^{\circ}C$, Cidlinsky & Polak 1969; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 7777.3/(T/K)] + 7.904664$; temp range -57 to $67.5^{\circ}C$ (Antoine eq., Weast 1972–73)

17778* ($22.489^{\circ}C$, ebulliometry, measured 284.779 – $365.122\ K$, Ambrose et al. 1976)

$\log(P/kPa) = 5.97678 - 1143.073/\{(T/K) + 53.810\}$; temp range 284 – $365\ K$ (Antoine eq., ebulliometry, Ambrose et al. 1976)

19954, 20120 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.78384 - 1050.657/(209.511 + t/^{\circ}C)$; temp range 0 – $60^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 5.97081 - 1137.408/(218.516 + t/^{\circ}C)$; temp range 23.5 – $67.21^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.8495 - 1139.34/(218.7 + t/^{\circ}C)$; temp range 23 – $67^{\circ}C$ (Antoine eq., Dean 1985, 1992)

19880 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 5.97678 - 1143.073/(219.340 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
19950, 19890 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.966496 - 1135.034/(-54.92 + T/\text{K})$; temp range 296–342 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.97661 - 1142.985/(-53.82 + T/\text{K})$; temp range 284–365 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.26597 - 1334.298/(-28.271 + T/\text{K})$; temp range 360–440 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 7.13537 - 2140.415/(80.78 + T/\text{K})$; temp range 436–500 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

19862, 10850 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 35.9552 - 2.0276 \times 10^3/(T/\text{K}) - 2.8551 \cdot \log(T/\text{K}) + 2.7662 \times 10^{-4} \cdot (T/\text{K}) - 9.9111 \times 10^{-14} \cdot (T/\text{K})^2$;
temp range 188–500 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

1010 (calculated as $1/K_{\text{AW}}, C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

483.3, 594.6 (calculated-group contribution calculated-bond contribution, Hine & Mookerjee 1975)

175.6 (computer value, Yaws et al. 1991)

208.8 (23°C , batch air stripping-IR, Nielsen et al. 1994)

212.4 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

231 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.52 (shake flask-GC, Funasaki et al. 1985)

1.56 (calculated-fragment const., Hansch & Leo 1979)

1.52 (recommended, Sangster 1989)

1.52 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.66 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = (1.07 \pm 0.20) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy, $k_{\text{OH}} = (1.13 \pm 0.20) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ by relative rate technique (Nelson et al. 1990)

$k_{\text{OH}}^* = (1.08 \pm 0.09) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–400 K (absolute rate, flash photolysis-resonance fluorescence, Wallington et al. 1993)

$k_{\text{OH}} = (9.9 \pm 0.2) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $(1.07 \pm 0.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1})$ at 298 K (relative rate method, Wallington et al. 1993)

$k_{\text{OH}} = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K using both relative (at 295 K) and absolute techniques over 240–440 K (FT-IR spectroscopy, Wallington et al. 1993)

$k_{\text{OH}} = 2.2 \times 10^{-12} \exp[(445 \pm 1450)/(T/\text{K})]$; temp range 240–440 K (Arrhenius eq., FT-IR, Wallington et al. 1993)

$k_{\text{OH}}(\text{calc}) = 33.3 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{exptl}) = 10.2 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.5.1

Reported aqueous solubilities of di-isopropyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	22800
9.7	10200
20	7900
31	5400
40.8	4100
50.7	2800
61	2200

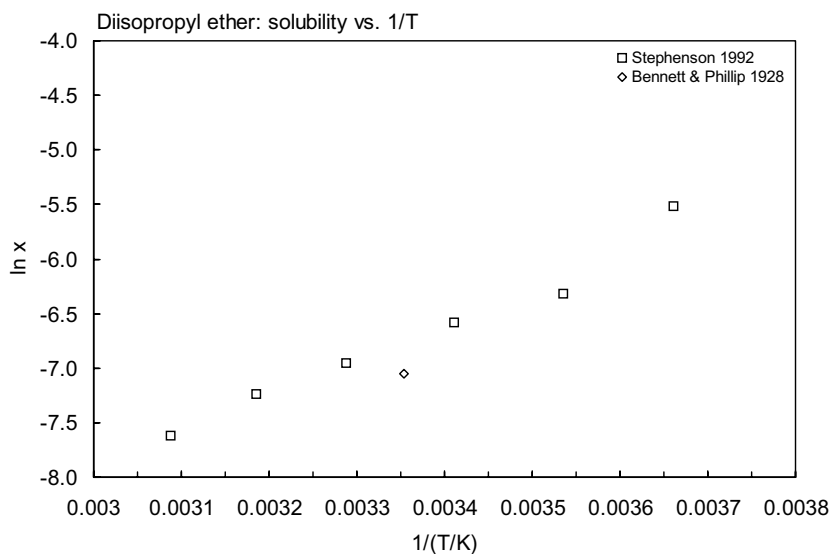


FIGURE 10.1.1.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for di-isopropyl ether.

TABLE 10.1.1.5.2

Reported vapor pressures of di-isopropyl ether at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log P = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Nicolini & Laffitte 1949		Cidlinsky & Polak 1969		Ambrose et al. 1976	
summary of literature data				in Boublik et al. 1984		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–57.0	133.3	0	5906	23.5	18654	11.629	10662
–37.4	666.6	5	7693	25.29	20194	15.253	12712
–27.4	1333	10	9932	27.42	22177	18.945	15122
–16.7	2666	15	12679	32	26963	22.489	17778
–4.50	5333	20	16092	34.22	29591	27.115	21812
3.4	7999	25	20093	36.93	32980	31.087	25839
13.7	13332	30	24891	41.17	39005	35.626	31160
30	26664	35	31651	44.08	43639	40.08	37199
48.2	53329	40	37530	46.7	48085	44.778	44561
67.5	101325	45	45329	48.57	51514	49.953	53861
mp/°C	–60.0	50	54382	50.96	56204	54.454	63367
		55	64821	54.52	63829	59.24	74743
		60	76727	56.12	67372	64.423	88818
				58.17	72427	68.397	100951
				60.68	78891	69.209	103576
Flom et al. 1951				63.21	89995	73.855	119720
dynamic-ebulliometry				64.66	89995	78.057	135878
t/°C	P/Pa			65.75	93316	83.078	157382
13.5	11466			67.21	97.734	87.857	180219
26.8	21532			bp/°C	68.339	91.972	201847
35.1	30491					25	19880
42.4	40423			eq. 2	P/kPa	Antoine	
47.9	50356						
53	60062			A	5.97081		
56.7	68541			B	1137.408		
59.8	76354			C	218.516	A	5.97678
63	85380					B	1143.073
66.3	95859					C	–53.810
69.5	104205					bp/K	341.66
70.6	109471					coefficients of Chebyshev also given in text.	

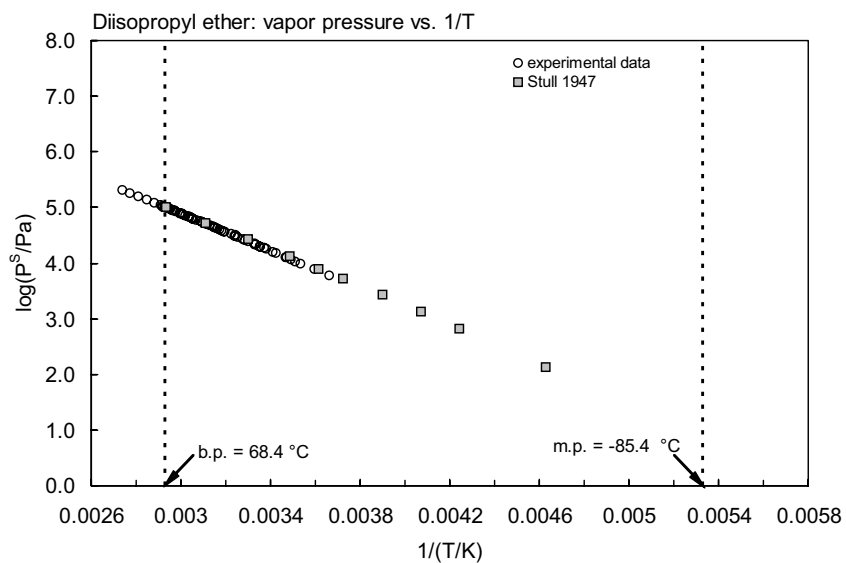
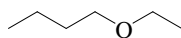


FIGURE 10.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for di-isopropyl ether.

10.1.1.6 Butyl ethyl ether



Common Name: Butyl ethyl ether

Synonym: butyl ethyl ether, 1-ethoxybutane, *n*-butylethyl ether, 3-oxaheptane

Chemical Name: butylethyl ether, 1-ethoxybutane, *n*-butylethyl ether

CAS Registry No: 628-81-9

Molecular Formula: $C_6H_{14}O$, $C_4H_9OCH_2CH_3$

Molecular Weight: 102.174

Melting Point ($^{\circ}C$):

-124 (Lide 2003)

Boiling Point ($^{\circ}C$):

92.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7495, 0.7448 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

136.3 ($20^{\circ}C$, calculated-density)

150.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6500* ($20^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.7^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

303164* ($126.67^{\circ}C$, static-Bourdon gauge, measured range 126.67 – $237.78^{\circ}C$, Kobe et al. 1956)

13912* ($38.18^{\circ}C$, ebulliometry, measured range 38.18 – $91.38^{\circ}C$, Cidlinsky & Polak 1969; quoted, Boublik et al. 1984)

$\log(P/kPa) = 6.06257 - 1252.485/(T/K + 56.685)$ (Antoine eq., Ambrose et al. 1976)

9090 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.06565 - 1234.258/(226.668 + t/^{\circ}C)$; temp range 38.18 – $91.38^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.9444 - 1256.4/(216.9 + t/^{\circ}C)$; temp range 38 – $92^{\circ}C$ (Antoine eq., Dean 1985, 1992)

7461 (quoted, Riddick et al. 1986)

$\log(P/kPa) = 6.06257 - 1252.485/(216.465 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

7510 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.062575 - 1252.485/(-56.685 + T/K)$; temp range 311 – $365 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 8.5224 - 2.4667 \times 10^3/(T/K) + 1.0513 \cdot \log(T/K) - 1.4047 \times 10^{-2} \cdot (T/K) + 9.2664 \times 10^{-6} \cdot (T/K)^2$; temp range 170 – $531 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

136 (calculated-P/C from selected data)

241 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.03 (shake flask-GC, Hansch & Anderson 1967)

2.03 (recommended, Sangster 1989)

2.03 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.89 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 2.28 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 1.34 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (relative rate, Bennett & Kerr 1989)

$k_{OH} = (13.4 - 22.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294–298 K (review, Atkinson 1989)

$k_{OH} = (18.7 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (pulse radiolysis-UV spectroscopy, Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.6.1
Reported aqueous solubilities of butyl ethyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	10900
9.3	8300
20	6500
31.2	5300
39.7	5800
50.8	4600
60.2	5100
70.2	3900
80.2	4300
90.7	4000

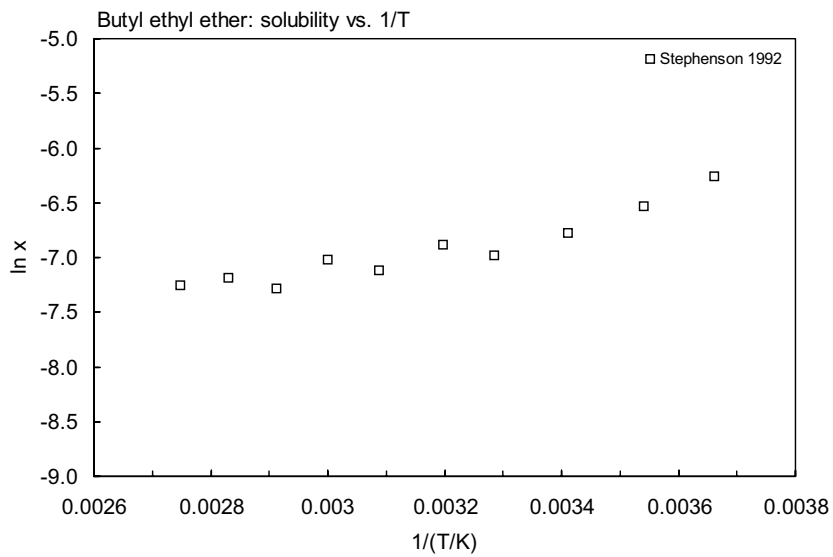


FIGURE 10.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for butyl ethyl ether.

TABLE 10.1.1.6.2
Reported vapor pressures of butyl ethyl ether at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Kobe et al. 1956				Cidlinsky & Polak 1969			
static-Bourdon gauge				in Boublik et al. 1984			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
126.67	303164	204.44	1329789	38.18	13912	79.64	67966
132.22	344505	210	1453811	42.31	16695	82.25	74080
137.78	385846	215.56	1591613	44	17950	85.08	81073
143.33	434076	221.11	1736305	49.04	22146	86.71	85441
148.89	489197	226.67	1894778	52.27	25259	89.73	92885
154.44	544318	232.22	2959149	55.1	28420	91.38	98581
160	613219	237.78	2232392	58.73	32451		
165.56	675230			61.25	35696	bp/°C	92.267
171.11	744131			63.22	38339	Antoine	
176.67	826812			65.85	42271	eq. 2	P/kPa
182.22	909493			68.51	46517	A	6.06565
187.78	1005955			71.66	51925	B	1254.258
193.33	1102416			73.74	55807	C	216.668
198.89	1212658			77.12	62513		

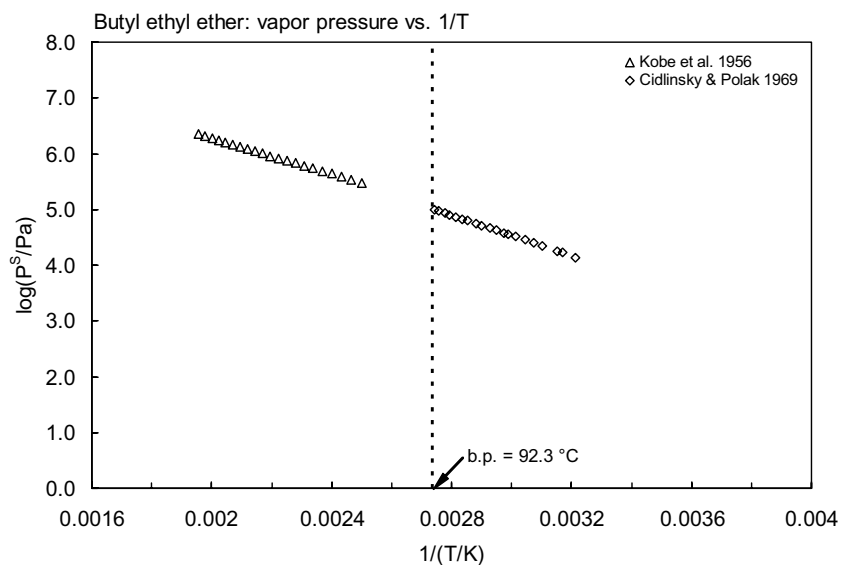
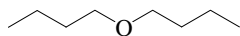


FIGURE 10.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for butyl ethyl ether.

10.1.1.7 Di-*n*-butyl ether

Common Name: Di-*n*-butyl ether

Synonym: 1-butoxybutane, butyl ether, dibutyl ether, *n*-butyl ether, 5-oxanonane, 1,1'-oxybisbutane

Chemical Name: butyl ether, dibutyl ether, di-*n*-butyl ether, *n*-butyl ether, 5-oxanonane, 1,1'-oxybisbutane

CAS Registry No: 142-96-1

Molecular Formula: C₈H₁₈O, (n-C₄H₉)₂O

Molecular Weight: 130.228

Melting Point (°C):

−95.2 (Riddick et al. 1986; Lide 2003)

Boiling Point (°C):

140.28 (Lide 2003)

Density (g/cm³ at 20°C):

0.76889, 0.76461 (20°C, 25°C, Dreisbach & Martin 1949)

0.7684, 0.7641 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

170.0 (calculated-density, Wang et al. 1992)

196.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

< 100 (17°C, synthetic method, Bennett & Phillip 1928)

300 (20°C, Verschueren 1983; Riddick et al. 1986)

230* (19.9°C, shake flask-GC/TC, measured range 0–90.6°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7605* (66.84°C, ebulliometry, measured range 67–142°C, Dreisbach & Shrader 1949)

log (P/mmHg) = 7.31540 – 1648.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

80612* (237.78°C, static method-Bourdon gauge, measured range 238–293°C, Kobe et al. 1956)

19529* (89.14°C, ebulliometry, measured range 89.14–140°C, Cidlinsky & Polak 1969)

log (P/kPa) = 5.93018 – 1302.768/(T/K – 81.481); temp range 89–140°C (Cidlinsky & Polak 1969)

log (P/kPa) = 5.93018 – 1302.768/{(T/K) – 81.481} (Antoine eq., ebulliometry, Ambrose et al. 1976)

640 (20°C, Verschueren 1983)

825, 874 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.151 – 1458.718/(141.982 + t/°C); temp range 66.8–141.97°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.92274 – 1298.256/(191.144 + t/°C); temp range 89.14–140.06°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 6.7963 – 1297.3/(191.03 + t/°C); temp range 89–140°C (Antoine eq., Dean 1985, 1992)

898 (select, Riddick et al. 1986)

log (P/kPa) = 5.930185 – 1302.768/(191.669 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P_L/kPa) = 6.4403 – 1648.4/(–42.15 + T/K); temp range 339–415 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.0537 – 1398.8/(–69.55 + T/K); temp range 336–415 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 12.9321 – 3.0416 × 10³/(T/K) + 0.42929 · log (T/K) – 1.237 × 10^{–2} · (T/K) + 7.5943 × 10^{–6} · (T/K)²; temp range 178–581 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

- 608.5 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
 350, 1362 (calculated-group contribution calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:

- 3.08 (calculated-f const., Hansch & Leo 1979)
 3.21 (shake flask-GC, Funasaki et al. 1984)
 3.21 (recommended, Sangster 1989)
 3.21 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

- 3.89 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:

k_{OH} = (27.8 ± 3.6) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

k_{OH} = 17 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 294 ± 2 K (relative rate method, Bennett & Kerr 1989)

k_{OH} = (17.0 – 27.8) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 294–298 K (review, Atkinson 1989)

k_{OH} = (27.2 ± 0.2) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ by pulse radiolysis-UV spectroscopy; k_{OH} = (28.8 ± 1.2) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance t_{1/2} < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.7.1
Reported aqueous solubilities of di-*n*-butyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	S/g·m ⁻³
0	400
9.3	320
19.9	230
30.9	230
40.3	200
50.3	220
61.3	120
70.5	150
80.7	90
90.5	100

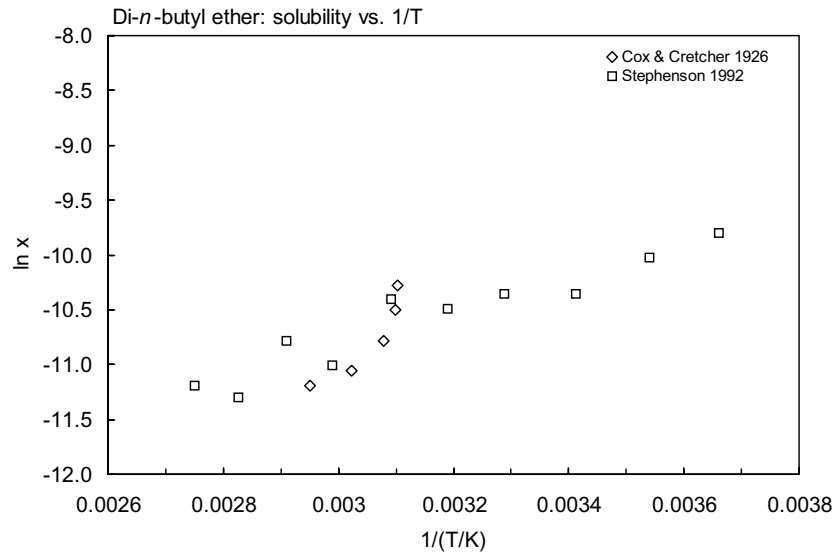
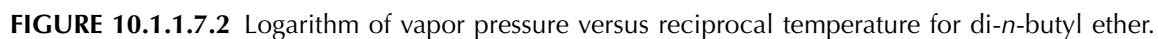


FIGURE 10.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for di-*n*-butyl ether.

TABLE 10.1.1.7.2
Reported vapor pressures of di-*n*-butyl ether at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)
log (P/mmHg) = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)
log (P/Pa) = A – B/(C + T/K)		(3)			
log (P/mmHg) = A – B/(T/K) – C·log (T/K)		(4)			
Dreisbach & Shrader 1949		Kobe et al. 1956		Cidlinsky & Polak 1969	
ebulliometry		static method-Bourdon gauge		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
66.84	7605	237.78	806142	89.14	19529
73.6	10114	243.33	895713	94.57	23957
85.75	16500	248.89	978394	106.43	36288
112.28	42066	254.44	1061075	110.54	41580
127.73	67661	260	1143757	113.28	45509
141.97	101325	265.56	1247108	114.85	47781
		271.11	1357350	118.2	53253
		276.67	1474481	121.05	58118
		282.22	1598503	123.18	62051
		287.78	1729415	123.41	62509
		293.33	1874107	125.27	66052
				127.67	70427



10.1.1.8 1,2-Propylene oxide

Common Name: 1,2-Propylene oxide

Synonym: 1,2-epoxypropane, methyloxirane, propylene oxide

Chemical Name: 1,2-propylene oxide, 1,2-epoxypropane, propylene oxide

CAS Registry No: 75-56-9

Molecular Formula: C₃H₆O

Molecular Weight: 58.079

Melting Point (°C):

–111.9 (Lide 2003)

Boiling Point (°C):

35 (Lide 2003)

Density (g/cm³ at 20°C):

0.859 (0°C, Verschueren 1983)

Molar Volume (cm³/mol):

69.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

6.57, 6.53 (exptl., Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

476000 (US EPA 1981; quoted, Howard 1989)

405000, 650000 (20°C, 30°C, Verschueren 1983)

259000 (literature data compilation, Yaws et al. 1990)

139320 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

74520* (calculated-Antoine eq. regression, temp range –75 to 34.5°C, Stull 1947)

530538* (87.78°C, static method, measured range 88–204°C, Kobe et al. 1956)

51969* (17.05°C, ebulliometry, measured range –24.17 to 34.75°C (McDonald et al. 1959)

$\log (P/\text{mmHg}) = 6.96997 - 1065.27/(226.283 + t/^{\circ}\text{C})$; temp range –24.17 to 34.75°C (ebulliometry, McDonald et al. 1959)

70112* (interpolated-Antoine eq., static method, measured range 19.0–71.8°C Bott & Sadler 1966)

$\log (P/\text{mmHg}) = 7.658 - 1472/(T/\text{K})$; temp range 19.0–71.8°C (Antoine eq., static method, Bott & Sadler 1966)

$\log (P/\text{mmHg}) = [-0.2185 \times 7295.8/(T/\text{K})] + 8.093473$; temp range –75 to 34.5°C (Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = 7.06492 - 1113.6/(232.0 + t/^{\circ}\text{C})$; temp range –35 to 130°C (Antoine eq., Dean 1985, 1992)

59300, 75900 (20, 25°C, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.09487 - 1065.27/(226.283 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

71700 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.09487 - 1065.27/(-46.867 + T/\text{K})$; temp range 225–308 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 38.5381 - 2.631 \times 10^3/(T/\text{K}) - 11.104 \cdot \log (T/\text{K}) + 4.2178 \times 10^{-10} \cdot (T/\text{K}) + 5.5025 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 161–482 K (vapor pressure eq., Yaws 1994)

$\log (P/\text{kPa}) = 6.14068 - 1086.37/[(T/\text{K}) - 44.556]$; temp range not specified (Antoine eq., Horstmann et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C):

8.653 (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

0.03 (shake flask, Hansch & Leo 1985, 1987)

0.03	(recommended, Sangster 1989)
0.03	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

−0.20, −0.40 (calculated, Howard 1989)

Sorption Partition Coefficient, log K_{OC} :

0.623	(estimated-S, Lyman et al. 1982; quoted, Howard 1989)
1.477	(calculated-QSAR, Sabljic 1984; quoted, Howard 1989)

Environmental Fate Rate Constants, k , and Half-Lives,:

Volatilization: $t_{1/2}(\text{calc}) \sim 3$ and 18 d from a representative or natural river and oligotrophic lake, respectively (USEPA 1986; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{exptl}) = 5.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas phase reactions;
 $k = 2.4 \times 10^8 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with photochemically produced OH radical in water at room temp. (Güesten et al. 1981; quoted, Howard 1989)

photooxidation $t_{1/2} = 19.3$ d can be calculated for the gas phase reaction with OH radical in air by using Güesten 1981 data and assuming an average OH radical concn. of 8×10^5 molecules/cm³ (GEMS 1986; quoted, Howard 1989)

$k_{OH} = (1.11 \pm 0.75) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to *n*-butane for the gas phase reaction with OH radical in air at $(23.1 \pm 1.1)^\circ\text{C}$ with an atmospheric lifetime of 10 d for an average concentration of 1×10^6 molecules/cm³ of OH radical (Edney et al. 1986)

$k_{OH}(\text{calc}) = 5.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH}(\text{exptl}) = 5.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{OH} = (4.95 \pm 0.52) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 4.95 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

Hydrolysis: estimated $t_{1/2} \sim 11.6$ d in fresh water at pH 7 to 9 and $t_{1/2} = 6.6$ d at pH 5 (Howard 1989).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

atmospheric lifetime of 10 d (Edney et al. 1986);

$t_{1/2} = 19.3$ d, based on estimated photooxidation half-life in air by using Güesten et al. 1981 data and assuming an average OH radical concn. of 8×10^5 molecules/cm³ (GEMS 1986; quoted, Howard 1989).

Surface water: calculated $t_{1/2} = 9.15$ yr in natural water by using Güesten et al. 1981 data and assuming an average OH radical concentration of 1×10^{-17} M in natural water (Howard 1989).

Ground water:

Sediment:

Soil:

Biota:

TABLE 10.1.1.8.1

Reported vapor pressures of 1,2-propylene oxide at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log (P/mmHg) = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log (P/Pa) = A – B/(C + T/K)		(3)					
log (P/mmHg) = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Kobe et al. 1956		McDonald et al. 1959		Bott & Sadler 1966	
summary of lit. data		static-Bourdon gauge		ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–75.0	133	87.78	530538	–24.7	6665	19	55462
–57.8	666.6	93.33	599439	–13.66	12170	27	76527
–49.0	1333	98.89	675230	0.77	25345	36.3	107457
–39.8	2666	104.44	771691	17.05	51969	40.8	126656
–28.4	5333	110	868153	33.11	97379	46.8	154253
–21.3	7999	115.56	978394	34.75	103298	50.2	168652
–12.0	13332	121.11	1102416			54	193583
2.1	26664	126.67	1226438			59.2	225847
17.8	53329	132.22	1378020	eq. 2	P/mmHg	64.7	265844
34.5	101325	137.78	1536492	A	6.96997	71.8	320373
		143.33	1701855	B	1065.27		
mp/°C	–112.1	148.89	1880997	C	233.386	eq. 1	P/mmHg
		154.44	2073920			A	7.658
		160	2273733	mp/°C	–112.13	B	1472
		165.56	2506996				
		171.11	2762930				
		176.67	3017864				
		182.22	3300358				
		187.78	3589742				
		193.33	3906687				
		198.89	4251192				
		204.44	4602587				

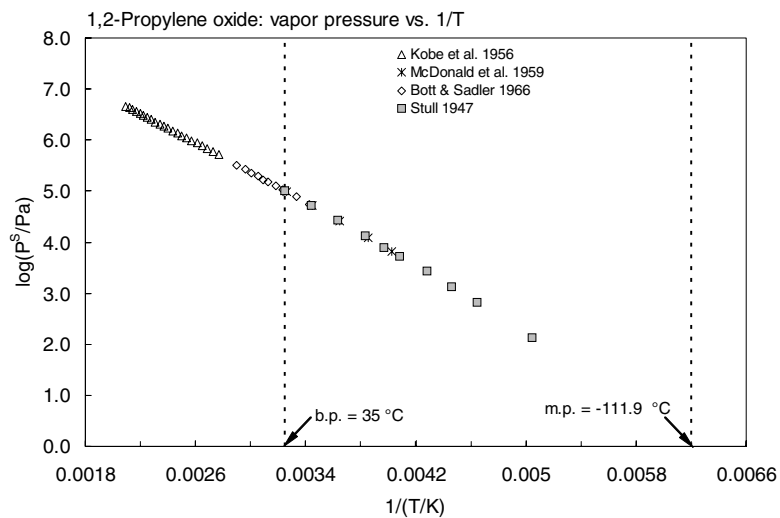


FIGURE 10.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2-propylene oxide.

10.1.1.9 Furan



Common Name: Furan

Synonym: 1,4-epoxy-1,3-butadiene, divinylene oxide, furfuran, oxole, tetrole

Chemical Name: 1,4-epoxy-1,3-butadiene, divinylene oxide, furan

CAS Registry No: 110-00-9

Molecular Formula: C_4H_4O

Molecular Weight: 68.074

Melting Point ($^{\circ}C$):

−85.61 (Lide 2003)

Boiling Point ($^{\circ}C$):

31.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9378 (Dreisbach 1955; Riddick et al. 1986)

0.9514 (Weast 1982–83)

Molar Volume (cm^3/mol):

72.6 ($20^{\circ}C$, calculated-density)

73.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

3.803 (Riddick et al. 1986)

2.05, 3.80 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

10070 (literature average, Valvani et al. 1981)

10000 (Verschueren 1983)

10000 (Riddick et al. 1986)

9900 (literature data compilation, Yaws et al. 1990)

26500 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

70109* ($21.614^{\circ}C$, comparative ebulliometry, measured range $2,552$ – $61.43^{\circ}C$, Guthrie et al. 1952)

$\log(P/mmHg) = 6.97523 - 1060.851/(t/^{\circ}C + 227.740)$; temp range 2.5 – $61.43^{\circ}C$ (Antoine eq., comparative ebulliometry, Guthrie et al. 1952)

79980 (calculated from determined data, Dreisbach 1955)

$\log(P/mmHg) = 6.97523 - 1060.851/(227.740 + t/^{\circ}C)$; temp range -35 to $90^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

627000* ($93.33^{\circ}C$, static-Bourdon gauge, measured range 93.33 – $210^{\circ}C$, Kobe et al. 1956)

$\log(P/mmHg) = [1 - 304.367/(T/K)] \times 10^4 \{0.858337 - 8.56435 \times 10^{-4} \cdot (T/K) + 9.32123 \times 10^{-7} \cdot (T/K)^2\}$; temp range 340.95 – $463.65\ K$ (Cox eq., Chao et al. 1983)

70110 ($21.61^{\circ}C$, quoted, Boublik et al. 1984)

79930 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.10017 - 1060.871/(227.742 + t/^{\circ}C)$; temp range: $2,552$ – $61.43^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.97527 - 1060.87/(227.74 + t/^{\circ}C)$; temp range: 2 – $61^{\circ}C$ (Antoine eq., Dean 1985, 1992)

84530 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.10013 - 1060.851/(227.74 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

79930 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.10013 - 1060.851/(-45.41 + T/K)$; temp range 238 – $363\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 24.9555 - 2.1624 \times 10^3/(T/K) - 6.1066 \cdot \log (T/K) - 2.4185 \times 10^{-10} \cdot (T/K) + 2.0858 \times 10^{-6} \cdot (T/K)^2;$$

temp range 188–490 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

575.5	(calculated-P/C using Riddick et al. 1986 data)
545.8	(computed-vapor liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.34	(Hansch & Leo 1979;)
1.13	(estimated-HPLC, Garst 1984)
1.14, 1.35	(estimated-MO, π substituent consts., Bodor et al. 1989)
1.34	(recommended, Sangster 1989)
1.34	(recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.50, 1.46; 1.48 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k = 1.4 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ oxidation rate by singlet oxygen in water (Mill 1980; quoted, Mill & Mabey 1985)

$k_{\text{OH}} = (4.01 \pm 0.30) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a atmospheric lifetime $\tau \sim 7 \text{ h}$, $k_{\text{O}_3} = (2.42 \pm 0.28) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$; and $k_{\text{O}(^3\text{P})} \sim 1.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom at 298 K (relative rate method, Atkinson et al. 1983)

$k_{\text{OH}} = (3.98 \pm 0.35) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $22 \pm 2^\circ\text{C}$ (relative rate method, Tuazon et al. 1984)

$k_{\text{OH}}^* = (40.8, 43.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K , measured range $254\text{--}424 \text{ K}$ (FP-RF flash photolysis-resonance fluorescence, Wine & Thompson 1984)

$k_{\text{O}_3} = 2.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.15 d^{-1} , $k_{\text{OH}} = 4.0 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 3.5 d^{-1} , and $k_{\text{NO}_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 29 d^{-1} at room temp. (review, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.15 d^{-1} , $k_{\text{OH}} = 4.0 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 1.7 d^{-1} , and $k_{\text{NO}_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 29 d^{-1} at room temp. (review, Atkinson 1985)

$k_{\text{NO}_3} = (1.4 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1985)

$k_{\text{O}_3} = 2.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 6.7 \text{ d}$, $k_{\text{OH}} = 4.0 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated $\tau = 6.9 \text{ h}$, and $k_{\text{NO}_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated $\tau = 50 \text{ min}$ at room temp. (Atkinson et al. 1985)

$k_{\text{OH}} = 4.07 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1987, 1988; quoted, Müller & Klein 1991)

$k_{\text{OH}} = 4.046 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , $k_{\text{NO}_3} = 1.439 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1986 and Atkinson et al. 1988, Sabljic & Güsten 1990; Atkinson 1991)

$k_{\text{NO}_3} = 1.44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (relative rate method, Atkinson et al. 1988, Atkinson 1991)

$k_{\text{OH}}^* = 4.05 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated atmospheric lifetimes: 6.7 d due to reaction with O_3 in 24-h, 6.9 h due to reaction with OH radical in daytime and 50 min with NO_3 radical at room temp. (Atkinson et al. 1985).

Surface water: $t_{1/2} = 1.0$ h, estimated from oxidation rate by singlet oxygen of $1.4 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ (Mill 1980; quoted, Mill & Mabey 1985).

Ground water:

Sediment:

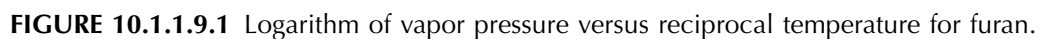
Soil:

Biota:

TABLE 10.1.1.9.1

Reported vapor pressures of furan at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Guthrie et al. 1952		Kobe et al. 1956					
comparative ebulliometry		static-Bourdon gauge					
t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa
2.552	31160	56.329	232087	93.33	627000	154.44	2156601
7.267	38547	61.43	270110	98.89	709680	160	2370194
12.018	47359			104.44	806142	165.56	1597568
16.797	57803	bp/ $^{\circ}C$	31.36	110	909493	171.11	2838721
21.614	70109	$\Delta H_v/(kJ\ mol^{-1}) = 27.09$		115.56	1019735	176.67	3107435
26.469	84525		at bp	121.11	1150647	182.22	3389929
31.357	101325			126.67	1295339	187.78	3686204
36.279	120790	eq. 2	P/mmHg	132.22	1440031	193.33	3996258
41.241	143268	A	6.97523	137.78	1605393	198.89	4326983
46.232	169052	B	1060.851	143.33	1770756	204.44	4671488
51.265	198530	C	227.74	149.89	1956788	210	5009103



10.1.1.10 2-Methylfuran



Common Name: 2-Methylfuran

Synonym: silvan, sylvan

Chemical Name: 2-methylfuran

CAS Registry No: 534-22-5

Molecular Formula: C₅H₆O

Molecular Weight: 82.101

Melting Point (°C):

−91.3 (Lide 2003)

Boiling Point (°C):

64.7 (Lide 2003)

Density (g/cm³ at 20°C):

0.913 (Verschuereen 1983)

Molar Volume (cm³/mol):

89.9 (20°C, calculated-density)

95.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

8.66 (exptl., Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

3000 (20°C, Verschuereen 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

358285* (110°C, static-Bourdon gauge, measured range 110–254.44°C, Kobe et al. 1956)

86126* (60.3°C, isotenoscope/manometry, measured range 60.3–100.3°C, Eon et al. 1971)

$\log (P/\text{mmHg}) = [1 - 338.704/(T/K)] \times 10^{\{0.871223 - 7.95690 \times 10^{-4} \cdot (T/K) + 7.81737 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 333.45–527.61 K (Cox eq., Chao et al. 1983)

18930, 29990 (20°C, 30°C, quoted, Verschuereen 1983)

23090 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.81244 - 1641.052/(276.164 + t/^\circ\text{C})$; temp range 60.3–100.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

23250 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.95585 - 1107.3/(-56.88 + T/K)$; temp range 251–338 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

518 (20°C, calculated-P/C using Verschuereen 1983 data)

Octanol/Water Partition Coefficient, log K_{ow}:

1.85 (shake flask, Log P Database, Hansch & Leo 1987)

1.85 (recommended, Sangster 1989)

1.85 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.1.10.1

Reported vapor pressures of 2-methylfuran at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$				(1)	$\ln P = A - B/(T/K)$			(1a)
$\log P = A - B/(C + t/^{\circ}C)$				(2)	$\ln P = A - B/(C + t/^{\circ}C)$			(2a)
$\log P = A - B/(C + T/K)$				(3)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$				(4)				
Kobe et al. 1956				Eon et al. 1971				
static-Bourdon gauge				isoteniscope/manometry				
$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	
110	358285	160	1088636	210	2521777	60.3	86126	
115.56	413406	165.56	1205768	215.56	2749150	70.3	119057	
121.11	468527	171.11	1329789	221.11	2990303	80.3	161720	
126.67	537428	176.67	1467591	226.67	3231457	90.3	215982	
132.22	606329	182.22	1612283	232.22	3493281	100.3	283977	
137.78	689010	187.78	1770756	237.78	3768885			
143.33	778581	193.33	1943008	243.33	4065159			
149.89	888823	198.89	2122151	248.89	4382104			$\Delta H_v/(kJ\ mol^{-1}) = 30.79$
154.44	978394	204.44	2321964	254.44	4719719			

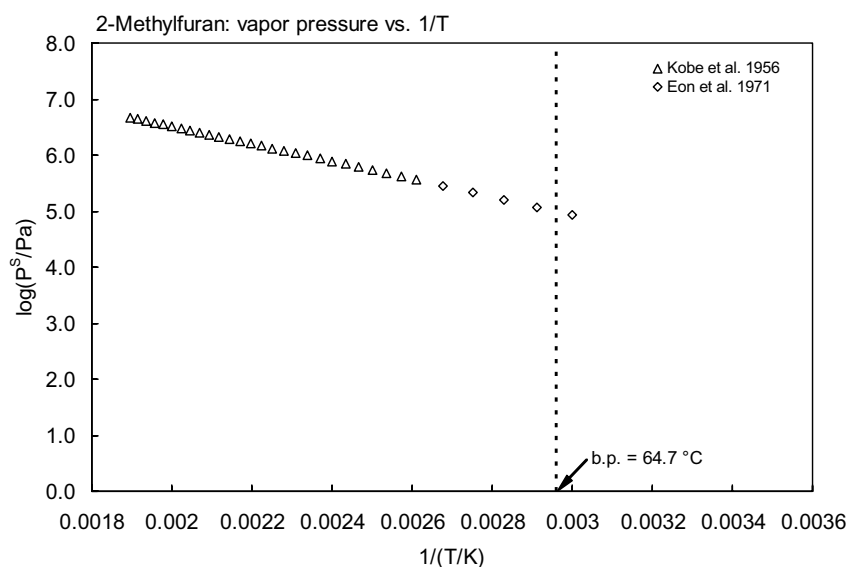


FIGURE 10.1.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for methylfuran.

10.1.1.11 Tetrahydrofuran



Common Name: Tetrahydrofuran

Synonym: 1,4-epoxybutane, diethylene oxide, oxacyclopentane, tetramethylene oxide

Chemical Name: 1,4-epoxybutane, diethylene oxide, oxacyclopentane, tetrahydrofuran, tetramethylene oxide

CAS Registry No: 109-99-9

Molecular Formula: C₄H₈O

Molecular Weight: 72.106

Melting Point (°C):

−108.44 (Lide 2003)

Boiling Point (°C):

65 (Lide 2003)

Density (g/cm³ at 20°C):

0.8880 (Verschuereen 1983)

0.8892 (Riddick et al. 1986)

Molar Volume (cm³/mol):

81.1 (20°C, calculated-density)

88.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.535 (quoted, Riddick et al. 1986)

8.54 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Verschuereen 1983; Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):

23465* (dynamic-ebulliometry, measured 15–65°C, Flom et al. 1951)

434076* (121.11°C, static-Bourdon gauge, measured range 121.11–265.56°C, Kobe et al. 1956)

19920* (23.139°C, measured range 23.2–99.7°C, Scott et al. 1970)

21646* (measured range 0.35–35°C, Koizumi & Ouchi 1970; quoted, Boublik et al. 1984)

$\log (P/\text{mmHg}) = [1 - 339.244/(T/K)] \times 10^4 \{0.830424 - 6.81525 \times 10^{-4} \cdot (T/K) + 6.84786 \times 10^{-7} \cdot (T/K)^2\}$; temp range 253.15–540.15 K (Cox eq., Chao et al. 1983)

17530, 26340 (20°C, 30°C, quoted, Verschuereen 1983)

21610, 21630 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.59372 - 1446.15/(249.982 + t/^\circ\text{C})$; temp range 0.35–35°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.12023 - 1202.394/(226.267 + t/^\circ\text{C})$; temp range 23.139–99.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 6.97231 - 540.5/(260.10 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Dean 1985, 1992)

19920, 21600, 26870 (23.139, 25, 30°C, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.79696 - 1157.06/(t/^\circ\text{C} + 206.75)$, temp range: 90–140°C, (Antoine eq., Riddick et al. 1986)

21620, 21900 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.92617 - 1101.47/(-57/95 + T/K)$; temp range 273–339 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.12052 - 1202.561/(-46.863 + T/K)$; temp range 296–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.63507 - 1626.656/(15.041 + T/K)$; temp range 399–479 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.73137 - 1702.922/(23.613 + T/\text{K})$; temp range 467–541 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 34.870 - 2.7523 \times 10^3/(T/\text{K}) - 9.5958 \cdot \log (T/\text{K}) + 1.9889 \times 10^{-10} \cdot (T/\text{K}) + 3.5465 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 165–540 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

7.15 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

10.33, 142.6 (calculated-group contribution calculated-bond contribution method, Hine & Mookerjee 1975)

Octanol Water Partition Coefficient, $\log K_{OW}$:

0.46 (calculated-f const., Hansch & Leo 1979)

0.22 (shake flask-GC, Funasaki et al. 1985)

0.46 (shake flask, Log P Database, Hansch & Leo 1987)

0.46 (recommended, Sangster 1989)

0.46 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.86 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.37, 1.26; 1.33 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.59 - 1.63) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (FP-RF flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)

$k_{OH}(\text{calc}) = 1.66 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}(\text{exptl}) = 1.50 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.28 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1986, 1987; quoted, Sabljic & Güsten 1990)

$k_{OH}(\text{calc}) = 1.28 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987, 1988; quoted, Müller & Klein 1991)

$k_{NO_3} = 4.875 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Atkinson 1991)

$k_{NO_3} = 4.88 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (relative rate method, Atkinson et al. 1988, Atkinson 1991)

$k_{OH} = 1.78 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 296 K (RP-RF method, Wallington et al. 1988b)

$k_{OH} = 1.61 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}^* = 18.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method; $k_{OH} = 16.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 16 h at $298 \pm 2 \text{ K}$; measured range 263–372 K (Moriarty et al. 2003)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water:

Ground water:

Sediment:

Soil: disappearance $t_{1/2} = 5.7$ d was calculated from measured first-order rate constant (Anderson et al. 1991).

Biota:

TABLE 10.1.1.11.1

Reported vapor pressures of tetrahydrofuran at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Flom et al. 1951	Kobe et al. 1956		Koizumi & Ouchi 1970	Scott 1970			
dynamic-ebulliometry	static-Bourdon gauge		in Boublik et al. 1984	comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
15	15199	121.11	434076	0.35	567	23.139	19920
25	23465	126.67	509867	10	10732	28.362	25007
35	35064	132.22	578768	15	13687	33.62	31160
45	51329	137.78	661450	20	17240	38.917	38547
55	73327	143.33	744131	25	21646	44.251	47359
65	101325	148.89	833702	30	26842	49.62	57803
		154.44	909493	35	35031	55.029	70109
bp/°C	66.1	160	1005955			60.475	84525
		165.56	1116196			65.965	101325
		171.11	1233328			71.489	120.789
		176.67	1364240			77.054	143.268
		182.22	1502042			82.659	169052
		187.78	1653624			88.3	198530
		193.33	1777646			93.98	232087
		198.89	1984349			99.7	270110
		204.44	2156601				
		210	2349524			mp/°C	
		215.56	2549337				
		21.11	2769820				
		226.67	3004084				
		232.22	3252127				
		237.78	3507061				
		243.33	3782655				
		248.89	4078939				
254.44	4388994						
260	4705938						
265.56	5050443						

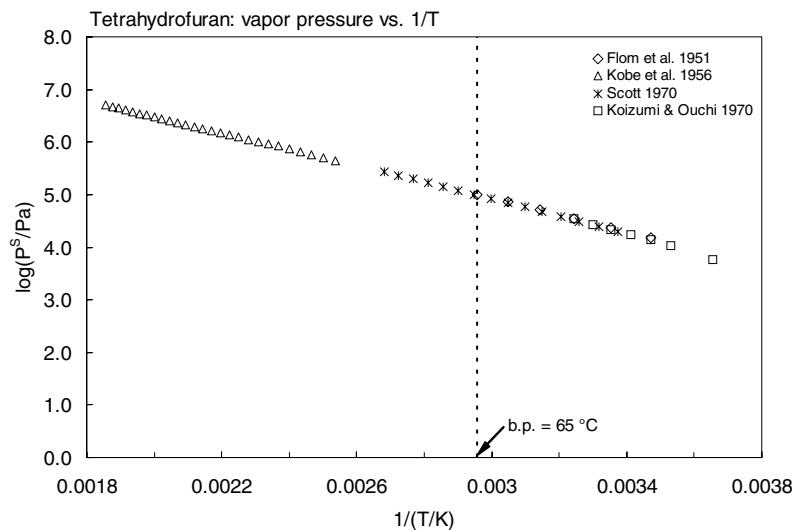


FIGURE 10.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for tetrahydrofuran.

10.1.1.12 Tetrahydropyran



Common Name: Tetrahydropyran

Synonym: pentamethylene oxide, oxacyclohexane

Chemical Name: 1,5-epoxypentane, pentamethylene oxide, oxacyclohexane, tetrahydro-2H-pyran

CAS Registry No: 142-68-7

Molecular Formula: $C_5H_{10}O$

Molecular Weight: 86.132

Melting Point ($^{\circ}C$):

−49.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

88.0 (Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8814, 0.8772 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

97.7 ($20^{\circ}C$, calculated-density)

107.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

80200 (selected, Riddick et al. 1986)

85700*, 68800 ($19.9^{\circ}C$, $31^{\circ}C$, shake flask-GC/TC, measured range $0-81.3^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

9536 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.01171 - 1249.062/(-49.943 + T/K)$; temp range $273-362 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

12.71 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

13.94, 215.9 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.64 (shake flask-GC, Funasaki et al. 1985)

0.82 (recommended, Sangster 1989)

1.00 (recommended, Sangster 1993)

0.95 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.22 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} \sim 13.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at 298 K (Atkinson 1989)
 $k_{\text{OH}}^* = 11.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method; $k_{\text{OH}} = 12.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 28 h at $298 \pm 2 \text{ K}$, measured range 263–372 K (Moriarty et al. 2003).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (Darnall et al. 1976);
 photodecomposition $t_{1/2} = 3.4 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976).

TABLE 10.1.1.12.1
Reported aqueous solubilities of tetrahydropyran at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
0	12900
9.4	10030
19.9	8670
31	6880
39.6	6040
50.5	5160
60.7	4620
71.3	4500
81.3	4290

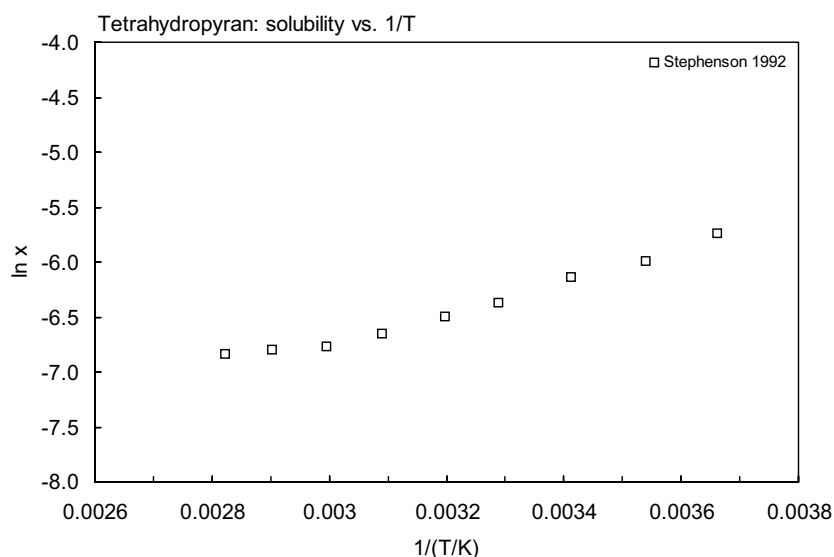


FIGURE 10.1.1.12.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tetrahydropyran.

10.1.1.13 1,4-Dioxane



Common Name: 1,4-Dioxane

Synonym: 1,4-diethylenedioxiide, glycoethyleneether, *p*-dioxane

Chemical Name: 1,4-dioxane

CAS Registry No: 123-91-1

Molecular Formula: $C_4H_8O_2$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

11.85 (Lide 2003)

Boiling Point ($^{\circ}C$):

101.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.03318, 1.02766 ($20^{\circ}C$, $25^{\circ}C$, Hovorka et al. 1936)

1.0336, 1.0280 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

85.2 ($20^{\circ}C$, calculated-density)

92.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.46 (quoted, Riddick et al. 1986)

12.84 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Verschueren 1983; Riddick et al. 1986; Howard 1990)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations, *data at other temperatures are tabulated at end of this section):

4920* (static method, measured range 10 – $80^{\circ}C$, Hovorka et al. 1936)

$\log (P/mmHg) = 8.0588 - 1933.8/(T/K)$; temp range 10 – $80^{\circ}C$ (Antoine eq., static method, Hovorka et al. 1936)

$\log (P/mmHg) = 7.8642 - 1866.7/(T/K)$; temp range ~ 10 – $110^{\circ}C$ (Antoine eq., differential manometer, Gallagher & Hibbert 1937)

4986* (static-Hg manometer, measured range 20 – $105^{\circ}C$, Crenshaw et al. 1938; quoted, Vinson & Martin 1963)

$\log (P/mmHg) = -2316.26/(T/K) - 2.77251 \cdot \log (T/K) + 16.2007$; temp range 20 – $105^{\circ}C$ (Hg manometer, Crenshaw et al. 1938)

5333* (summary of literature data, Stull 1947)

406516* ($154.44^{\circ}C$, static-Bourdon gauge, measured range 154.44 – $310^{\circ}C$, Kobe et al. 1956)

$\log (P/mmHg) = [-0.2185 \times 8546.2/(T/K)] + 7.864110$; temp range -35.8 to $101^{\circ}C$ (Antoine eq., isomer not specified, Weast 1972–73)

5065 (Boublik et al. 1984)

4932 (quoted, Verschueren 1983)

$\log (P/kPa) = 6.66014 - 1556.983/(240.366 + t/^{\circ}C)$; temp range 20 – $105^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 6.56891 - 1550.445/(240.459 + t/^{\circ}C)$; temp range 20 – $125^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

4950, 6135 (25 , $30^{\circ}C$, Riddick et al. 1986)

$\log (P/kPa) = 6.9891 - 1866.7/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

4915 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.40318 - 1457.97/(-42.888 + T/\text{K})$; temp range 285–375 K (Antoine eq., Stephenson & Malanowski 1987)

5060, 6092 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 20.5761 - 2.4658 \times 10^3/(T/\text{K}) - 4.3645 \cdot \log (T/\text{K}) - 2.7053 \times 10^{-10} \cdot (T/\text{K}) + 8.5235 \times 10^{-6} (T/\text{K})^2$; temp range 285–587 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

0.495 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975; quoted, Howard 1990)

0.431, 1.564 (calculated-group contribution, calculated-bond contribution method Hine & Mookerjee 1975)

0.698 (computer value, Yaws et al. 1991)

1.609, 4.314, 6.925, 10.19 (dioxane, 40, 60, 70, 80°C, equilibrium headspace-GC, Kolb et al. 1992)

$\ln (1/K_{AW}) = -7.940 + 4798/(T/\text{K})$, temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)

0.496 (quoted from Howard 1989–1991, Capel & Larson 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

−0.42, 0.01 (observed, calculated-f const., Chou & Jurs 1979)

−0.42 (quoted, Verschuereen 1983; quoted, Pinal et al. 1990)

−0.27 (Hansch & Leo 1985; quoted, Howard 1990; Capel & Larson 1995)

−0.27 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.17 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.23 (soil, estimated- K_{OW} , Lyman et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated Henry' law constant suggests that volatilization for 1,4-dioxane from water and moist soil should be slow; however, it has a moderate vapor pressure, so volatilization from dry soil is possible (Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 67$ d to 9.1 yr in water, based on measured rates for the reaction with hydroxyl radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; quoted, Howard et al. 1991)

photooxidation $t_{1/2} = 8.1$ –81 h in air, based on measured rate constant for the reaction of 1,3,5-trioxane with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

photooxidation $t_{1/2} = 6.69$ –9.6 h in the atmosphere, based on estimated reaction rate with photochemically produced hydroxyl radicals (Howard 1990)

$k_{OH} = 10.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 38.6 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 10.9 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

$k_{OH}^* = 9.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method; $k_{OH} = 12.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 25 h at 298 ± 2 K; measured range 263–372 K (Moriarty et al. 2003)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672$ –4320 h, based on unacclimated aerobic aqueous screening test data with confirmed resistance to biodegradation (Sasaki 1978; Kawasaki 1980; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688$ –17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 28$ d, $t_{1/2}(\text{anaerobic}) = 110$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 8.1\text{--}81$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);
 $t_{1/2} = 6.69\text{--}9.6$ h in the atmosphere, based on estimated reaction rate with photochemically produced hydroxyl radical (Howard 1990).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 10.1.1.13.1

Reported vapor pressures of 1,4-dioxane at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Hovorka et al. 1936		Crenshaw et al. 1938		Stull 1947		Kobe et al. 1956	
static method		ebulliometry-Hg manometer		summary of literature data		static method-Bourdon gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
10	2266	20	3853	–35.8	133.3	154.44	406516
20	3746	25	4986	–12.8	666.6	160	461637
25	4920	30	6386	–1.20	1333	165.56	523648
30	6346	40	10239	12	2666	171.11	585659
40	10212	50	15905	25.2	5333	176.67	654560
50	15972	60	23985	33.8	7999	182.22	730351
60	24171	70	35224	45.1	13332	187.78	806142
70	35583	80	50503	62.3	26664	193.33	902603
80	51036	90	70821	81.8	53329	198.89	992174
		100	97350	101.1	101325	204.44	1095526
eq. 1	P/mmHg	105	113351			210	1205768
A	8.0588			mp/°C	10	215.56	1322899
B	1933.8	bp/°C	101.26			221.11	1440031
						226.67	1577833
		eq. 4	P/mmHg			232.22	1722525
		A	16.2007			237.78	1874107
		B	2316.26			243.33	2039470
		C	2.77251			248.89	2211722
						254.44	2397755
						260	2597568
						265.56	2797381
						271.11	3052314
						276.67	3259017
						282.22	3507061
						287.78	3755105
						293.33	4037599
						298.89	4333873
						204.44	4595697
						310	4933312

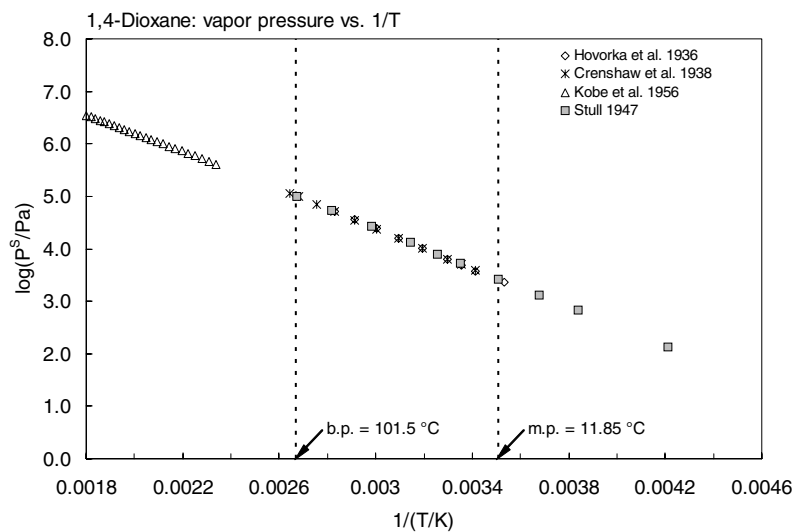
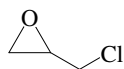


FIGURE 10.1.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for dioxane.

10.1.2 HALOGENATED ETHERS

10.1.2.1 Epichlorohydrin



Common Name: Epichlorohydrin

Synonym: 1-chloro-2,3-epoxypropane, (chloromethyl)oxirane, α -epichlorohydrin, γ -chloropropylene oxide

Chemical Name: epichlorohydrin, 1-chloro-2,3-epoxypropane, α -epichlorohydrin, γ -chloropropylene oxide

CAS Registry No: 106-89-8

Molecular Formula: C_3H_5OCl

Molecular Weight: 92.524

Melting Point ($^{\circ}C$):

–57.2 (Riddick et al. 1986; Howard 1989)

–26 (Lide 2003)

Boiling Point ($^{\circ}C$):

118 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1807, 1.1746 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

78.4 ($20^{\circ}C$, calculated-density)

90.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

65800 ($20^{\circ}C$, selected, Riddick et al. 1986)

65800 ($20^{\circ}C$, Krijgsheld & Van der Gen 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2400 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.5958 - 1587.9/(230 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

2192 (Daubert & Danner 1985)

$\log(P_L/kPa) = 6.5958 - 1587.9/(-43.15 + T/K)$; temp range 328–388 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 24.764 - 2.8846 \times 10^3/(T/K) - 5.6252 \cdot \log(T/K) - 1.1011 \times 10^{-10} \cdot (T/K) + 5.3331 \times 10^{-7} \cdot (T/K)^2$; temp range 216–610 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

3.375 (calculated-P/C using Riddick et al. 1986 data)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.30 (Krijgsheld & Van der Gen 1986)

0.45 (shake flask-GC, Deneer et al. 1988)

0.45 (recommended, Sangster 1993)

0.45 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

0.66 (estimated, Santodonato et al. 1980; quoted, Howard 1989)

Sorption Partition Coefficient, $\log K_{oc}$:

2.09 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2} \sim 29$ h for a model river 1 m deep with a 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} \sim 4.0$ d, based on estimation for the photooxidation with hydroxyl radical in air (Cupitt 1980; quoted, Howard 1989)

$k_{OH}(\text{calc}) = 9.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 4.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} \geq 5.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to *n*-butane for the gas phase reaction with OH radical at $23.3 \pm 0.9^\circ\text{C}$ with an atmospheric lifetime of < 21 d for an average OH radical concentration of 1×10^6 molecules/cm³ (Edney et al. 1986)

$k_{OH}(\text{exptl}) = 4.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 6.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{O_3}(\text{aq.}) \leq 0.003 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 4.1 and 22°C , with $t_{1/2} \sim 130$ d at pH 7 (Yao & Haag 1991).

Hydrolysis: half-life of 8.2 d in distilled water to hydrolyze to 1-chloropropan-2,3-diol at 20°C and pH 5–9 (Mabey & Mill 1978; quoted, Howard 1989; Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Bridie et al. 1979; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ –2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photodecomposition $t_{1/2} = 16.0$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976); $t_{1/2} \sim 4.0$ d, based on estimation for the photooxidation with hydroxyl radical in air (Cupitt 1980; quoted, Howard 1989);

$t_{1/2} = 146$ –1458 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991); atmospheric lifetime < 21 d due to reactions with OH radical (Edney et al. 1986).

Surface water: evaporation $t_{1/2} = 29$ h for a model river 1 m deep with a 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured rate constant $k \leq 0.003 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 4.1 and 22°C , with $t_{1/2} \sim 130$ d at pH 7 (Yao & Haag 1991).

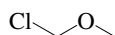
Ground water: 336–1344 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

10.1.2.2 Chloromethyl methyl ether



Common Name: Chloromethyl methyl ether

Synonym: chloromethyl ether, chloromethoxymethane, CMME, monochlorodimethyl ether

Chemical Name: chloromethyl methyl ether

CAS Registry No: 107-30-2

Molecular Formula: C_2H_5ClO , $ClCH_2-O-CH_3$

Molecular Weight: 80.513

Melting Point ($^{\circ}C$):

−103.5 (Verschuereen 1983; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

59.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0703 (Dean 1985)

1.0605 (Budavari 1989)

Molar Volume (cm^3/mol):

75.2 ($20^{\circ}C$, calculated-density)

81.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

decomposes (Verschuereen 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

24900 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.259 - 1240/(-43.15 + T/K)$; temp range 290–332 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 22.7\text{--}227$ h, based on estimated rate constant for the reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $k = 21\text{ h}^{-1}$ at pH 7 and $25^{\circ}C$ with a calculated $t_{1/2} = 2.0$ min (Van Duuren et al. 1972; quoted, Ellington 1989);

$t_{1/2} = 0.0108\text{--}0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991);

hydrolyzed very fast in aqueous solutions with $t_{1/2} < 1.0$ s (Verschuereen 1983).

Biodegradation: aqueous aerobic $t_{1/2} = 168\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 672\text{--}2688$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 22.7\text{--}227$ h, based on estimated rate constant for the reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 0.0108\text{--}0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

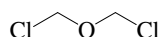
Ground water: $t_{1/2} = 0.0108\text{--}0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 0.0108\text{--}0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biota:

10.1.2.3 Bis(chloromethyl)ether



Common Name: Bis(chloromethyl)ether

Synonym: BCME, Bis-CME, chloro(chloromethoxy)methane, dichloromethylether, (dichloro-dimethyl)ether, sym-dichloromethyl ether, oxybis(chloromethane)

Chemical Name: chloromethyl ether, sym-dichloromethyl ether

CAS Registry No: 542-88-1

Molecular Formula: $C_2H_4Cl_2O$, $ClCH_2-O-CH_2Cl$

Molecular Weight: 114.958

Melting Point ($^{\circ}C$):

−41.5 (Weast 1977; Weast 1982–83; Verschueren 1983; Howard 1989; Lide 2003)

Boiling Point ($^{\circ}C$):

106 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.328 ($15^{\circ}C$, Weast 1982–83)

1.315 (Verschueren 1983)

Molar Volume (cm^3/mol):

102.7 (calculated-Le Bas method at normal boiling point)

87.4 (calculated-density, Stephenson & Malanowski 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

22000 (calculated as per Moriguchi 1975 using Quayle 1953 data, Callahan et al. 1979)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3999 ($22^{\circ}C$, Dreisbach 1952)

$\log(P/mmHg) = -3.4945 - 2.2305 \times 10^3/(T/K) + 6.774 \cdot \log(T/K) - 1.7332 \times 10^{-2} \cdot (T/K) + 9.5511 \times 10^{-6} \cdot (T/K)^2$;
temp range 232–579 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

21.27 (calculated-P/C, Mabey et al. 1982)

21.27 (20 – $25^{\circ}C$ and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

213.18 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

−0.38 (calculated, Radding et al. 1977)

2.40 (calculated, Mabey et al. 1982)

Bioconcentration Factor, $\log BCF$:

1.041 (bluegill sunfish, Veith et al. 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

1.20 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $k \ll 360\ M^{-1}\ h^{-1}$ for singlet oxygen and $k = 3.0\ M^{-1}\ h^{-1}$ for peroxy radical (Mabey et al. 1982)

photooxidation $t_{1/2} = 0.196$ – $1.96\ h$, based on estimated rate constant for reaction with hydroxyl radical in air
(Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: hydrolyzed very fast in aqueous solution with half-life in the order of 10 s when extrapolated to pure water (Hammond & Alexander 1972; quoted, Verschueren 1983);
rate constant $k = 0.018 \text{ s}^{-1}$ with $t_{1/2} = 38 \text{ s}$ (Tou et al. 1974; quoted, Callahan et al. 1979; Howard et al. 1991);
hydrolysis $t_{1/2} = 10\text{--}38 \text{ s}$ and will rapidly disappear from any aquatic system (Fishbein 1979; quoted, Howard 1989);

$k = 65 \text{ h}^{-1}$ at pH 7.0 at 20°C (quoted, Mabey et al. 1982).

Biodegradation: aqueous aerobic $t_{1/2} = 168\text{--}672 \text{ h}$, based on scientific judgement; aqueous anaerobic $t_{1/2} = 672\text{--}2688 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.196\text{--}1.96 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 0.0106\text{--}0.106 \text{ h}$, based on estimated hydrolysis half-life in water (Howard et al. 1991).

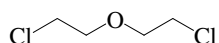
Ground water: $t_{1/2} = 0.0106\text{--}0.106 \text{ h}$, based on estimated hydrolysis in water (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} < 10 \text{ d}$, via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

$t_{1/2} = 0.0106\text{--}0.106 \text{ h}$, based on estimated hydrolysis half-life in water (Howard et al. 1991).

Biota:

10.1.2.4 Bis(2-chloroethyl)ether

Common Name: Bis(2-chloroethyl)ether

Synonym: 2-chloroethyl ether, 1,1'-oxybis(2-chloroethane), bis(β -chloroethyl)ether, Chlorex, 1-chloro-2-(β -chloroethoxy)-ethane, β,β' -dichloroethyl ether, 2,2'-dichloroethyl ether, di(2-chloroethyl)ether, di(chloroethyl)ether, dichlorodiethyl ether, sym-dichlorodiethyl ether

Chemical Name: 2-chloroethyl ether, bis(β -chloroethyl)ether, 1-chloro-2-(β -chloroethoxy)-ethane

CAS Registry No: 111-44-4

Molecular Formula: $C_4H_8Cl_2O$, $ClCH_2CH_2-O-CH_2CH_2Cl$

Molecular Weight: 143.012

Melting Point ($^{\circ}C$):

-51.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

178.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2200 (Verschuereen 1983)

1.2192 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

117.3 ($20^{\circ}C$, calculated-density)

147.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.66 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

10200 ($20^{\circ}C$, Du Pont 1966; Verschuereen 1983)

17195 (shake flask-LSC, Veith et al. 1980)

10200 ($20^{\circ}C$, Riddick et al. 1986)

10400*, 10300 ($20^{\circ}C$, $31^{\circ}C$, shake flask-GC/TC, measured range $0-91.7^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

156.2 (Antoine eq. regression, temp range $23.5-178.5^{\circ}C$, Stull 1947)

94.64, 186 (20, $25^{\circ}C$, Verschuereen 1977,1983)

207 (selected, Riddick et al. 1986)

$\log(P/kPa) = 7.2289 - 2359.6/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

143.6 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.7637 - 1948.62/(-41.974 + T/K)$: temp range $297-452 K$ (Antoine eq., Stephenson & Malanowski 1987)

857.1 (calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

28.97 (calculated-P/C, Lyman et al. 1982; Howard 1989)

1.320 ($20^{\circ}C$, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.58 (calculated, Leo et al. 1971)

1.12 (shake flask-LSC, Veith et al. 1980)

1.29 (shake flask, Hansch & Leo 1985)

1.29 (recommended, Sangster 1993)

1.29 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.041	(bluegill sunfish, Barrows et al. 1980)
1.040	(bluegill sunfish, LSC- ¹⁴ C, Veith et al. 1980; Veith & Kosian 1983)
0.964	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
1.15	(calculated, Sabljic 1987)

Sorption Partition Coefficient, log K_{OC} :

1.38	(soil, calculated-S, Lyman et al. 1982)
1.14	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: calculated $t_{1/2} = 5.78$ d (as per Mackay & Wolkoff 1973 by Durkin et al. 1975);

$t_{1/2} = 3.5, 4.4$ and 180.5 d for the streams, rivers and lakes, respectively, were estimated using Henry's law constant (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 4.0$ h, based on an estimated half-life for ethyl ether in the smog chamber (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);

$k \ll 360 \text{ M}^{-1} \cdot \text{h}^{-1}$ for the reaction with singlet oxygen and $k = 24.0 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 9.65\text{--}96.5$ h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $t_{1/2} = 40.0$ d was estimated at pH 7 from ethyl chloride data in water at an unspecified temperature (Brown et al. 1975; quoted, Howard 1989);

$t_{1/2} = 0.5\text{--}2.0$ yr, based on data from chlorinated ethanes and propanes (Dilling et al. 1975; quoted, Callahan et al. 1979);

first-order hydrolysis $t_{1/2} = 22$ yr, based on neutral hydrolysis rate constant at 20°C which was extrapolated from data for hydrolysis of dioxane at 100°C (Mabey et al. 1982; quoted, Howard et al. 1991);

$k = 2.6 \times 10^{-5} \text{ h}^{-1}$ at pH 7 and 25°C with a calculated $t_{1/2} = 3.0$ yr (Ellington et al. 1987; quoted, Ellington 1989).

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on river die-away test data (Ludzack & Ettinger 1963 and Doljido 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $k = 3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ for the bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} = 13.44$ h was estimated for the reaction with OH radical (GEMS 1986; quoted, Howard 1989);

photooxidation $t_{1/2} = 9.65\text{--}96.5$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

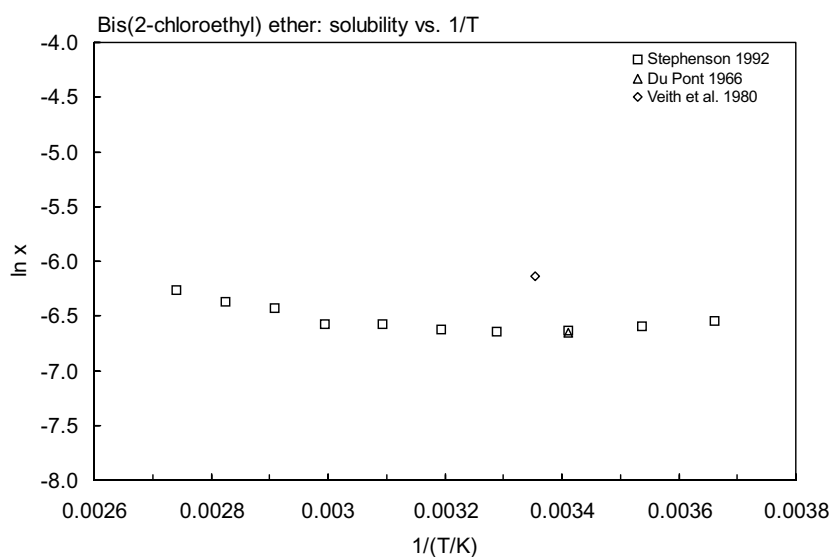
Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

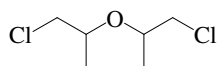
Biota: $t_{1/2} > 4.0$ d but less than 7.0 d in fish tissues (Barrows et al. 1980).

TABLE 10.1.2.4.1**Reported aqueous solubilities of bis(2-chloroethyl) ether at various temperatures**

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	11400
9.6	10900
20	10400
31	10300
40	10500
50.1	11100
60.7	11100
70.6	12800
80.9	13600
91.7	15100

**FIGURE 10.1.2.4.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for bis(2-chloroethyl)ether.

10.1.2.5 Bis(2-chloroisopropyl)ether



Common Name: Bis(2-chloroisopropyl)ether

Synonym: bis(2-chloro-1-methylethyl)ether, dichlorodiisopropyl ether, dichloroisopropyl ether, 2,2'-dichloroisopropyl ether, 2,2'-oxybis(1-chloropropane)

Chemical Name: bis(2-chloroisopropyl)ether, dichlorodiisopropyl ether, dichloroisopropyl ether

CAS Registry No: 108-60-1

Molecular Formula: $C_6H_{12}Cl_2O$, $ClCH_2CH(CH_3)-O-CH(CH_3)CH_2Cl$

Molecular Weight: 171.064

Melting Point ($^{\circ}C$):

-97 (Weast 1977; Verschueren 1983)

Boiling Point ($^{\circ}C$):

187 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1100 (Verschueren 1983)

1.1122 (Dean 1985)

Molar Volume (cm^3/mol):

154.1 ($20^{\circ}C$, calculated-density)

193.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1700* (room. temp., Verschueren 1977,1983)

2450*, 2370 ($19.1^{\circ}C$, $31.0^{\circ}C$, shake flask-GC, measured range $9.5-91.4^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

103.95 (Antoine eq. regression, temp range $24.7-180^{\circ}C$, Stull 1947)

113.31 ($20^{\circ}C$, Verschueren 1977,1983)

112.30 ($28.85^{\circ}C$, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.68233 - 1856.14/(-58.793 + T/K)$; temp range 302–456 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

11.14 ($20^{\circ}C$, calculated-P/C, Mabey et al. 1982)

11.40 (calculated-P/C from Verschueren 1977/83 data)

116.5 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.58 (calculated, Leo et al. 1971)

2.10 (calculated, Mabey et al. 1982)

2.48 (HPLC-RT correlation, Kawamoto & Urano 1989)

2.48 (recommended, Sangster 1993)

Bioconcentration Factor, $\log BCF$:

1.544 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{oc}$:

1.785 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: calculated $t_{1/2} = 1.37$ d (calculated as per Mackay & Wolkoff 1973, Durkin et al. 1975; quoted, Callahan et al. 1979).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 4.0$ h, based on estimated half-life for ethyl ether in a smog chamber (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with singlet oxygen and $k = 2.0 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with peroxy radical (Mabey et al. 1982).

Hydrolysis: $t_{1/2} = 0.5\text{--}2.0$ yr, based on data from chlorinated ethanes and propanes (Dilling et al. 1975; quoted, Callahan et al. 1979);

$k = 4 \times 10^{-6} \text{ h}^{-1}$ at pH 7.0 and 25°C (Mabey et al. 1982).

Biodegradation: aqueous aerobic $t_{1/2} = 432\text{--}4320$ h, based on river die-away test data (Kleopfer & Fairless 1972; quoted, Howard et al. 1991) and aerobic soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 1728\text{--}17280$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 4.61\text{--}46.1$ h, based on photooxidation half-life in air (Howard et al. 1991).

Surface water: estimated $t_{1/2} = 3.1$ d for surface waters in case of a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 432\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 864\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 432\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 10.1.2.5.1
Reported aqueous solubilities of bis(2-chloroisopropyl) ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
9.5	4090
19.1	2450
31	2370
40.3	2180
51.1	1820
60.6	2090
80.7	2650
91.4	2410

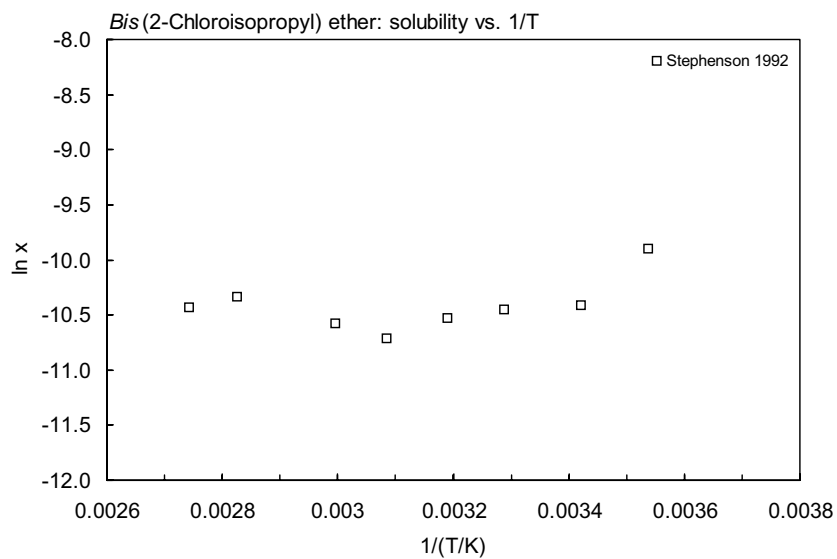
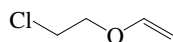


FIGURE 10.1.2.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for bis(2-chloroisopropyl)ether.

10.1.2.6 2-Chloroethyl vinyl ether

Common Name: 2-Chloroethyl vinyl ether

Synonym: (2-chloroethoxy)-ethene, β -chloroethyl vinyl ether, vinyl 2-chloroethyl ether

Chemical Name: β -chloroethyl vinyl ether, 2-chloroethyl vinyl ether, vinyl 2-chloroethyl ether

CAS Registry No: 110-75-8

Molecular Formula: $C_4H_7Cl_2O$, $ClCH_2CH_2-O-CH=CH_2$

Molecular Weight: 106.551

Melting Point ($^{\circ}C$):

-70 (Lide 2003)

Boiling Point ($^{\circ}C$):

108 (Weast 1977; Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0475 (Weast 1982–83)

1.0480 (Dean 1985)

Molar Volume (cm^3/mol):

101.7 ($20^{\circ}C$, calculated-density)

119.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

15000 (calculated as per Moriguchi 1975, Callahan et al.)

6000 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

3566 ($20^{\circ}C$, calculated, Dreisbach 1952)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

0.0253 (20 – $25^{\circ}C$, calculated-P/C, Mabey et al. 1982)

25.33 (20 – $25^{\circ}C$ and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

24.79 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.28 (calculated as per Leo et al. 1971, Callahan et al. 1979)

1.14 (calculated, Mabey et al. 1982)

Bioconcentration Factor, $\log BCF$:

0.672 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

0.820 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 30$ min, based on half-life estimated for 2-methyl-2-butene from smog chamber data (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);

$k = 1 \times 10^{10} M^{-1} \cdot h^{-1}$ for singlet oxygen and $k = 34 M^{-1} h^{-1}$ for peroxy radical (Mabey et al. 1982).

Hydrolysis: $k = 4.4 \times 10^{-10} s^{-1}$, minimum rate at pH 7 and $25^{\circ}C$ in pure water with a maximum $t_{1/2} = 0.48$ yr (Jones & Wood 1964; quoted, Callahan et al. 1979);

$k \sim 4 \times 10^{-6} h^{-1}$ at pH 7.0 and $25^{\circ}C$ with reference to that of bis(2-chloroethyl)ether (Mabey et al. 1982).

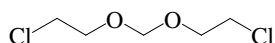
Biodegradation:

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation to water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Soil: $t_{1/2} < 10 \text{ d}$, via volatilization subject to plant uptake from the soil (Ryan et al. 1988).

10.1.2.7 Bis(2-chloroethoxy)methane

Common Name: Bis(2-chloroethoxy)methane

Synonym: bis(β -chloroethyl)formal, β , β -dichlorodiethyl formal, dichlorodiethyl methylal

Chemical Name: bis(2-chloroethoxy)methane

CAS Registry No: 111-91-1

Molecular Formula: $C_5H_{10}Cl_2O_2$, $ClCH_2CH_2-O-CH_2-O-CH_2CH_2Cl$

Molecular Weight: 173.037

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

215 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

180.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

81000 (calculated as per Moriguchi 1975, Callahan et al. 1979;)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

21.58 (Antoine eq. regression, temp range 53 – $215^{\circ}C$, Stull 1947)

< 13.3 (calculated as per Dreisbach 1952 using data of Webb et al. 1962, Callahan et al. 1979)

21.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.54778 - 2641.33/(-11.518 + T/K)$; temp range 326 – $486 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$ or as indicated):

0.0284 (20 – $25^{\circ}C$, calculated-P/C, Mabey et al. 1982)

0.0273 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.260 (calculated as per Leo et al. 1971, Callahan et al. 1979; Ryan et al. 1988)

1.029 (calculated, Mabey et al. 1982)

Bioconcentration Factor, $\log BCF$:

0.568 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

0.716 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $k \ll 360 M^{-1} h^{-1}$ for singlet oxygen and $k = 52 M^{-1} h^{-1}$ for peroxy radical (Mabey et al. 1982).

Hydrolysis: minimum rate $k = 2.53 \times 10^{-6} L mol^{-1} s^{-1}$ for acid-catalyzed hydrolysis of the acetal linkage at $25^{\circ}C$ (Kankaanperä 1969; quoted, Callahan et al. 1979; Mabey et al. 1982);

$t_{1/2} = 0.5$ – 2.0 yr, based on data of Dilling et al. 1975 on chlorinated ethanes and propanes (quoted, Callahan et al. 1979);

estimated rate constant $k \sim 4 \times 10^{-6} h^{-1}$ at pH 7.0 and $25^{\circ}C$ by analogy to bis(2-chloroethyl)ether (Mabey et al. 1982).

Biodegradation:

Biotransformation:

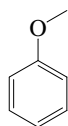
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Soil: $t_{1/2} > 50$ d, via volatilization subject to plant uptake from the soil (Ryan et al. 1988).

10.1.3 AROMATIC ETHERS

10.1.3.1 Anisole (Methoxybenzene)



Common Name: Anisole

Synonym: methoxybenzene

Chemical Name: anisole, methoxybenzene, methyl phenyl ether

CAS Registry No: 100-66-3

Molecular Formula: C_7H_8O , $C_6H_5OCH_3$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

-37.13 (Lide 2003)

Boiling Point ($^{\circ}C$):

153.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.99402, 0.98932 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

0.9940, 0.9893 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

108.8 ($20^{\circ}C$, calculated-density)

127.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1514 (shake flask-UV, McGowan et al. 1966)

1536 (shake flask-UV, Vesala 1974)

2030*, 1860 ($20^{\circ}C$, $29.7^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.7^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

497* (calculated-Antoine eq. regression, temp range 5.4 – $155.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.35950 - 1718.7/(230 + t/^{\circ}C)$ (Antoine eq., temp range 73 – $154^{\circ}C$, Dreisbach & Martin 1949)

6287* ($73.34^{\circ}C$, ebulliometry, measured range 73.34 – $153.75^{\circ}C$, Dreisbach & Shrader 1949)

26547* ($109.876^{\circ}C$, ebulliometry, measured range 109.876 – $164.114^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.05236 - 1489.756/(203.543 + t/^{\circ}C)$; temp range 109.876 – $164.114^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 22.84299 - 3033.20/(T/K) - 4.88720 \cdot \log(T/K)$; temp range 109.876 – $164.114^{\circ}C$ (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = [-0.2185 \times 10440.9/(T/K)] + 8.221443$; temp range 5.4 – $155.5^{\circ}C$ (Antoine eq., Weast 1972–73)

472* (“recomputed” reported data, ebulliometry, measured range 383 – 437 K, Ambrose et al. 1976)

$\log(P/kPa) = 6.17595 - 1489.502/(T/K - 69.577)$; temp range 383 – 437 K (Antoine eq., ebulliometry, Ambrose et al. 1976)

$\log(P/mmHg) = [1 - 426.827/(T/K)] \times 10^{0.942238 - 10.2065 \times 10^{-4} \cdot (T/K) + 10.6819 \times 10^{-7} \cdot (T/K)^2}$; temp range 346.49 – 415.52 K (Cox eq., Chao et al. 1983)

$\log(P/kPa) = 6.23361 - 1529.735/(208.062 + t/^{\circ}C)$; temp range 73.3 – $153.75^{\circ}C$ (Antoine eq. derived from exptl data of Dreisbach & Shrader 1949, Boublik et al. 1984)

$\log(P/kPa) = 6.17900 - 1490.93/(203.675 + t/^{\circ}C)$; temp range 109.9 – $164.1^{\circ}C$ (Antoine eq. derived from reported exptl data of Collerson et al. 1965, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.05269 - 1489.99/(203.57 + t/^{\circ}\text{C})$; temp range 110–164°C (Antoine eq., Dean 1985, 1992)
 472 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.17595 - 1489.502/(203.573 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P_L/\text{kPa}) = 6.17622 - 1489.957/(-69.525 + T/\text{K})$; temp range 382–437 K (Antoine eq., Stephenson & Malanowski 1987)
 204, 383 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
 $\log (P/\text{mbar}) = 7.11773 - 1451.742/[(T/\text{K}) - 73.252]$; temp range 382–429 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)
 $\log (P/\text{mmHg}) = -8.1053 - 2.5386 \times 10^3/(T/\text{K}) + 9.0289 \cdot \log (T/\text{K}) - 2.0426 \times 10^{-2} \cdot (T/\text{K}) + 1.0536 \times 10^{-5} \cdot (T/\text{K})^2$;
 temp range 236–642 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

430.8 (exptl. $1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975)
 430.8, 358.3 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.11 (shake flask-UV, Fujita et al. 1964)
 2.04 (shake flask-UV, Rogers & Cammarata 1969)
 2.10 (HPLC-RT correlation, Mirrlees et al. 1976)
 2.08 (Hansch & Leo 1979)
 2.24 (HPLC- k' correlation, Haky & Young 1984)
 2.16 (HPLC-RT correlation, Ge et al. 1987)
 2.15 (HPLC-RT correlation, Minick et al. 1988)
 2.01 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
 2.11 (recommended, Sangster 1989, 1993)
 2.17 (dual-mode centrifugal partition chromatography, Gluck 1990)
 1.67, 1.79 (shake flask-UV/VIS spec.: 25, 60°C, Kramer & Henze 1990)
 2.11 (recommended, Hansch et al. 1995)
 2.41, 2.31, 2.58, 2.55 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovsaky et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

4.01 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

1.34 (Isnard & Lambert 1988)

Sorption Partition Coefficient, $\log K_{OC}$:

6.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 1.054 \times 10^{-2} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.57 \pm 0.24) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K, measured range 299–435 K (overall rate constant, flash photolysis-resonance fluorescence technique, Perry et al. 1977)

$k_{OH} = 1.57 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985; quoted, Sabljic & Güsten 1990)

$k_{NO_3} = 9.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (re-evaluated value, Atkinson et al. 1987)

$k_{OH} = 1.35 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air, extrapolated from lit. data to 25°C (Dilling et al. 1988)

$k_{NO_3} = 2.08 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{OH} = (14.1 - 19.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. to 299.9 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation: degradation $k = 2.86 \times 10^{-17} \text{ mol cell}^{-1} \text{ h}^{-1}$ in pure culture system (Banerjee et al. 1984).
 Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.3.1.1
Reported aqueous solubilities of anisole at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	
10.2	2370
20	2030
29.7	1860
39.9	1840
50.2	1990
60.2	2550
70.2	2530
81.2	2940
90.7	3520

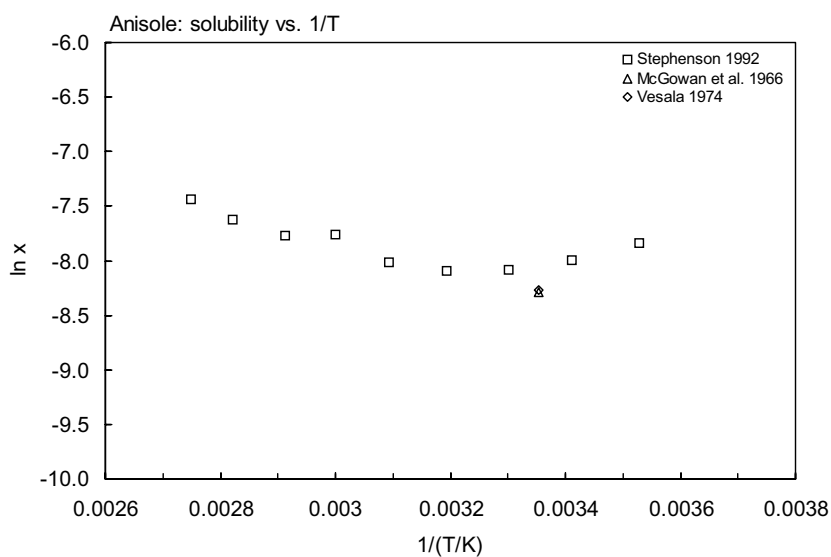


FIGURE 10.1.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for anisole.

TABLE 10.1.3.1.2

Reported vapor pressures of anisole at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log P = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1976	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
5.4	133.3	73.34	6287	109.876	26547	109.88	26547
30	666.6	81.31	8851	116.255	33024	116.261	33024
42.2	1333	84.55	10114	122.045	39966	122.053	39966
55.8	2666	99.89	16500	126.854	46587	126.864	46587
70.7	5333	123.77	42066	131.266	55425	131.279	53424
80.1	7999	139.37	67661	136.078	59950	135.092	59950
93	13332	153.75	101325	138.64	66614	138.655	66614
112.3	26664			141.919	73266	141.936	73266
133.8	53329			145.003	79992	145.021	79992
155.5	101325	Antoine eq. given by		147.89	86731	147.91	86732
		Dreisbach & Martin 1949		150.429	93021	150.45	93021
mp/°C	–37.3	Eq. 2	P/mmHg	153.143	100135	153.164	100137
		A	7.3595	155.554	106819	155.576	106820
		B	1718.7	157.81	113382	157.834	113381
		C	230	160.009	120086	160.033	120084
				162.087	126698	162.113	126697
		bp/°C	153.75	164.114	133429	164.141	133427
		mp/°C	–37.38			25	472
				bp/°C	153.598		
						Antoine eq.	
				Antoine eq.		eq. 2	P/kPa
				eq. 2	P/mmHg	A	6.17595
				A	705236	B	1489.502
				B	1489.756	C	–69.577
				C	203.543		
				Kirchhoff eq.		Coefficients of Chebyshev eq. are	
				eq. 4	P/mmHg	also given in text.	
				A	22.842 99		
				B	3033.2		
				C	4.8872		
				ΔH _v /(kJ mol ^{–1}) = 39.04			

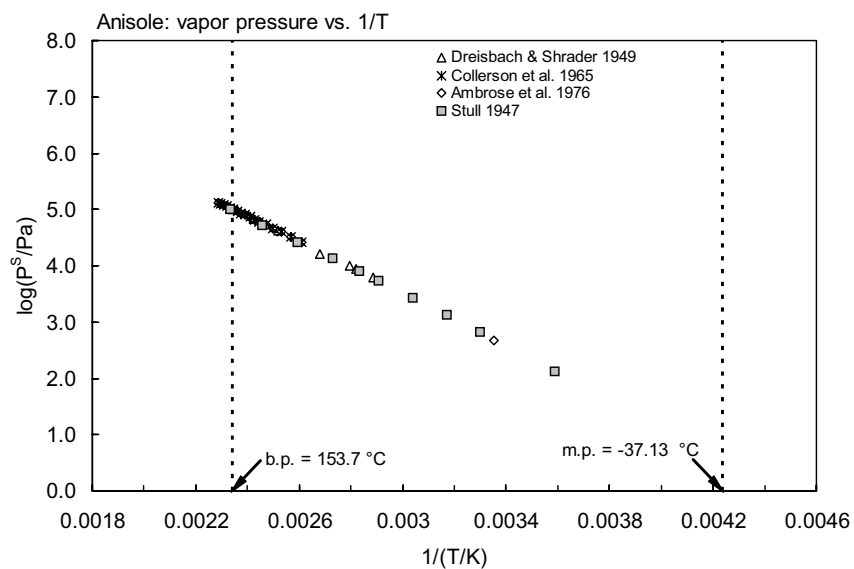
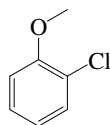


FIGURE 10.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for anisole.

10.1.3.2 2-Chloroanisole



Common Name: 2-Chloroanisole

Synonym: 1-chloro-2-methoxybenzene

Chemical Name: 2-chloroanisole

CAS Registry No: 766-51-8

Molecular Formula: C_7H_7ClO , $C_6H_4Cl(OCH_3)$

Molecular Weight: 142.583

Melting Point ($^{\circ}C$): liquid

-26.8 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

198.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1911 (Lide 2003)

Molar Volume (cm^3/mol):

119.7 ($20^{\circ}C$, calculated-density)

148.2 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

490 (shake flask-HPLC/UV, Lun et al. 1995)

766 (liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

6287 ($115.13^{\circ}C$, ebulliometry, measured range 115.13 – $186.19^{\circ}C$, Dreisbach & Shrader 1949)

$\log(P/mmHg) = 7.54073 - 2012.4/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

$\log(P/kPa) = 6.25236 - 1660.008/(189.207 + t/^{\circ}C)$, temp range 115.13 – $186.19^{\circ}C$ (Antoine eq. derived from exptl data of Dreisbach & Shrader 1949, Boublik et al. 1984)

0.0594 (P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.66563 - 2012.4/(-43.15 + T/K)$, temp range 388 – 460 K, (Antoine eq., Stephenson & Malanowski 1987)

0.0302 (liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

9.50 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.68 (shake flask-UV, Nakagawa et al. 1992)

2.50 (shake flask-HPLC/UV both phases, Lun et al. 1995)

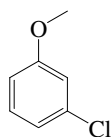
2.72 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.13 (calculated- K_{ow}/K_{aw} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

10.1.3.3 3-Chloroanisole

Common Name: 3-Chloroanisole

Synonym:

Chemical Name:

CAS Registry No: 2845-89-8

Molecular Formula: C_7H_7ClO , $C_6H_4Cl(OCH_3)$

Molecular Weight: 142.583

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

193.5 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

148.2 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

235 (shake flask-HPLC/UV, Lun et al. 1995)

231 (liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0282 (liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

21.4 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.60 (shake flask-HPLC/UV both phases, Lun et al. 1995)

3.09 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

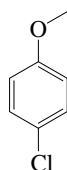
Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.15 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

10.1.3.4 4-Chloroanisole



Common Name: 4-Chloroanisole

Synonym: 1-chloro-4-methoxy-benzene

Chemical Name: 4-chloroanisole

CAS Registry No: 623-12-1

Molecular Formula: C_7H_7ClO , $C_6H_4Cl(OCH_3)$

Molecular Weight: 142.583

Melting Point ($^{\circ}C$):

< -18 (Lide 2003)

Boiling Point ($^{\circ}C$):

197.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.201 (Lide 2003)

Molar Volume (cm^3/mol):

118.7 ($20^{\circ}C$, calculated-density)

148.2 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

237 (shake flask-HPLC/UV, Lun et al. 1995)

312 (liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0324 (liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

18.2 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.78 ($23^{\circ}C$, shake flask-LSC, Banerjee et al. 1980)

2.78 (recommended, Sangster 1993)

2.70 (shake flask-HPLC/UV both phases, Lun et al. 1995)

3.00 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.13 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

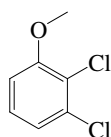
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Biodegradation: degradation rate constants $k = 2.29 \times 10^{-18} mol cell^{-1} h^{-1}$ from pure culture studies (Banerjee et al. 1984).

Half-Lives in the Environment:

10.1.3.5 2,3-Dichloroanisole

Common Name: 2,3-Dichloroanisole

Synonym:

Chemical Name:

CAS Registry No: 1984-59-4

Molecular Formula: $C_7H_6Cl_2O$, $C_6H_3Cl_2(OCH_3)$

Molecular Weight: 177.028

Melting Point ($^{\circ}C$):

32 (Lun et al. 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

169.1 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.854 (mp at $32^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

86.9 (shake flask-GC/ECD, Lun et al. 1995)

140.6 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0468 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

44.1 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.24 (shake flask-HPLC/UV both phases, Lun et al. 1995)

3.30 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.05 (calculated- K_{ow}/K_{Aw} , Pfeifer et al. 2001)

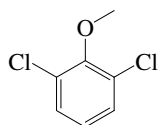
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Half-Lives in the Environment:

10.1.3.6 2,6-Dichloroanisole



Common Name: 2,6-Dichloroanisole

Synonym:

Chemical Name:

CAS Registry No: 1984-65-2

Molecular Formula: $C_7H_6Cl_2O$, $C_6H_3Cl_2(OCH_3)$

Molecular Weight: 177.028

Melting Point ($^{\circ}C$):

10 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

169.1 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

13.12 (shake flask-GC/ECD, Lun et al. 1995)

21.8 (liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0110 (liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

113.7 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.96 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

3.14 (shake flask-HPLC/UV both phases, Lun et al. 1995)

3.10 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.53 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

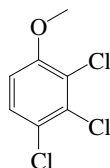
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.3.7 2,3,4-Trichloroanisole



Common Name: 2,3,4-Trichloroanisole

Synonym:

Chemical Name:

CAS Registry No: 54135-80-7

Molecular Formula: $C_7H_5Cl_3O$, $C_6H_2Cl_3(OCH_3)$

Molecular Weight: 211.473

Melting Point ($^{\circ}C$):

70 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

190.0 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.362 (mp at $70^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

10.8 (shake flask-GC/ECD, Lun et al. 1995)

22.1 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.263 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

74.7 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.74 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)

4.03 (shake flask-GC/ECD, both phases, Lun et al. 1995)

3.92 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.44 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.09 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

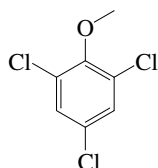
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 1450 mL g^{-1} d^{-1}$; $k_2 = 1.9 d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

10.1.3.8 2,4,6-Trichloroanisole



Common Name: 2,4,6-Trichloroanisole

Synonym:

Chemical Name:

CAS Registry No: 87-40-1

Molecular Formula: $C_7H_5Cl_3O$, $C_6H_2Cl_3(OCH_3)$

Molecular Weight: 211.473

Melting Point ($^{\circ}C$): 61.5 (Lide 2003)

Boiling Point ($^{\circ}C$): 241 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

190.0 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.438 (mp at $61.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

13.2 (shake flask-GC/ECD, Lun et al. 1995)

14.6 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

2.065 (GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0724 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

218.7 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.20 (HPLC-relative retention time correlation, Neilson et al. 1984)

4.11 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)

3.96 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

4.02 (shake flask-GC/ECD, both phases, Lun et al. 1995)

4.05 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.10 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.90 (zebra fish, Neilson et al. 1984)

2.86 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

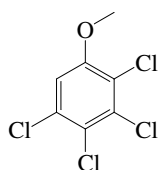
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 1600 mL g^{-1} d^{-1}$; $k_2 = 2.5 d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: biological $t_{1/2} < 1 d$ for all trichloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.9 2,3,4,5-Tetrachloroanisole

Common Name: 2,3,4,5-Tetrachloroanisole

Synonym:

Chemical Name:

CAS Registry No: 938-86-3

Molecular Formula: $C_7H_4Cl_4O$, $C_6HCl_4(OCH_3)$

Molecular Weight: 245.918

Melting Point ($^{\circ}C$):

88 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

210.9 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.241 (mp at $88^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.35 (shake flask-GC/ECD, Lun et al. 1995)

2.76 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

1.202 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

153.0 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.51 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)

4.50 (shake flask-GC/ECD, both phases, Lun et al. 1995)

4.57 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.78 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.67 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

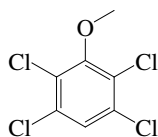
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 940$ $mL\ g^{-1}\ d^{-1}$; $k_2 = 0.42\ d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: biological $t_{1/2} \sim 1-4$ d for all tetrachloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.10 2,3,5,6-Tetrachloroanisole



Common Name: 2,3,5,6-Tetrachloroanisole

Synonym:

Chemical Name:

CAS Registry No: 6936-40-9

Molecular Formula: $C_7H_4Cl_4O$, $C_6HCl_4(OCH_3)$

Molecular Weight: 245.918

Melting Point ($^{\circ}C$):

84 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

210.9 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.264 (mp at $84^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.82 (shake flask-GC/ECD, Lun et al. 1995)

3.64 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzene as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.427 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

318.4 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.68 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)

4.40 (shake flask-GC/ECD, both phases, Lun et al. 1995)

4.52 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.41 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.69 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

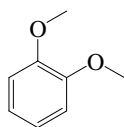
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 1480 mL g^{-1} d^{-1}$; $k_2 = 0.44 d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: biological $t_{1/2} \sim 1-4 d$ for all tetrachloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.11 Veratrole (1,2-Dimethoxybenzene)

Common Name: Veratrole

Synonym: 1,2-dimethoxybenzene

Chemical Name: 1,2-dimethoxybenzene

CAS Registry No: 91-16-7

Molecular Formula: C₈H₁₀O₂, C₆H₄(OCH₃)₂

Molecular Weight: 138.164

Melting Point (°C):

22 (Stephenson & Malanowski 1987)

22.5 (Lide 2003)

Boiling Point (°C):

206.7 (Stephenson & Malanowski 1987)

206 (Lide 2003)

Density (g/cm³):

Molar Volume (cm³/mol):

127.1 (calculated-density)

158.6 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

7160*, 7060 (19.9, 31°C, shake flask-GC, measured range 19.9–91.8°C, Stephenson 1992)

6690 (shake flask-HPLC/UV, Lun et al. 1995)

Vapor Pressure (Pa at 25°C):

$\log (P_L/\text{kPa}) = 8.705 - 3492/(T/\text{K})$, temp range not specified (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.79 (Log P Database, Hansch & Leo 1987, quoted, Sangster 1993)

1.79 (HPLC-RT correlation, average value, Ritter et al. 1994)

1.60 (recommended, Hansch et al. 1995)

2.18 (shake flask-HPLC/UV both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

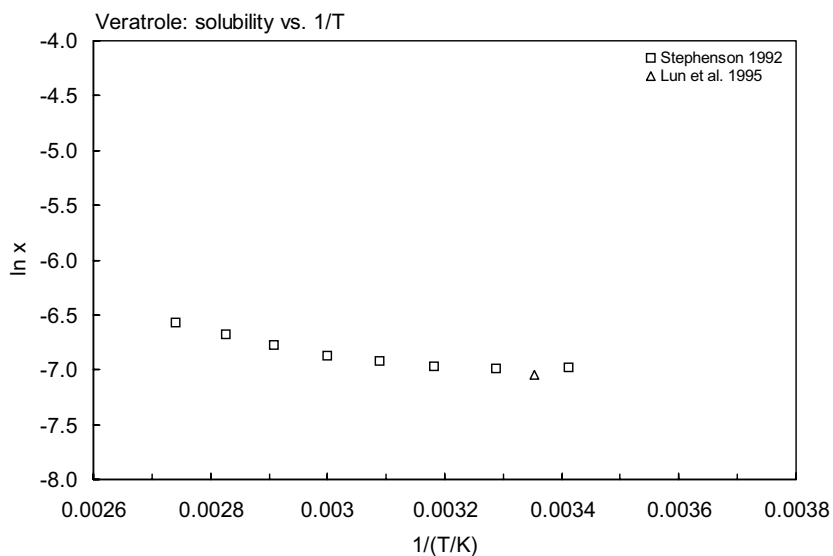
Sorption Partition Coefficient, $\log K_{\text{OC}}$:

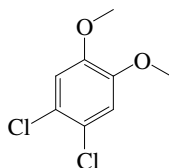
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.3.11.1**Reported aqueous solubilities of veratrole at various temperatures**

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
19.9	7160
31	7060
41.1	7230
50.6	7580
60.2	7940
70.6	8770
80.7	9700
91.8	10730

**FIGURE 10.1.3.11.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for veratrole.

10.1.3.12 4,5-Dichloroveratrole

Common Name: 4,5-dichloroveratrole

Synonym:

Chemical Name:

CAS Registry No: 2772-46-5

Molecular Formula: $C_8H_8Cl_2O_2$, $C_6H_2Cl_2(OCH_3)_2$

Molecular Weight: 207.054

Melting Point ($^{\circ}C$):

83 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

200.4 (Le-Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.27 (mp at $83^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

71.9 (shake flask-HPLC/UV, Lun et al. 1995)

72.6 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.11 (shake flask-GC/ECD, both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

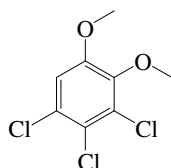
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.3.13 3,4,5-Trichloroveratrole



Common Name: 3,4,5-trichloroveratrole

Synonym:

Chemical Name:

CAS Registry No: 16766-29-3

Molecular Formula: $C_8H_7Cl_3O_2$, $C_6HCl_3(OCH_3)_2$

Molecular Weight: 241.499

Melting Point ($^{\circ}C$):

66 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

221.3 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.396 (mp at $66^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.50 (shake flask-GC, Neilson et al. 1984)

10.3 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.60, 5.25 (HPLC-RT correlation, calculated-solubility, Neilson et al. 1984)

4.01 (shake flask-GC/ECD, both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

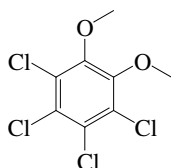
3.50, 3.30 (zebra fish, calculated, Neilson et al. 1984)

Sorption Partition Coefficient, $\log K_{oc}$:

3.20 (sediment, $K_p = 1.6 ml/(kg \text{ of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.3.14 Tetrachloroveratrole

Common Name: Tetrachloroveratrole

Synonym: 1,2,3,4-tetrachloro-5,6-dimethoxybenzene

Chemical Name: tetrachloroveratrole

CAS Registry No: 944-61-6

Molecular Formula: $C_8H_6Cl_4O_2$, $C_6Cl_4(OCH_3)_2$

Molecular Weight: 275.944

Melting Point ($^{\circ}C$):

90 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.23 (mp at $90^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.70 (shake flask-GC, Neilson et al. 1984)

1.59 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.80, 5.90 (HPLC-RT correlation, calculated-solubility, Neilson et al. 1984)

4.70 (Sarrikoski et al. 1986)

5.90 (Part et al. 1992, quoted, Sangster 1993)

4.86 (shake flask-GC/ECD both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.40, 4.50 (zebra fish, calculated, Neilson et al. 1984)

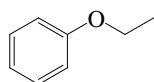
Sorption Partition Coefficient, $\log K_{oc}$:

3.45 (sediment, $K_p = 2.8$ $ml \cdot (kg \text{ of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.3.15 Phenetole



Common Name: Phenetole

Synonym: ethoxybenzene, ethyl phenyl ether

Chemical Name: ethoxybenzene, ethyl phenyl ether

CAS Registry No: 103-73-1

Molecular Formula: $C_8H_{10}O$, $C_6H_5-O-C_2H_5$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

-29.52 (Riddick et al. 1986)

-33.00 (Stephenson & Malanowski 1987)

-29.43 (Lide 2003)

Boiling Point ($^{\circ}C$):

169.84 (Riddick et al. 1986)

172.00 (Stephenson & Malanowski 1987)

169.81 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9651, 0.9605 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949; Riddick et al. 1986)

Molar Volume (cm^3/mol):

126.6 ($20^{\circ}C$, calculated-density)

150.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1160 (residual volume, Booth & Everson 1948)

550 (shake flask-AS, McGowan et al. 1966)

569 (shake flask-UV, Vesala 1974)

1114 (calculated- K_{OW} , Valvani et al. 1981)

1200 (selected, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($18^{\circ}C$, compiled and evaluated data, temp range $18-172^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.40281 - 1808.8/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

7605* ($91.89^{\circ}C$, ebulliometry, measured range $91.89-170^{\circ}C$, Dreisbach & Shrader 1949)

20441* ($117.43^{\circ}C$, ebulliometry, measured range $117.43-180.608^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.01980 - 1507.267/(194.357 + t/^{\circ}C)$; temp range $117.43-180.608^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 24.97404 - 3295.20/(T/K) - 5.53743 \cdot \log(T/K)$; temp range $117.43-180.608^{\circ}C$ (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)

204* (comparative ebulliometry-extrapolated, measured range $117.438-180.642^{\circ}C$, Ambrose et al. 1976)

$\log(P/kPa) = 6.14658 - 1509.276/\{(T/K) - 78.502\}$; temp range $391-454 K$ (Antoine eq., Ambrose et al. 1976)

$\log(P/kPa) = 6.17151 - 1529.38/(197.132 + t/^{\circ}C)$; temp range $91.89-170^{\circ}C$ (Antoine eq. derived from exptl data of Dreisbach & Martin 1949, Boublik et al. 1984)

$\log(P/kPa) = 6.14656 - 1508.583/(194.512 + t/^{\circ}C)$; temp range $117.4-180.68^{\circ}C$ (Antoine eq. derived reported exptl data of Collerson et al. 1965, Boublik et al. 1984)

204 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.14658 - 1509.276/(194.648 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.14524 - 1508.326/(-78.613 + T/\text{K})$; temp range 390–454 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -8.3543 - 2.7728 \times 10^3/(T/\text{K}) + 9.4482 \cdot \log (T/\text{K}) - 2.1842 \times 10^{-2} \cdot (T/\text{K}) + 1.1038 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 244–647 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

44.5 (calculated-P/C from selected data)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

2.51 (shake flask, Hansch & Leo 1979; 1987)

2.68 (HPLC- k' correlation, Haky & Young 1984)

2.51 (recommended, Sangster 1993)

2.51 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.3.15.1

Reported vapor pressures of phenetole at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1976	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
18.1	133.3	91.89	7605	117.432	20441	117.438	20441
43.7	666.6	95.6	8850	124.908	26526	124.918	26526
56.4	1333	98.84	10114	131.478	33024	131.49	33024
70.3	2666	111.56	16500	137.43	39978	137.445	39978
86.6	5333	139.17	42066	142.338	46566	142.355	46566
95.4	7999	155.16	67661	146.908	53454	146.927	53453
108.4	13332	170	101325	150.795	59940	150.816	59940
127.9	26664			154.432	66655	154.455	66570
149.8	53329			157.829	73278	157.853	73277
172	101325	Antoine eq. given by		160.982	79972	161.008	79972
		Dreisbach & Martin 1949		163.972	86762	163.999	86762
mp/°C	–30.2	eq. 2	P/mmHg	166.622	93152	166.65	93152
		A	7.40281	169.315	100033	169.344	100033
		B	1808.8	171.821	106789	171.852	106788
		C	230	174.19	113487	174.221	113486
				176.407	120058	176.439	120057
		bp/°C	170	178.511	126572	178.544	126571
		mp/°C	–29.52	180.608	133334	180.642	133334
						25	204

(Continued)

TABLE 10.1.3.15.1 (Continued)

Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1976	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				bp/°C	169.806		
				Antoine eq.		Antoine eq.	
				eq. 2	P/mmHg	eq. 2	P/kPa
				A	7.0198	A	6.14658
				B	1507.267	B	1509.276
				C	194.357	C	-78.502
				Kirchhoff eq.			
				eq. 4	P/mmHg	Coefficients of Chebyshev eq.	
				A	24.97404	also given in text.	
				B	3295.2		
				C	5.53743		
				$\Delta H_v/(\text{kJ mol}^{-1}) = 40.71$			

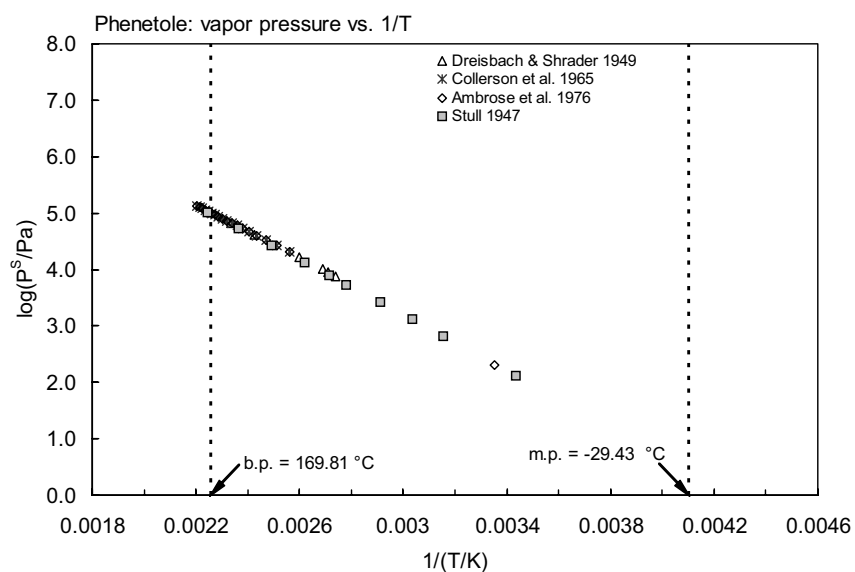
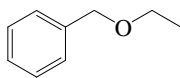


FIGURE 10.1.3.15.1 Logarithm of vapor pressure versus reciprocal temperature for phenetole.

10.1.3.16 Benzyl ethyl ether



Common Name: Benzyl ethyl ether

Synonym: (ethoxymethyl)benzene, α -ethoxytoluene

Chemical Name: benzyl ethyl ether, (ethoxymethyl)benzene, α -ethoxytoluene

CAS Registry No: 539-30-0

Molecular Formula: $C_9H_{12}O$, $C_6H_5CH_2-O-C_2H_5$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

185.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9490 (Weast 1982–83)

0.9478 (Dean 1985)

Molar Volume (cm^3/mol):

143.5 ($20^{\circ}C$, calculated-density)

172.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

135* (calculated-Antoine eq. regression, Stull 1947)

100 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.6496 - 1927.21/(230 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

135 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.92406 - 2133.29/(-24.38 + T/K)$; temp range 299–460 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 27.6421 - 3.4249 \times 10^3/(T/K) - 6.5804 \cdot \log(T/K) + 9.3417 \times 10^{-10} \cdot (T/K) + 1.0547 \times 10^{-6} \cdot (T/K)^2$; temp range 309–660 K (vapor pressure eq., Yaws 1994)

95.44* ($25.35^{\circ}C$, transpiration method, measured range 278.3–313.7 K, Krasnykh et al. 2002)

$\ln(P/Pa) = (305.859/R) - [79968.084/R(T/K)] - (88.80/R) \cdot \ln[(T/K)/298.15]$; temp range 278–313.7 K (transpiration method, Krasnykh et al. 2002)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.64 (calculated-f const. as per Rekker 1977, Hanai et al. 1981)

2.16 (Wang et al. 1987)

2.16 (recommended, Sangster 1993)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.3.16.1

Reported vapor pressures of benzyl ethyl ether at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Krasnykh et al. 2002			
summary of lit. data		transpiration method			
t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
26	133	278.3	19.44	298.6	95.44
52	666.6	278.7	19.59	300.1	105.16
65	1333	283.8	30.11	302.3	117.65
79.6	2666	285.1	35.31	303.2	128.09
95.4	5333	288.8	44.78	303.6	135.21
105.5	7999	290.2	52.97	307.4	177.63
118.9	13332	292.6	61.54	308.4	188.48
139.6	26664	293.7	65.53	310.2	223.55
161.5	53329	295.2	77.81	312.2	244.83
185	101325	297.3	88.33	313.7	259.37

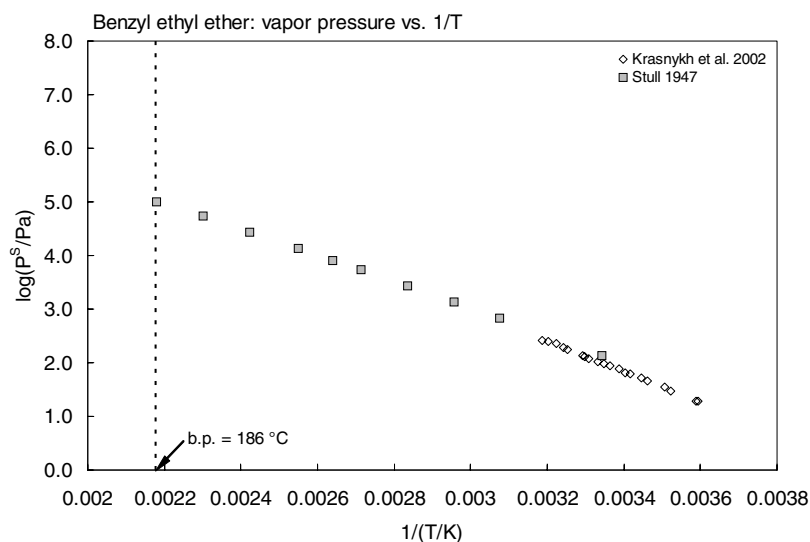
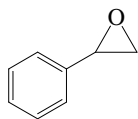


FIGURE 10.1.3.16.1 Logarithm of vapor pressure versus reciprocal temperature for benzyl ethyl ether.

10.1.3.17 Styrene oxide



Common Name: Styrene oxide

Synonym: (1,2-epoxyethyl)benzene, phenylepoxyethane

Chemical Name: (1,2-epoxyethyl)benzene, phenylepoxyethane, styrene oxide

CAS Registry No: 96-09-3

Molecular Formula: C_8H_8O

Molecular Weight: 120.149

Melting Point ($^{\circ}C$):

-35.6 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

194.1 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0523 ($16^{\circ}C$, Weast 1982–83; Dean 1985)

1.0500 (Verschueren 1983)

Molar Volume (cm^3/mol):

114.4 ($20^{\circ}C$, calculated-density)

136.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2800 (quoted, Verschueren 1983)

3020; 4570 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

40.0 (Verschueren 1983)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.84 (shake flask-HPLC, Pratesi et al. 1979)

1.51 (shake flask-GC, Serrentino et al. 1983)

1.61 (shake flask, Log P Database, Hansch & Leo 1987)

1.43 (Deneer et al. 1988)

1.61 (recommended, Sangster 1989, 1993)

1.51 (pH 7.5, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} = 12.3\text{--}123\text{ h}$, based on estimated photooxidation rate constant with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: rate constants $k = (434 \pm 12) \times 10^{-8}\text{ s}^{-1}$ at pH 7.25 and $k = (1690 \pm 620) \times 10^{-8}\text{ s}^{-1}$ at pH 7.3 in sediment pores both at $25^{\circ}C$ for water containing 0.1% w/w CH_2O as sterilant with 1-phenyl-1,2-ethanediol as major hydrolyzed product (Haag & Mill 1988);

$t_{1/2} = 0.00385\text{--}27.5$ h, based on an estimation from measured first-order rate constants at 25°C, the hydrolysis half-lives at pH 5, 7 and 9 are 0.00385, 21.4 and 27.5 h (Haag & Mill 1988; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on biological screening test data (Schmidt-Bleek et al. 1982; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 12.3\text{--}123$ h, based on estimated photooxidation rate constant with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 0.00385\text{--}27.5$ h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

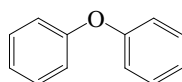
Ground water: $t_{1/2} = 0.00385\text{--}27.5$ h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 0.00385\text{--}27.5$ h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

Biota:

10.1.3.18 Diphenyl ether



Common Name: Diphenyl ether

Synonym: phenyl ether, diphenyl oxide, phenyl ether, 1,1'-oxybisbenzene, phenoxybenzene

Chemical Name: diphenyl ether, diphenyloxide, phenylether, phenoxybenzene

CAS Registry No: 101-84-8

Molecular Formula: $C_{12}H_{10}O$, $(C_6H_5)_2O$

Molecular Weight: 170.206

Melting Point ($^{\circ}C$):

26.87 (Lide 2003)

Boiling Point ($^{\circ}C$):

258 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0748 (Weast 1982–83)

Molar Volume (cm^3/mol):

158.6 ($20^{\circ}C$, calculated-density)

166.6 (Ruelle & Kesselring 1997)

195.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.217 (quoted, Riddick et al. 1986)

16.16 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.923 (mp $28.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4000 (shake flask-residue-volume, Booth & Everson 1948)

18.7 (shake flask-UV, Vesala 1974)

18.0 (shake flask-HPLC, Banerjee et al. 1980; Pearlman et al. 1984)

21.0 (Verschuereen 1983)

18, 3900 (quoted values, Riddick et al. 1986)

46.88 (supercooled liquid S_L , RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($66.1^{\circ}C$, summary of literature data, temp range 66.1 – $258.5^{\circ}C$, Stull 1947)

10.01* ($40^{\circ}C$, dynamic method, measured range 40 – $60^{\circ}C$, Bent & Francel 1948)

$\log(P/mmHg) = 9.6842 - 3351.9/(t/^{\circ}C + 273.1)$; measured range 40 – $60^{\circ}C$ (dynamic method-gas saturation, Bent & Francel 1948)

$\log(P/mmHg) = 7.65339 - 2330.5/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

26555* ($204.213^{\circ}C$, ebulliometry, measured range 204.2 – $270.9^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.06376 - 1261.455/(221.982 + t/^{\circ}C)$; temp range 204.2 – $270.9^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 19.48322 - 2328.0/(T/K) - 3.92657 \cdot \log(T/K)$; temp range 204.2 – $270.9^{\circ}C$ (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = [-0.2185 \times 12325.5/(T/K)] + 7.955679$; temp range 66.1 – $258.5^{\circ}C$ (Antoine eq., Weast 1972–73)

3.0* (“recomputed” reported data, temp range 204.257 – $271^{\circ}C$, Ambrose et al. 1976)

$\log(P/kPa) = 6.13913 - 1802.984/\{(T/K) - 95.013\}$; temp range 477 – $544\ K$ (Antoine eq., Ambrose et al. 1976)

2.67 (Verschuereen 1983)

1.82 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.01104 - 1799.712/(177.744 + t/^{\circ}C)$; temp range 204 – $270^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.13606 - 1799.811/(177.756 + t/^{\circ}\text{C})$; temp range 204.2–271 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.01104 - 1799.71/(177.74 + t/^{\circ}\text{C})$; temp range: 204–271 $^{\circ}\text{C}$ (Antoine eq., Dean 1985, 1992)
2.84 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.13913 - 1902.984/(178.137 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
2.93 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{kPa}) = 8.7109 - 3351.9/(T/\text{K})$; temp range 313–333K (Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log (P/\text{kPa}) = 6.1553 - 1800.743/(T/\text{K} - 95.275)$; temp range 477–544K (Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -26.9635 - 2.5909 \times 10^3/(T/\text{K}) + 16.42 \cdot \log (T/\text{K}) - 2.4334 \times 10^{-2} \cdot (T/\text{K}) + 1.0244 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 300–763 K (vapor pressure eq., Yaws 1994)

2.40 (P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$):

25.1 (calculated-P/C using selected data)

8.71 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.21, 4.36 (shake flask values, Leo et al. 1971)

4.20 (shake flask-GC, Chiou et al. 1977)

4.25 (calculated-fragment const., Rekker 1977)

4.26 (Hansch & Leo 1979)

4.08 (shake flask-HPLC, Banerjee et al. 1980)

3.79 (estimated-HPLC/MS correlation, Burkhard et al. 1985)

4.24 (calculated-f const., Burkhard et al. 1985)

3.87 (HPLC-RT correlation, Eadsforth 1986)

4.28 (shake flask, Log P Database, Hansch & Leo 1987)

4.21 (recommended, Sangster 1989, 1993)

3.949, 4.014 (shake flask method, Brooke et al. 1990)

4.21 (recommended, Hansch et al. 1995)

3.97 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

6.42 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log \text{BCF}$:

2.29 (rainbow trout, calculated, Veith et al. 1979)

2.29; 2.89 (quoted exptl., calculated- K_{OW} , Mackay 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

3.29; 3.41 (soil, quoted exptl.; calculated-MCI χ , Meylan et al. 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 5.5 \text{ h}^{-1}$, $k_2 = 0.0275 \text{ h}^{-1}$ (trout, Hawker & Connell 1985)

$1/k_2 = 36 \text{ h}$ (trout, Hawker & Connell 1988)

$k_2 = 0.676 \text{ h}^{-1}$ (fish, quoted, Thomann 1989)

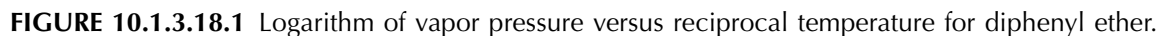
Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.3.18.1

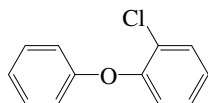
Reported vapor pressures of diphenyl ether at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)			
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)			
log P = A – B/(C + T/K)		(3)						
log P = A – B/(T/K) – C·log (T/K)		(4)						
Stull 1947		Bent & Francel 1948		Collerson et al. 1965		Ambrose et al. 1976		
summary of lit. data		dynamic method		ebulliometry		comparative ebulliometry		
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	
66.1	133.3	40	10.01	204.13	26555	204.257	26555	
97.8	666.6	50	21.96	212.102	33073	212.15	33074	
114	1333	60	43.97	219.226	40022	219.276	40022	
130.8	2666			225.105	46611	225.157	46611	
150	5333	eq. 2	P/mmHg	230.561	53482	230.616	53481	
162	7999	A	9.5842	235.186	59915	235.242	59915	
178.8	13332	B	3351.9	239.618	66654	239.676	66654	
203	26664	C	273.1	243.667	73327	243.726	73327	
230.7	53329			250.991	86741	247.473	79956	
258.5	101325	ΔH _v = 64.02 kJ/mol		254.089	92971	251.052	86740	
				257.458	100143	254.152	92971	
mp/°C	27			260.469	106906	257.522	100144	
				263.29	113569	260.534	106906	
				268.939	120124	263.355	113568	
		Dreisbach & Shrader 1949		268.416	126525	266.005	120124	
		ebulliometry		270.949	133333	268.482	126525	
		No data				271.015	133332	
				bp/°C	257.997	25	3	
		Antoine eq. given by		Antoine eq.				
		Dreisbach & Martin 1949		eq. 2	P/mmHg	bp	531.21 K	
		eq. 2	P/mmHg	A	7.01188	Antoine equation:		
		A	7.65339	B	1800.415		eq. 3	P/kPa
		B	2330.5	C	177.826		A	6.12913
		C	230	Kirchhoff eq.			B	1802.984
				eq. 4	P/mmHg	C	–95.013	
		bp/°C	258.31	A	24.66548	Coefficients of Chebyshev eq. also given in text.		
		mp/°C	26.9	B	3897.5			
				C	5.30117			
				ΔH _v = 48.62 kJ/mol				



10.1.4 POLYCHLORINATED DIPHENYL ETHERS (PCDEs)

10.1.4.1 2-Chlorodiphenyl ether (PCDE-1)



Common Name: 2-Chlorodiphenyl ether

Synonym: 2-CDPE, PCDE-1, 2-chlorobiphenyl ether

Chemical Name: 2-chlorodiphenyl ether

CAS Registry No: 2689-07-8

Molecular Formula: $C_{12}H_9ClO$

Molecular Weight: 204.652

Melting Point ($^{\circ}C$):

45 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

216.5 (calculated-Le Bas method at normal boiling point)

179.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.634 (mp at $45^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.40; 4.80 (quoted exptl.; calculated-molar volume and MP, Ruelle & Kesselring 1997)

3.40 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.537 (P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

32.36 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.45 (HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

6.33 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Photolysis: photolysis rate $k_p = 0.0035$ d^{-1} with a half-life of 200 d in summer sunlight; $k_p(exptl) = 3.4 \times 10^{-8}$ s^{-1} with $t_{1/2} = 240$ h, $k_p(calc) = 3.1 \times 10^{-9}$ s^{-1} in winter sunlight, at $40^{\circ}C$ in surface waters (Dulin et al. 1986)

Half-Lives in the Environment:

Air:

Surface water: photolysis $t_{1/2} = 200$ d in summer sunlight and $t_{1/2} = 240$ d in winter sunlight at $40^{\circ}C$ in surface waters (Dulin et al. 1986)

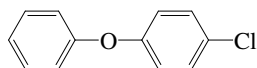
Ground water:

Sediment:

Soil:

Biota: $t_{1/2} = 4-63$ d in trout Cl_1 -DPEs to Cl_4 -DPEs (Niimi et al. 1994).

10.1.4.2 4-Chlorodiphenyl ether



Common Name: 4-Chlorodiphenyl ether

Synonym: 4-chlorophenyl phenyl ether, 1-chloro-4-phenoxybenzene, p-chlorophenyl phenyl ether, 4-chlorodiphenyl ether, monochlorodiphenyl oxide

Chemical Name: 4-chlorophenyl phenyl ether, 4-chlorodiphenyl ether

CAS Registry No: 7005-72-3

Molecular Formula: $C_{12}H_9ClO$

Molecular Weight: 204.652

Melting Point ($^{\circ}C$):

−6.0 (Callahan et al. 1979)

−8.0 (Mabey et al. 1982)

Boiling Point ($^{\circ}C$):

284.5 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2026 ($15^{\circ}C$, Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

216.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.30 (Branson 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

59.04 (Isnard & Lambert 1988,1989)

Vapor Pressure (Pa at $25^{\circ}C$):

0.360 (calculated, Branson 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$ or as indicated):

22.19 (calculated-P/C, Mabey et al. 1982)

22.29 (20 – $25^{\circ}C$ and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)

24.79 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.08 (Branson 1977; quoted, Callahan et al. 1979; Ryan et al. 1988; Isnard & Lambert 1988,1989)

5.079 (calculated, Mabey et al. 1982)

Bioconcentration Factor, $\log BCF$:

2.867 (rainbow trout muscle, Branson 1977; quoted, Callahan et al. 1979)

4.255 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)

2.87 (quoted, Isnard & Lambert 1988)

Sorption Partition Coefficient, $\log K_{oc}$:

4.763 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolysis rate $k_p = 0.19 d^{-1}$ with $t_{1/2} = 3.6 d$ in summer sunlight; $k_p(exptl) < 2.0 \times 10^{-8} s^{-1}$ with $t_{1/2} > 400 h$, $k_p(calc) = 3.7 \times 10^{-8} s^{-1}$ in winter sunlight, both at $40^{\circ}C$ in surface waters (Dulin et al. 1986)

Oxidation: $k \ll 360 M^{-1} h^{-1}$ for singlet oxygen and $k \ll 1.0 M^{-1} h^{-1}$ for peroxy radical (Mabey et al. 1982)

Hydrolysis:

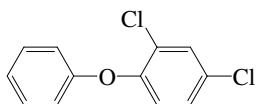
Biodegradation: $t_{1/2} = 4.0$ h, measured only in activated sludge (Branson 1978; quoted, Callahan et al. 1979).

Biotransformation: estimated rate constant $k = 1 \times 10^{-7}$ mL cell⁻¹ h⁻¹ for bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: photolysis $t_{1/2} = 3.6$ d summer sunlight and $t_{1/2} > 400$ d in winter sunlight at 40° L surface waters (Dulin et al. 1986)

10.1.4.3 2,4-Dichlorodiphenyl ether (PCDE-8)

Common Name: 2,4-Dichlorodiphenyl ether

Synonym: 2,4-DCDPE, PCDE-8

Chemical Name:

CAS Registry No: 51892-26-3

Molecular Formula: $C_{12}H_8Cl_2O$

Molecular Weight: 239.097

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

237.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.605 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.123 (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.25 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.62 (Oliver & Niimi 1984)

4.93 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.60 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

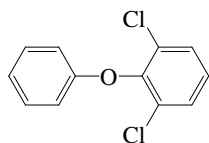
3.97 (rainbow trout, Oliver & Niimi 1984)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 3\text{--}63\ d$ for Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.4 2,6-Dichlorodiphenyl ether (PCDE-10)

Common Name: 2,6-Dichlorodiphenyl ether

Synonym: 2,6-DCDPE, PCDE-10

Chemical Name:

CAS Registry No: 28419-69-4

Molecular Formula: $C_{12}H_8Cl_2O$

Molecular Weight: 239.097

Melting Point ($^{\circ}C$):

39 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

237.4 (calculated-Le Bas method at normal boiling point)

192.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.729 (mp at $39^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.08; 0.213 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

2.08 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.174 (supercooled liquid P_L , GC-RI correlation, Kurz & Kesselring 1997)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

19.95 (calculated-P/C, Kurz & Kesselring 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.64 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

6.73 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

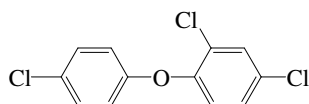
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 4-63$ d Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.5 2,4,4'-Trichlorodiphenyl ether (PCDE-28)



Common Name: 2,4,4'-Trichlorodiphenyl ether

Synonym: 2,4,4'-TCDPE, PCDE-28

Chemical Name: 2,4,4'-trichlorodiphenyl ether

CAS Registry No: 59030-21-3

Molecular Formula: $C_{12}H_7Cl_3O$

Molecular Weight: 273.543

Melting Point ($^{\circ}C$):

oil (Navalainen et al. 1994)

40 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

258.3 (calculated-Le Bas method at normal boiling point)

205.3 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.712 (mp at $40^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.102; 0.0385 (quoted exptl.; calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.101 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0204 (supercooled liquid P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

33.88 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.53 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.19 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.98; 3.36 (concn of 2,4,4'-trichloro-DPE 39.3; 118 $\mu g/L$, juvenile Atlantic salmon, 96-h exposure, Zitko & Carson 1977)

Sorption Partition Coefficient, $\log K_{OC}$:

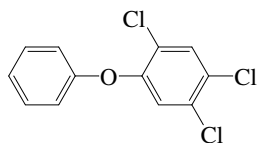
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 235$ h following uptake from water, excretion $t_{1/2} = 15$ d following uptake from food for Juvenile salmon (Zitko & Carson 1977);

average $t_{1/2} = 15$ d in salmon for trichloro-DPE congeners; biological $t_{1/2} = 63$ d (range 46–104 d) in rainbow trout (average value for trichlorodiphenyl ethers (Niimi 1986);

$t_{1/2} = 4$ –63 d Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.6 2,4,5-Trichlorodiphenyl ether (PCDE-29)

Common Name: 2,4,5-Trichlorodiphenyl ether

Synonym: 2,4,5-TCDPE, PCDE-29

Chemical Name: 2,4,5-trichlorodiphenyl ether

CAS Registry No: 52322-80-2

Molecular Formula: $C_{12}H_7Cl_3O$

Molecular Weight: 273.543

Melting Point ($^{\circ}C$):

oil (Opperhuizen & Voors 1987)

61 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

258.3 (calculated-Le Bas method at normal boiling point)

205.3 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.443 (mp at $61^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.050 (Opperhuizen 1986)

0.072; 0.0486 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.072 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0288 (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

112.2 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.0 (estimated, Opperhuizen 1986)

5.44 (Opperhuizen & Voors 1987; quoted, Niimi et al. 1994)

5.58 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

6.92 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.18 (guppy, 8-d exposure, Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Biotransformation: rate of metabolism $k = 0.27$ d^{-1} (guppy, 8-d exposure, Opperhuizen & Voors 1987)

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

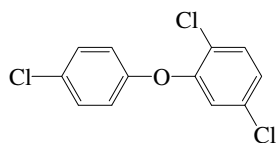
$k_1 > 5 \times 10^2$ d^{-1} (guppy, Opperhuizen 1986)

$k_1 = 1.5 \times 10^3$ mL g^{-1} d^{-1} (guppy, 8-d exposure, Opperhuizen & Voors 1987)

$k_2 = 0.34$ d^{-1} (guppy, elimination period 56 d, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: average excretion $t_{1/2} = 15$ d for trichloro-DPE congeners in salmon; biological $t_{1/2} = 63$ d in rainbow trout (average value for trichlorodiphenyl ethers, Niimi 1986);
 $t_{1/2} = 4\text{--}63$ d for Cl₁-DPEs to Cl₄-DPEs in trout (Niimi et al. 1994).

10.1.4.7 2,4',5-Trichlorodiphenyl ether (PCDE-31)

Common Name: 2,4',5-Trichlorodiphenyl ether

Synonym: 2,4',5-TCDPE, PCDE-31

Chemical Name: 2,4',5-trichlorodiphenyl ether

CAS Registry No: 65075-00-5

Molecular Formula: $C_{12}H_7Cl_3O$

Molecular Weight: 273.543

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

258.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0993 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0229 (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.31 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.66 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

5.70 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.25 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.30; 2.93 (ave. concn of 2,4',5-trichloro-DPE 2.37; 7.01 $\mu g/L$, juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, $\log K_{OC}$:

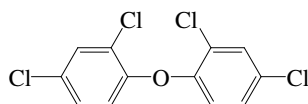
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 310\ h$ following uptake from water; $t_{1/2} = 26\ d$ following uptake from food for juvenile Atlantic salmon (Zitko & Carson 1976);

average excretion $t_{1/2} = 15\ d$ for trichloro-DPE congeners in salmon; biological $t_{1/2} = 63\ d$ in rainbow trout (average value for trichlorodiphenyl ethers, Niimi 1986);

$t_{1/2} = 4\text{--}63\ d$ Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.8 2,2',4,4'-Tetrachlorodiphenyl ether (PCDE-47)

Common Name: 2,2',4,4'-Tetrachlorodiphenyl ether

Synonym: 2,2',4,4'-TCDPE, PCDE-47, 2,2',4,4'-tetrachlorobiphenyl ether, 2,2',4,4'-TCBP

Chemical Name: 2,2',4,4'-tetrachlorodiphenyl ether

CAS Registry No: 28076-73-5

Molecular Formula: $C_{12}H_6Cl_4O$

Molecular Weight: 307.988

Melting Point ($^{\circ}C$):

69–70 (Navalainen et al. 1994)

69 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

279.2 (calculated-Le Bas method at normal boiling point)

218.2 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.366 (mp at $69.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0466; 0.0154 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.0466 (supercooled liquid, RP-HPLC-RI, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00525 (P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

34.67 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.95 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{AO}$:

7.80 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

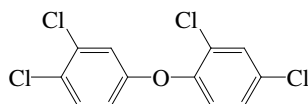
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: average excretion $t_{1/2} = 55$ d in salmon for tetrachloro-DPE congeners; mean biological $t_{1/2} = 119$ d (range 82–213 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 4$ –63 d for Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.9 2,3',4,4'-Tetrachlorodiphenyl ether (PCDE-66)

Common Name: 2,3',4,4'-Tetrachlorodiphenyl ether

Synonym: 2,3',4,4'-DCPE, PCDE-66

Chemical Name: 2,3',4,4'-tetrachlorodiphenyl ether

CAS Registry No: 61328-46-9

Molecular Formula: $C_{12}H_6Cl_4O$

Molecular Weight: 307.988

Melting Point ($^{\circ}C$):

oil (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

279.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0308 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00407 (supercooled liquid P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

40.74 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.13 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{AO}$:

7.91 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.43; 3.01 (ave. concn of 2,3',4,4'-tetrachloro-DPE 2.07; 6.03 $\mu g/L$, juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

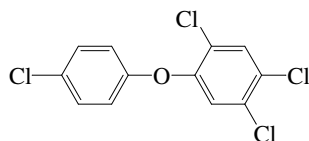
Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 370$ h following uptake from water, $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1976);

average excretion $t_{1/2} = 55$ d in salmon for tetrachloro-DPE congeners; mean biological $t_{1/2} = 119$ d (range 82–213 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 4$ –63 d in trout for Cl_1 -DPEs to Cl_4 -DPEs (Niimi et al. 1994).

10.1.4.10 2,4,4',5-Tetrachlorodiphenyl ether (PCDE-74)



Common Name: 2,4,4',5-Tetrachlorodiphenyl ether

Synonym: 2,4,4',5-PCDE, PCDE-74

Chemical Name: 2,4,4',5-tetrachlorodiphenyl ether

CAS Registry No: 61328-45-8

Molecular Formula: $C_{12}H_6Cl_4O$

Molecular Weight: 307.988

Melting Point ($^{\circ}C$):

62–63 (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

279.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0281 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

4.79×10^{-3} (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa· m^3/mol at $25^{\circ}C$):

52.48 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.99 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.66 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

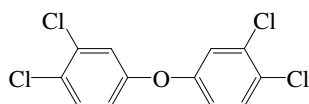
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for tetrachloro-DPE congeners (Zitko & Carson 1977; quoted, Niimi 1986); mean biological $t_{1/2} = 108$ d (range 62–407 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 4$ –63 d in trout for Cl_1 -DPEs to Cl_4 -DPEs; $t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.11 3,3',4,4'-Tetrachlorodiphenyl ether (PCDE-77)

Common Name: 3,3',4,4'-Tetrachlorodiphenyl ether

Synonym: 3,3',4,4'-PCDE, PCDE-77

Chemical Name: 3,3',4,4'-tetrachlorodiphenyl ether

CAS Registry No: 56348-72-2

Molecular Formula: $C_{12}H_6Cl_4O$

Molecular Weight: 307.988

Melting Point ($^{\circ}C$):

oil (Opperhuizen & Voors 1987)

69–71 (Navalainen et al. 1994)

70 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

279.2 (calculated-Le Bas method at normal boiling point)

218.2 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.362 (mp at $70^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.020 (Opperhuizen 1986)

0.0323; 0.00991 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.0323 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

2.57×10^{-3} (P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

24.55 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.0 (estimated, Opperhuizen 1986)

5.78 (Opperhuizen & Voors 1987; quoted, Niimi et al. 1994)

6.36 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.36 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.50 (guppy, 8-d exposure, Opperhuizen & Voors 1987)

4.51; 4.09 (guppy; trout muscle, Niimi et al. 1994)

4.46–4.99 (calculated- K_{OW} , Niimi et al. 1994)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 > 5 \times 10^2\ d^{-1}$ (Guppy, Opperhuizen 1986)

$k_1 = 9.6 \times 10^2 \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, 8-d exposure, Opperhuizen & Voors 1987)

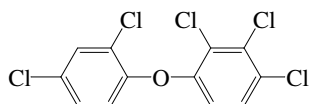
$k_2 = 0.03 \text{ d}^{-1}$ (guppy, elimination period 56 d, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: average $t_{1/2} = 55 \text{ d}$ in salmon for tetrachloro-DPE congeners (Zitko & Carson 1977; quoted, Niimi 1986)

mean biological $t_{1/2} = 134 \text{ d}$ (range 73–792 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 23 \text{ d}$ in guppy, $t_{1/2} = 29 \text{ d}$ in trout muscle (Niimi et al. 1994).

10.1.4.12 2,2',3,4,4'-Pentachlorodiphenyl ether (PCDE-85)

Common Name: 2,2',3,4,4'-Pentachlorodiphenyl ether

Synonym: PDCE-85

Chemical Name: 2,2',3,4,4'-pentachlorodiphenyl ether

CAS Registry No: 71585-37-0

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

65–67 (Navalainen et al. 1994)

66 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.396 (mp at $66^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0124; 0.00609 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.0124 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

6.92×10^{-4} (supercooled liquid P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

19.05 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.28 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.39 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

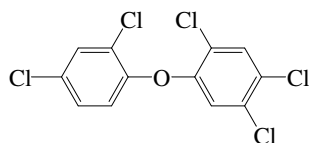
Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977; Niimi 1986)

biological $t_{1/2} \sim 113$ d (range 81–144 d, average value for pentachloro-DPE congeners, Niimi 1986);

$t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.13 2,2',4,4',5-Pentachlorodiphenyl ether (PCDE-99)



Common Name: 2,2',4,4',5-Pentachlorodiphenyl ether

Synonym: 2,2',4,4',5-PCDE, PCDE-99

Chemical Name: 2,2',4,4',5-pentachlorodiphenyl ether

CAS Registry No: 60123-64-0

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

oil (Navalainen et al. 1994)

25 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (calculated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

1.0 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

5.06×10^{-3} ; 0.0153 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

8.406×10^{-3} (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.392 - 866.2/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.35×10^{-3} (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

1.34×10^{-3} ; 1.34×10^{-3} (liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 11.90 - 4404/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.95 - 3525/(T/K)$ (liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

54.95 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 10.34 - 2659/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.38 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.46, 7.20 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.03 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.15; 2.77 (4.01; 12.0 $\mu g/L$, ave. concn of 2,2',4,4',5-PCDPE (reported as 2,2'4',5-TCDDPE), juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, $\log K_{OC}$:

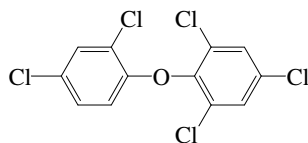
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 370$ h following uptake from water, $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1977);

average excretion $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners; mean biological $t_{1/2} = 144$ d (range 93–311 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.14 2,2',4,4',6-Pentachlorodiphenyl ether (PCDE-100)

Common Name: 2,2',4,4',6-Pentachlorodiphenyl ether

Synonym: 2,2',4,4',6-PCDE, PCDE-100

Chemical Name: 2,2',4,4',6-pentachlorodiphenyl ether

CAS Registry No: 104294-16-8

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

45–46 (Navalainen et al. 1994)

46 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (calculated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

1.0 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

0.0160 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.392 - 943.0/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.19×10^{-3} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

2.17×10^{-3} ; 1.34×10^{-3} (liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 11.90 - 4408/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.95 - 3467/(T/K)$ (liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

46.77 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 10.34 - 2524/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.11 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.11, 6.31 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.83 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B :

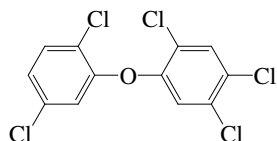
Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

- Biota: excretion $t_{1/2} = 370$ h following uptake from water, $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1977);
- average excretion $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners; mean biological $t_{1/2} = 144$ d (range 93–311 d) in rainbow trout (Niimi 1986);
- $t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.15 2,2',4,5,5'-Pentachlorodiphenyl ether (PCDE-101)



Common Name: 2,2',4,5,5'-Pentachlorodiphenyl ether

Synonym: PDCE-101

Chemical Name: 2,2',4,5,5'-pentachlorodiphenyl ether

CAS Registry No: 131138-21-1

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

oil (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00943; 0.0153 (quoted exptl.; calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.00943 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

1.74×10^{-3} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

63.10 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.22 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.81 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

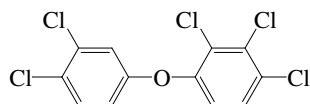
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 370$ d following uptake from water; $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1976);
average $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977; Niimi 1986);
biological $t_{1/2} = 113$ d (range 81–144 d) in rainbow trout (average value of pentachloro-DPE, Niimi 1986);
 $t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.16 2,3,3',4,4'-Pentachlorodiphenyl ether (PCDE-105)

Common Name: 2,3,3',4,4'-Pentachlorodiphenyl ether

Synonym: PCDE-105

Chemical Name: 2,3,3',4,4'-pentachlorodiphenyl ether

CAS Registry No: 85918-31-6

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 324.433

Melting Point ($^{\circ}C$):

64–66 (Navalainen et al. 1994)

65 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.405 (mp at $65^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00732; 0.0059 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.00732 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

5.13×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

23.99 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.51 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.52 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

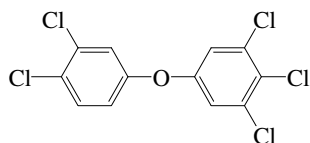
Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977, Niimi 1986)

biological $t_{1/2} \sim 113$ d (range 81–144 d) in rainbow trout (average value for pentachloro-DPE congeners, Niimi 1986);

$t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.17 3,3',4,4',5-Pentachlorodiphenyl ether (PCDE-126)



Common Name: 3,3',4,4',5-Pentachlorodiphenyl ether

Synonym: PCDE-126

Chemical Name: 3,3',4,4',5-pentachlorodiphenyl ether

CAS Registry No: 94339-59-0

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

68–70 (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.93×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

5.62×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

100 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.83 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

6.88 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.22 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

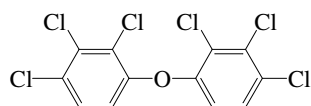
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977, Niimi 1986)

biological $t_{1/2} \sim 113$ d (range 81–144 d) in rainbow trout (average value for pentachloro-DPE congeners, Niimi 1986);

$t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.18 2,2',3,3',4,4'-Hexachlorodiphenyl ether (PCDE-128)

Common Name: 2,2',3,3',4,4'-Hexachlorodiphenyl ether

Synonym: PCDE-128

Chemical Name: 2,2',3,3',4,4'-hexachlorodiphenyl ether

CAS Registry No: 71585-39-2

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

141–142 (Navalainen et al. 1994)

95 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.206 (mp at $95^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.73×10^{-3} ; 4.33×10^{-4} (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

2.73×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

8.71×10^{-5} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

12.02 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.82 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.13 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

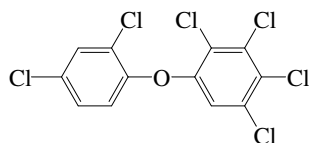
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: biological $t_{1/2} > 170\ d$ (range 100 to $> 300\ d$) in rainbow trout (average value for hexachloro-DPE congeners, Niimi 1986)

10.1.4.19 2,2',3,4,4',5-Hexachlorodiphenyl ether (PCDE-137)



Common Name: 2,2',3,4,4',5-Hexachlorodiphenyl ether

Synonym: PCDE-137

Chemical Name: 2,2',3,4,4',5-hexachlorodiphenyl ether

CAS Registry No: 71585-36-9

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

78–80 (Navalainen et al. 1994)

69 (Ruelle & Kesselring 1997)

80 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.285 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.85×10^{-3} ; 2.18×10^{-3} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.61×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1043/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.0×10^{-4} (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

2.04×10^{-4} ; 5.80×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.17 - 4878/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.22 - 3837/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

54.95 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 11.09 - 2794/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.72 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

6.72, 6.83 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

7.11 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.37 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

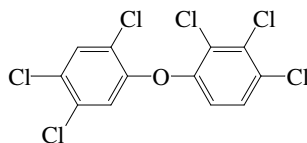
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 100$ d (range 69–179 d) in rainbow trout, mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.20 2,2',3,4,4',5'-Hexachlorodiphenyl ether (PCDE-138)



Common Name: 2,2',3,4,4',5'-Hexachlorodiphenyl ether

Synonym: PCDE-138

Chemical Name: 2,2',3,4,4',5'-hexachlorodiphenyl ether

CAS Registry No: 71585-38-1

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

69–70 (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.359 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

1.84×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1014/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.70×10^{-4} (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

1.73×10^{-4} ; 6.23×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.15 - 4866/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.21 - 3854/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

34.67 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 11.08 - 2840/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.01 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.01, 6.77 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.86 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

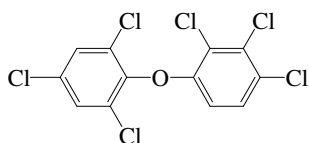
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 100$ d (range 69–179 d) in rainbow trout; mean $t_{1/2} > 170$ d (range 100 to >300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.21 2,2',3,4,4',6'-Hexachlorodiphenyl ether (PCDE-140)

Common Name: 2,2',3,4,4',6'-Hexachlorodiphenyl ether

Synonym: PCDE-140

Chemical Name: 2,2',3,4,4',6'-hexachlorodiphenyl ether

CAS Registry No: 106220-82-0

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

120–122 (Navalainen et al. 1994)

121 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.114 (mp at $121^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.99×10^{-3} ; 6.4×10^{-4} (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

2.99×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

2.69×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

33.88 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.76 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.51 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

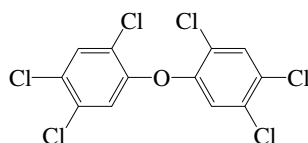
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 149$ d (range 99–302 d) in rainbow trout; mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.22 2,2',4,4',5,5'-Hexachlorodiphenyl ether (PCDE-153)



Common Name: 2,2',4,4',5,5'-Hexachlorodiphenyl ether

Synonym: PCDE-153

Chemical Name: 2,2',4,4',5,5'-hexachlorodiphenyl ether

CAS Registry No: 71859-30-8

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

113–115 (Navalainen et al. 1994)

114 (Ruelle & Kesselring 1997)

115 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.134 (mp at $114^{\circ}C$)

0.126 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

1.65×10^{-4} ; 7.52×10^{-4} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.65×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1047/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.47×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

3.74×10^{-4} ; 4.71×10^{-5} (quoted supercooled liquid P_L from Hinckley et al. 1998; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.19 - 4916/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.24 - 3771/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

79.43 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log (H/(Pa m^3/mol)) = 11.11 - 2724/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.72 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

6.72, 6.84 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.21 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, \log BCF or $\log K_B$:

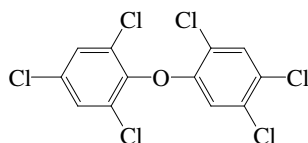
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 167$ d (range 98–553 d) in rainbow trout ; mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.23 2,2',4,4',5,6'-Hexachlorodiphenyl ether (PCDE-154)



Common Name: 2,2',4,4',5,6'-Hexachlorodiphenyl ether

Synonym: PCDE-154

Chemical Name: 2,2',4,4',5,6'-hexachlorodiphenyl ether

CAS Registry No: 106220-81-9

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

94–96 (Navalainen et al. 1994)

95 (Ruelle & Kesselring 1997)

96 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997); quoted Passivirta et al. 1999

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.206 (mp at $95^{\circ}C$)

0.198 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

3.44×10^{-3} ; 1.16×10^{-3} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

3.44×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1090/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

6.46×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

6.64×10^{-4} ; 1.32×10^{-4} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.10 - 4760/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.15 - 4465/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

70.79 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa\ m^3/mol)] = 11.02 - 2582/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.49 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

6.49, 6.93 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.03 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

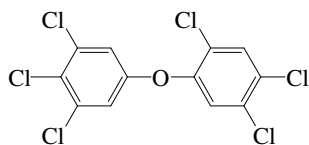
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 142$ d (range 90–330 d) in rainbow trout; mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.24 2,3',4,4',5,5'-Hexachlorodiphenyl ether (PCDE-167)



Common Name: 2,3',4,4',5,5'-Hexachlorodiphenyl ether

Synonym: PCDE-167

Chemical Name: 2,3',4,4',5,5'-hexachlorodiphenyl ether

CAS Registry No: 131138-20-0

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

104–105 (Navalainen et al. 1994)

84 (Ruelle & Kesselring 1997)

105 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997; quoted Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F :

0.161 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

7.18×10^{-4} ; 1.51×10^{-3} (quoted exptl., calculated-molar volume, MP and mobile order thermodynamics, Ruelle & Kesselring 1997)

7.18×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1117/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25 and reported temperature dependence equations $^{\circ}C$):

2.29×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

2.49×10^{-4} ; 4.0×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/Pa) = 12.20 - 4938/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.25 - 3822/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

120.23 (calculated-P/C, Kurz & Ballschmiter 1997)

$\log [H/(Pa m^3/mol)] = 11.12 - 2705/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.11 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.11, 6.99 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.42 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

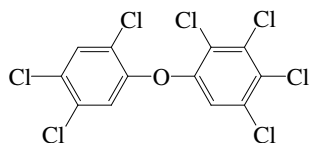
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} > 170$ d (range 100 to > 300 d) in rainbow trout for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.25 2,2',3,4,4',5,5'-Heptachlorodiphenyl ether (PCDE-180)



Common Name: 2,2',3,4,4',5,5'-Heptachlorodiphenyl ether

Synonym: PCDE-180

Chemical Name: 2,2',3,4,4',5,5'-heptachlorodiphenyl ether

CAS Registry No: 83992-69-2

Molecular Formula: $C_{12}H_3Cl_7O$

Molecular Weight: 411.324

Melting Point ($^{\circ}C$):

88–90 (Navalainen et al. 1994; quoted, Passivirta et al. 1999)

89 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

341.9 (calculated-Le Bas method at normal boiling point)

256.9 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.236 (mp at $89^{\circ}C$)

0.227 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

1.30×10^{-4} ; 4.83×10^{-4} (quoted exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.30×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -2.344 - 1073/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

6.31×10^{-6} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

5.14×10^{-5} ; 1.17×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.31 - 5117/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.36 - 4046/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

199.53 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 11.70 - 2973/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.46 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.46, 7.20 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

7.39 (GC-RT correlation, Hankenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.55 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B :

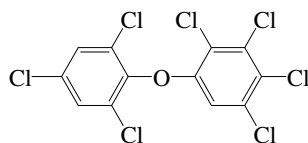
Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 146$ d (range 90–380 d) in rainbow trout; mean $t_{1/2} > 300$ d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);
 $t_{1/2} = 6$ –13 d for Cl₇-DPEs to Cl₇-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.26 2,2',3,4,4',5,6'-Heptachlorodiphenyl ether (PCDE-182)



Common Name: 2,2',3,4,4',5,6'-Heptachlorodiphenyl ether

Synonym: PCDE-182

Chemical Name: 2,2',3,4,4',5,6'-heptachlorodiphenyl ether

CAS Registry No: 88467-63-4

Molecular Formula: $C_{12}H_3Cl_7O$

Molecular Weight: 411.324

Melting Point ($^{\circ}C$):

136–138 (Navalainen et al. 1994)

136 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

341.9 (calculated-Le Bas method at normal boiling point)

256.9 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.076 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

$\log [S_L/(mol/L)] = -2.344 - 1215/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.01×10^{-4} ; 7.66×10^{-6} (supercooled liquid P_L , GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.35 - 5188/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.49 - 3976/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

$\log [H/(Pa \cdot m^3/mol)] = 11.74 - 2761/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.50 (calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

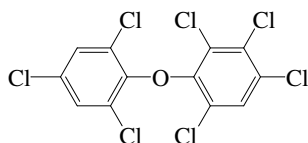
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean $t_{1/2} > 300$ d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);

$t_{1/2} = 6$ –13 d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.27 2,2',3,4,4',6,6'-Heptachlorodiphenyl ether (PCDE-184)



Common Name: 2,2',3,4,4',6,6'-Heptachlorodiphenyl ether

Synonym: PCDE-184

Chemical Name: 2,2',3,4,4',6,6'-heptachlorodiphenyl ether

CAS Registry No: 106220-84-2

Molecular Formula: $C_{12}H_3Cl_7O$

Molecular Weight: 411.324

Melting Point ($^{\circ}C$):

142 (calculated, Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

341.9 (calculated-Le Bas method at normal boiling point)

256.9 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.080 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

$\log [S_L/(mol/L)] = -2.344 - 1227/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.32×10^{-4} ; 1.06×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.73 - 5858/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.78 - 4633/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

$\log [H/(Pa \cdot m^3/mol)] = 12.12 - 3406/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.53 (calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

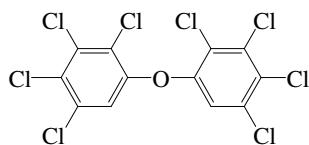
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean $t_{1/2} > 300$ d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);

$t_{1/2} = 6-13$ d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.28 2,2',3,3',4,4',5,5'-Octachlorodiphenyl ether (PCDE-194)



Common Name: 2,2',3,3',4,4',5,5'-Octachlorodiphenyl ether

Synonym: PCDE-194

Chemical Name: 2,2',3,3',4,4',5,5'-octachlorodiphenyl ether

CAS Registry No:

Molecular Formula: $C_{12}H_2Cl_8O$

Molecular Weight: 445.769

Melting Point ($^{\circ}C$):

125–128 (Navalainen et al. 1994)

126 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

362.8 (calculated-Le Bas method at normal boiling point)

269.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.102 (mp at $126^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.30×10^{-5} ; 7.57×10^{-5} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

3.30×10^{-5} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

1.74×10^{-5} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

234.42 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.78 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.80 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

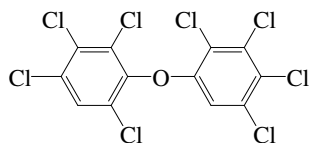
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 6 - 13$ d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.29 2,2',3,3',4,4',5,6'-Octachlorodiphenyl ether (PCDE-196)



Common Name: 2,2',3,3',4,4',5,6'-Octachlorodiphenyl ether

Synonym: PCDE-196

Chemical Name: 2,2',3,3',4,4',5,6'-octachlorodiphenyl ether

CAS Registry No: 85918-38-3

Molecular Formula: $C_{12}H_2Cl_8O$

Molecular Weight: 445.769

Melting Point ($^{\circ}C$):

147–149 (Navalainen et al. 1994)

149 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

362.8 (calculated-Le Bas method at normal boiling point)

269.8 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.0595 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

$\log [S_L/(mol/L)] = -2.819 - 1247/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

8.86×10^{-6} ; 5.27×10^{-6} (supercooled liquid P_L , GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.57 - 5586/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.62 - 4341/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

$\log [H/(Pa \cdot m^3/mol)] = 12.44 - 3094/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.88 (calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

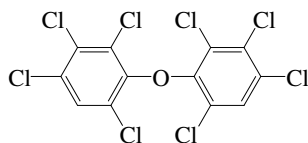
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 6 - 13$ d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.30 2,2',3,3',4,4',6,6'-Octachlorodiphenyl ether (PCDE-197)



Common Name: 2,2',3,3',4,4',6,6'-Octachlorodiphenyl ether

Synonym: PCDE-197

Chemical Name: 2,2',3,3',4,4',6,6'-octachlorodiphenyl ether

CAS Registry No: 117948-62-6

Molecular Formula: $C_{12}H_2Cl_8O$

Molecular Weight: 445.769

Melting Point ($^{\circ}C$):

124–126 (Navalainen et al. 1994)

126 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

362.8 (calculated-Le Bas method at normal boiling point)

269.8 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56.6 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F :

0.100 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

$\log [S_L/(mol/L)] = -2.819 - 1179/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.75×10^{-5} ; 1.75×10^{-6} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/Pa) = 12.47 - 5405/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.52 - 4228/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

$\log [H/(Pa\ m^3/mol)] = 12.34 - 3049/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.73 (calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

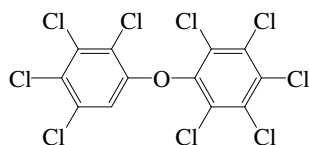
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 6 - 13\ d$ for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.31 2,2',3,3',4,4',5,5',6-Nonachlorodiphenyl ether (PCDE-206)

Common Name: 2,2',3,3',4,4',5,5',6-Nonachlorodiphenyl ether

Synonym: PCDE-206

Chemical Name: 2,2',3,3',4,4',5,5',6-nonachlorodiphenyl ether

CAS Registry No: 83992-73-8

Molecular Formula: $C_{12}HCl_9O$

Molecular Weight: 480.214

Melting Point ($^{\circ}C$):

176–177 (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

383.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.704×10^{-6} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

6.92×10^{-6} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1949.84 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.07 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.08 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

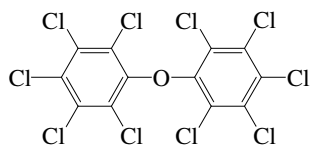
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 6 - 13$ d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.32 Decachlorodiphenyl ether (PCDE-209)



Common Name: Decachlorodiphenyl ether

Synonym: PCDE-209

Chemical Name: decachlorodiphenyl ether

CAS Registry No: 31710-30-2

Molecular Formula: $C_{12}Cl_{10}O$

Molecular Weight: 514.659

Melting Point ($^{\circ}C$):

220–222 (Navalainen et al. 1994)

131 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

404.6 (calculated-Le Bas method at normal boiling point)

295.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.64×10^{-8} ; 1.13×10^{-9} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

5.64×10^{-8} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

1.58×10^{-6} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

14125 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.16 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.40 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

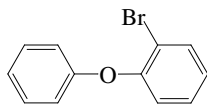
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 46\ d$ (range 27–164 d) in rainbow trout (Niimi 1986)

10.1.5 BROMINATED DIPHENYL ETHERS

10.1.5.1 2-Bromodiphenyl ether (BDE-1)



Common Name: 2-Bromodiphenyl ether

Synonym: BDE-1, PBDE-1, 1-bromo-2-phenoxybenzene, 2-bromophenyl phenyl ether, *o*-bromophenyl phenyl ether

Chemical Name: 2-monobromodiphenyl ether

CAS Registry No: 7025-06-1

Molecular Formula: $C_{12}H_9BrO$

Molecular Weight: 249.103

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

218.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

63.7 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.163; 0.163 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -3327/(T/K) + 10.37$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.24; 7.34 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: first-order degradation $t_{1/2} = 50$ h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first-order degradation $t_{1/2} = 900$ h (estimated by EPIWIN, Wania & Dugani 2003)

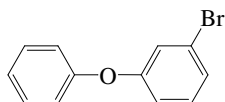
Ground water:

Sediment: first-order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first-order degradation $t_{1/2} = 900$ h (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

10.1.5.2 3-Bromodiphenyl ether (BDE-2)



Common Name: 3-Bromodiphenyl ether

Synonym: BDE-2, PBDE-2, 1-bromo-3-phenoxybenzene, *m*-bromophenyl phenyl ether, 3-bromophenyl phenyl ether, 3-phenoxybromobenzene, 3-phenoxyphenyl bromide, *m*-bromodiphenyl ether, *m*-phenoxybromobenzene, *m*-phenoxyphenyl bromide

Chemical Name: 3-monobromodiphenyl ether

CAS Registry No: 6876-00-2

Molecular Formula: C₁₂H₉BrO

Molecular Weight: 249.103

Melting Point (°C):

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):

218.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

65.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):

0.128; 0.125 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

log (P_L/Pa) = -3416/(T/K) + 10.56, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

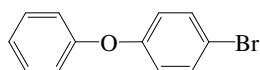
7.36; 7.44 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

10.1.5.3 4-Bromodiphenyl ether (BDE-3)

Common Name: 4-Bromophenyl phenyl ether

Synonym: BDE-3, PBDE-3, *p*-bromophenyl phenyl ether, 1-bromo-4-phenoxybenzene, 4-bromophenyl phenyl ether, 4-phenoxybromobenzene, 4-phenoxyphenyl bromide, *p*-bromodiphenyl ether, *p*-bromophenoxybenzene, *p*-phenoxybromobenzene, *p*-phenoxyphenyl bromide

Chemical Name: 4-bromodiphenyl ether, bromophenyl ether

CAS Registry No: 101-55-3

Molecular Formula: $C_{12}H_9BrO$, $C_6H_5-O-C_6H_4Br$

Molecular Weight: 249.103

Melting Point ($^{\circ}C$):

18.72 (Weast 1977, 1982–83)

18.0 (Dean 1985, 1992)

Boiling Point ($^{\circ}C$):

310.1 (Weast 1977, 1982–83)

305 (Dean 1985, 1992)

Density (g/cm^3 at $20^{\circ}C$):

1.423 (Dean 1985)

Molar Volume (cm^3/mol):

154.8 ($20^{\circ}C$, Stephenson & Malanowski 1987)

218.9 (calculated-Le Bas method at normal boiling point)

175.1 (calculated-density)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

47.9 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.80 (calculated- K_{ow} , Mabey et al. 1982)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.20 ($20^{\circ}C$, calculated, Dreisbach 1952; quoted, Callahan et al. 1979; Mabey et al. 1982)

$\log(P_L/kPa) = 5.80633 - 1683.84/(-140.25 + T/K)$, temp range 463–673 K, (Antoine eq., Stephenson & Malanowski 1987)

0.259 (supercooled liquid PL, GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -2503/(T/K) + 7.81$, (Clausius-Clapeyron eq. from GC-RT correlation measurement, Tittlemier et al. 2002)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated):

10.13 (20 – $25^{\circ}C$, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.28 (calculated as per Leo et al. 1971 using data of Branson 1977, Callahan et al. 1979; quoted, Ryan et al. 1988)

4.94 (calculated, Mabey et al. 1982)

5.24 (quoted, Van Leeuwen et al. 1992)

4.85 (estimated, Tittlemier et al. 2002)

Bioconcentration Factor, log BCF:

4.114 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC} :

4.623 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $\ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $\ll 1.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982).

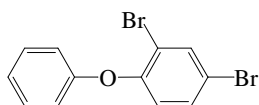
Hydrolysis:

Biodegradation: estimated half-life of 4.0 h in activated sludge, based on biodegradation of 4-chlorophenyl phenyl ether in activated sewage sludge (Branson 1978; quoted, Callahan et al. 1979).

Biotransformation: estimated rate constant of $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ for the bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

10.1.5.4 2,4-Dibromodiphenyl ether (BDE-7)

Common Name: 2,4-Dibromodiphenyl ether

Synonym: BDE-7, PBDE-7, 2,4-dibromo-1-phenoxybenzene

Chemical Name: 2,4-dibromodiphenyl ether

CAS Registry No: 171977-44-9

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

75.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0168; 0.0153 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -3941/(T/K) + 11.34$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.03 (for dibromodiphenyl ethers, RP-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.37; 8.36 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

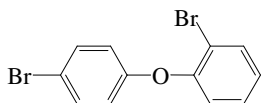
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.5 2,4'-Dibromodiphenyl ether (BDE-9)



Common Name: 2,4'-Dibromodiphenyl ether

Synonym: BDE-8, PBDE-8, 1-bromo-2-(4-bromophenoxy)-benzene

Chemical Name: 2,4'-dibromodiphenyl ether

CAS Registry No: 147217-71-8

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

76.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0137; 0.0124 (supercooled liquid P_L ; calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -3991/(T/K) + 11.42$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.03 (dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

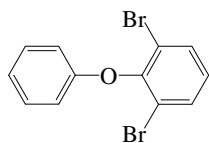
8.47; 8.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.6 2,6-Dibromodiphenyl ether (BDE-10)

Common Name: 2,6-Dibromodiphenyl ether

Synonym: BDE-10, PBDE-10, 1,3-dibromo-2-phenoxybenzene

Chemical Name: 2,6-dibromodiphenyl ether

CAS Registry No: 51930-04-2

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

73.1 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0277; 0.0256 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -3818/(T/K) + 11.25$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.03 (dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.12; 8.13 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

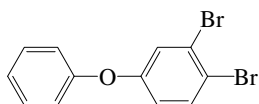
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.7 3,4-Dibromodiphenyl ether (BDE-12)



Common Name: 3,4-Dibromodiphenyl ether

Synonym: BDE-12, PBDE-12, 1,2-dibromo-4-phenoxybenzene

Chemical Name: 3,4-dibromodiphenyl ether

CAS Registry No: 189084-59-1

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0119; 0.107 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4020/(T/K) + 11.56$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

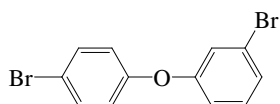
8.55; 8.52 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.8 3,4'-Dibromodiphenyl ether (BDE-13)

Common Name: 3,4'-Dibromodiphenyl ether

Synonym: BDE-13, PBDE-13, 1-bromo-3-(4-bromophenoxy)-benzene

Chemical Name: 3,4'-dibromodiphenyl ether

CAS Registry No: 83694-71-7

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.0 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0113; 0.0101 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4044/(T/K) + 11.62$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.57; 8.54 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

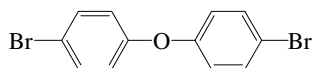
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.9 4,4'-Dibromodiphenyl ether (BDE-15)



Common Name: 4,4'-Dibromodiphenyl ether

Synonym: BDE-15, PBDE-15, 1,1-oxybis[4-bromo]benzene, bis(4-bromophenyl)ether, *p*, *p'*-dibromodiphenyl ether

Chemical Name: 4,4'-dibromodiphenyl ether

CAS Registry No: 2050-47-7

Molecular Formula: C₁₂H₈Br₂O

Molecular Weight: 327.999

Melting Point (°C):

57–58 (Tittlemier et al. 2002)

57.7 (Wania & Dugani 2003)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.0 (Wong et al. 2001)

67.7 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

0.477 (mp at 57.5°C, Wania & Dugani 2003)

Water Solubility (g/m³ or mg/L at 25°C):

0.130 (generator column-GC/ECD, Tittlemier et al. 2002)

0.273, 0.79 (supercooled S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

9.84 × 10⁻³; 8.80 × 10⁻³ (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

log (P_L/Pa) = -4074/(T/K) + 11.65, (GC-RT correlation, Wong et al. 2001)

0.0173 (supercooled liquid P_L, GC-RT correlation, Tittlemier et al. 2002)

log (P_L/Pa) = -3528/(T/K) + 10.08, (Clausius-Clapeyron equation from GC-RT correlation measurements, Tittlemier et al. 2002)

0.0143, 0.010 (supercooled, P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant (Pa·m³/mol at 25°C):

21 (calculated-P_L/C_L, Tittlemier et al. 2002)

4.11 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (value for dibromodiphenyl ether, Pijnenburg et al. 1995)

5.55 (estimated, Tittlemier et al. 2002)

5.03, 5.48 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

8.64; 8.60 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

8.79, 8.63 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photochemical degradation pathway of BDE15 undergoes strict debromination via first-order decay, $k = 1.98 \times 10^{-2} \text{ min}^{-1}$ in 100% CH_3CN and $k = 3.10 \times 10^{-2} \text{ min}^{-1}$ in CH_3OH , corresponding to $t_{1/2} \sim 30 \text{ min}$. (Rayne et al. 2003)

Photooxidation:

Hydrolysis:

Biodegradation: complete debromination under anaerobic microbial degradation in a fixed-film plug-flow bioreactor (Rayne et al. 2003)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 120 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 1440 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

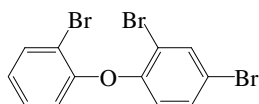
Ground water:

Sediment: first order degradation $t_{1/2} = 5760 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 1440 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

10.1.5.10 2,2',4-Tribromodiphenyl ether (BDE-17)



Common Name: 2,2',4-Tribromodiphenyl ether

Synonym: PBDE-17

Chemical Name: 2,2',4-tribromodiphenyl ether

CAS Registry No: 147217-75-2

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)

0.00219 (supercooled P_L , GC-RT correlation on a CPSil-8 column, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted range of value for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

9.30* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -3.54 + 3803/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

9.966, 9.385, 8.841, 8.332 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

9.919, 9.339, 8.789, 8.290 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.10.1

Reported octanol-air partition coefficients of 2,2',4-tribromodiphenyl ether (PBDE 17) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
		QRSETP* model 3	
15	9.777	15	9.966
25	9.27	25	9.385
35	8.901	35	8.841
45	8.517	45	8.332
25	9.3	QRSETP model 5	
		15	9.919
		25	9.339
		35	8.798
		45	9.29
log K _{OA} = A + B/(T/K)			
A	-3.45		
B	3803		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 72.8$			

Quantitative relationships between structures, environmental temperatures and properties.

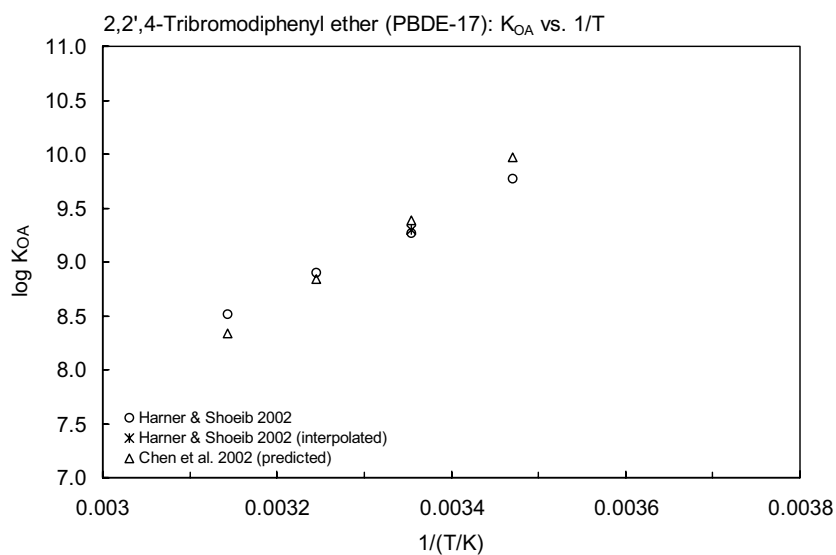
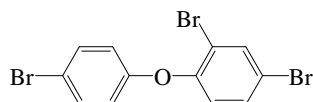


FIGURE 10.1.5.10.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4-tribromodiphenyl ether (PBDE-17).

10.1.5.11 2,4,4'-Tribromodiphenyl ether (BDE-28)



Common Name: 2,4,4'-Tribromodiphenyl ether

Synonym: PBDE-28, 2,4-dibromo-1-(4-bromophenoxy)-benzene, p-bromophenyl 2,4-dibromophenyl ether

Chemical Name: 2,4,4'-tribromodiphenyl ether

CAS Registry No: 41318-75-6

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

64–64.5 (Tittlemier et al. 2002)

64.25 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

94.05 (Tittlemier & Tomy 2001)

79.7 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.409 (at mp $64.25^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for triBDE, Alcock et al. 1999)

0.070 (solid S_s , generator column-GC/ECD, Tittlemier et al. 2002)

0.173, 0.334 (supercooled liquid S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)

1.78×10^{-4} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -4912/(T/K) + 12.73$, (GC-RT correlation, Tittlemier & Tomy 2001)

0.00160 (supercooled P_L , GC-RT correlation on a CPSil-8 column, Wong et al. 2001)

2.19×10^{-3} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -4160/(T/K) + 11.30$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

1.96×10^{-3} , 1.57×10^{-3} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.1 (calculated- P_L/C_L , Tittlemier et al. 2002)

1.924 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

5.98 (estimated from PCDEs and fragment constant, Tittlemier et al. 2002)

5.53, 5.80 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

9.50* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -3.54 + 3889/(T/K)$, temp range 15–45°C (generator column-GC, Harner & Shoeib 2002)

10.279, 9.689, 9.154, 8.645 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)

10.213, 9.634, 9.092, 8.585 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

9.50, 9.41 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.019 \text{ d}^{-1}$ with $t_{1/2} = 36.5 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 128 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 1440 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 5760 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 1440 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota: depuration $t_{1/2} = 36.5 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.11.1
Reported octanol-air partition coefficients of 2,4,4'-tribromodiphenyl ether (PBDE 28) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	9.994	15	10.279
25	9.46	25	9.698
35	9.077	35	9.154
45	8.709	45	8.645
25	9.5	QRSETP model 5	
		15	10.213
		25	9.634
		35	9.092
		45	8.585
$\log K_{OA} = A + B/(T/K)$			
A	-3.54		
B	3889		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 74.5$			

Quantitative relationships between structures, environmental temperatures and properties.

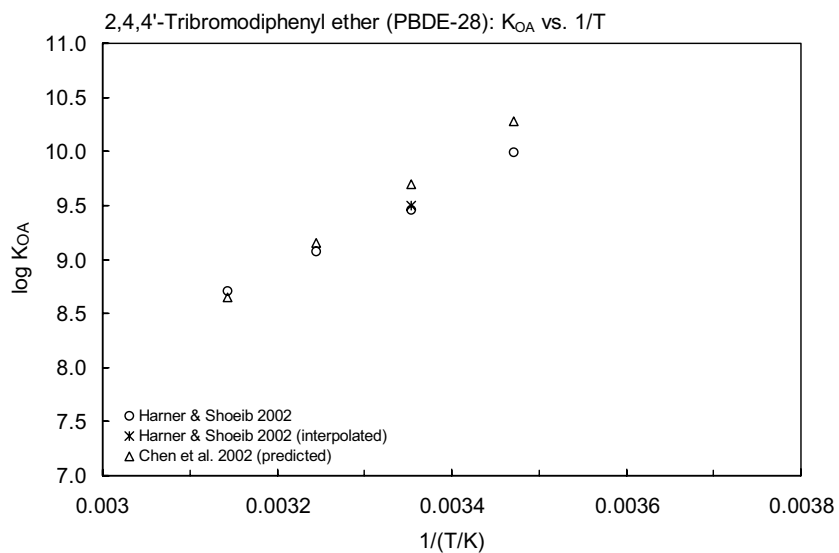
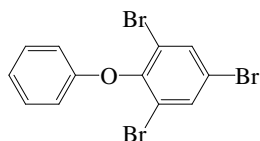


FIGURE 10.1.5.11.1 Logarithm of K_{OA} versus reciprocal temperature for 2,4,4'-tribromodiphenyl ether (PBDE-28).

10.1.5.12 2,4,6-Tribromodiphenyl ether (BDE-30)

Common Name: 2,4,6-Tribromodiphenyl ether

Synonym: PBDE-30, BDE-30, 1,3,5-tribromo-2-phenoxybenzene

Chemical Name: 2,4,6-tribromodiphenyl ether

CAS Registry No: 155999-95-4

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.1 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for triBDE, Alcock et al. 1999)

4.56×10^{-3} ; 3.96×10^{-3} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4232/(T/K) + 11.85$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.02; 8.94 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

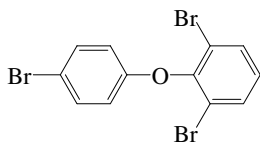
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.13 2,4',6-Tribromodiphenyl ether (BDE-32)



Common Name: 2,4',6-Tribromodiphenyl ether

Synonym: PBDE-32, BDE-32, 1,3-dibromo-2-(4-bromophenoxy)-benzene

Chemical Name: 2,4',6-tribromodiphenyl ether

CAS Registry No: 189083-60-4

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.3 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for triBDE, Alcock et al. 1999)

2.25×10^{-3} ; 1.90×10^{-3} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4352/(T/K) + 11.94$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.59 (quoted values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

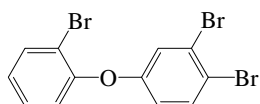
9.28; 9.18 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.14 2',3,4-Tribromodiphenyl ether (BDE-33)

Common Name: 2',3,4-Tribromodiphenyl ether

Synonym: PBDE-33, BDE-33. 1,2-dibromo-4-(2-bromophenoxy)-benzene

Chemical Name: 2',3,4-tribromodiphenyl ether

CAS Registry No: 147217-78-5

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

81.0 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.01150 (estimated for tri-BDE, Alcock et al. 1999)

1.78×10^{-3} ; 1.49×10^{-3} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4443/(T/K) + 12.15$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted range of values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

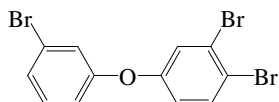
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.15 3,3',4-Tribromodiphenyl ether (BDE-35)



Common Name: 3,3',4-Tribromodiphenyl ether

Synonym: PBDE-35, BDE-35, 1,2-dibromo-4-(4-bromophenoxy)-benzene

Chemical Name: 3,3',4-tribromodiphenyl ether

CAS Registry No: 147217-80-9

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00155 (estimated for triBDE, Alcock et al. 1999)

1.39×10^{-3} ; 1.15×10^{-3} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4512/(T/K) + 12.28$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted range of values for tribromodiphenyl ethers, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

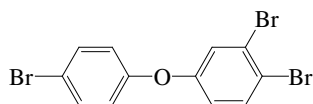
9.61; 9.48 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.16 3,4,4'-Tribromodiphenyl ether (BDE-37)

Common Name: 3,4,4'-Tribromodiphenyl ether

Synonym: PBDE-37, BDE-37, 1,2-dibromo-4-(4-bromophenoxy)-benzene

Chemical Name: 3,4,4'-tribromodiphenyl ether

CAS Registry No: 147217-81-0

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.7 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)

1.02×10^{-3} ; 8.0×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4528/(T/K) + 12.20$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted range of values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.68; 9.54 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

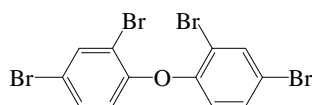
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.17 2,2',4,4'-Tetrabromodiphenyl ether (BDE-47)



Common Name: 2,2',4,4'-Tetrabromodiphenyl ether

Synonym: PBDE-47, BDE-47, 1,1'-oxybis[2,4-dibromo-benzene], NSC 21724

Chemical Name: 2,2',4,4'-tetrabromodiphenyl ether

CAS Registry No: 5436-43-1

Molecular Formula: $C_{12}H_6Br_4O$

Molecular Weight: 485.791

Melting Point ($^{\circ}C$):

83.5–84.5 (Tittlemier et al. 2002)

84.0 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

288.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

103.13 (Tittlemier & Tomy 2001)

92.0 (Wong et al. 2001)

94.6 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.261 (calculated at mp $84^{\circ}C$, Wania & Dugani 2002)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00007 (calculated for tetra-BDE, Alcock et al. 1999)

0.015 (solid S_s , generator column-GC/ECD, Tittlemier et al. 2002)

0.0496, 0.0947 (supercooled liquid S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.35×10^{-4} – 2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

2.19×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -5386/(T/K) + 13.42$, (GC-RT correlation, Tittlemier & Tomy 2001)

3.19×10^{-4} ; 2.50×10^{-4} (supercooled P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4805/(T/K) + 12.62$, (GC-RT correlation, Wong et al. 2001)

1.86×10^{-4} (supercooled liquid P_L , GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -4940/(T/K) + 12.85$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

2.66×10^{-4} , 2.15×10^{-4} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.5 (calculated-P/C, Tittlemier et al. 2002)

1.107 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.02 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)

6.55 (estimated, Tittlemier et al. 2002)

6.11, 6.39 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

10.53* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -6.47 + 5068/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)

10.987, 10.406, 9.863, 9.353 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)

10.928, 10.349, 9.807, 9.300 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

10.34; 10.14 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

10.53, 10.44 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 120 \text{ L d}^{-1} \text{ g}^{-1} \text{ dry wt}$, $k_2 = 0.090 \text{ d}^{-1}$ in blue mussels (Gustafsson et al. 1999)

$k_1 = 0.108 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$ in Lake Höytiäinen sediment; $0.251 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$ in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)

$k_2 = 0.034 \text{ d}^{-1}$ in Lake Höytiäinen sediment; 0.071 d^{-1} in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)

$k_2 = 0.023 \text{ d}^{-1}$ with $t_{1/2} = 30.1 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 256 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota: depuration half-life of 7.7 d in blue mussels (Gustafsson et al. 1999);

biphasic depuration kinetics observed in oligochaete tissues with half-life of 10.5–47.5 h in compartment A for sediment ingesting oligochaetes (Leppänen & Kukkonen 2004)

depuration $t_{1/2} = 30.1 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.17.1

Reported octanol-air partition coefficients of 2,2',4,4'-tetrabromodiphenyl ether (PBDE 47) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
15	11.129	15	10.987
25	10.499	25	10.406
35	10.063	35	9.863
45	9.428	45	9.353
25	10.53	QRSETP model 5	
		15	10.928
		25	10.349
		35	9.807
		45	9.3
log K _{OA} = A + B/(T/K)			
A	-6.47		
B	5068		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 97.0$			

Quantitative relationships between structures, environmental temperatures and properties.

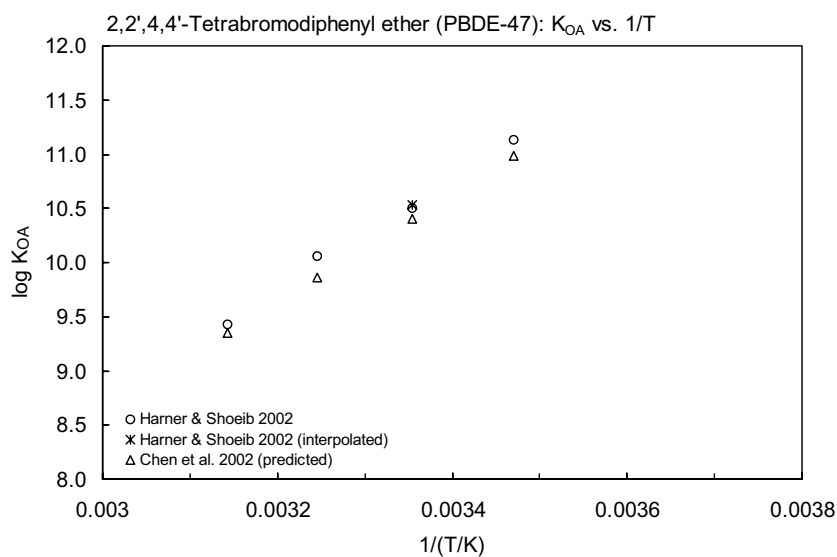
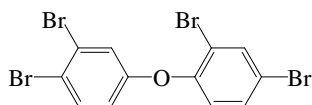


FIGURE 10.1.5.17.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4'-tetrabromodiphenyl ether (PBDE-47).

10.1.5.18 2,3',4,4'-Tetrabromodiphenyl ether (BDE-66)



Common Name: 2,3',4,4'-Tetrabromodiphenyl ether

Synonym: PBDE-66, BDE-66, 1,2-dibromo-4-(2,4-dibromophenoxy)-benzene

Chemical Name: 2,3',4,4'-tetrabromodiphenyl ether

CAS Registry No: 189084-61-5

Molecular Formula: $C_{12}H_6Br_4O$

Molecular Weight: 485.791

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

288.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

93.5 (Wong et al. 2001)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00007 (calculated for tetraBDE, Alcock et al. 1999)

0.018 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.35×10^{-4} – 2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

2.38×10^{-4} ; 1.90×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4882/(T/K) + 12.75$, (GC-RT correlation, Wong et al. 2001)

1.22×10^{-4} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5109/(T/K) + 13.23$, (Clausius-Clapeyron eq. form GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.50 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.73 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

10.82* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -7.88 + 5576/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

11.348, 10.767, 10.223, 9.714 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

11.281, 10.702, 10.161, 9.653 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

10.49; 10.28 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.18.1

Reported octanol-air partition coefficients of 2,3',4,4'-tetrabromodiphenyl ether (PBDE 66) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^{\circ}\text{C}$	log K_{OA}	$t/^{\circ}\text{C}$	log K_{OA}
QRSETP* model 3			
15	11.516	15	11.348
25	10.773	25	10.767
35	10.224	35	10.223
45	9.673	45	9.714
25	10.82	QRSETP model 5	
		15	11.281
		25	10.702
		35	10.161
		45	9.653
log $K_{OA} = A + B/(T/K)$			
A	-7.88		
B	5576		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 107.0$			

Quantitative relationships between structures, environmental temperatures and properties.

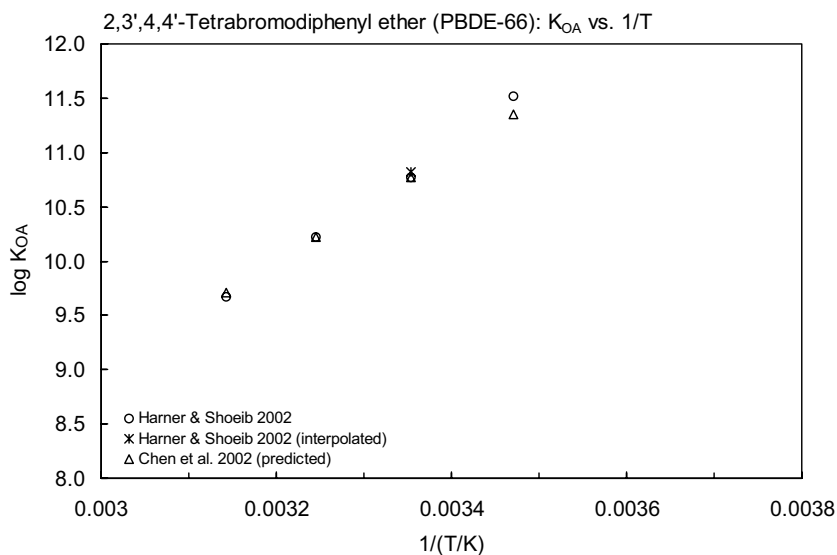
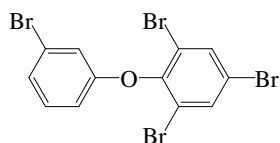


FIGURE 10.1.5.18.1 Logarithm of K_{OA} versus reciprocal temperature for 2,3',4,4'-tetrabromodiphenyl ether (PBDE-66).

10.1.5.19 2,3',4,6-Tetrabromodiphenyl ether (BDE-69)

Common Name: 2,3',4,6-Tetrabromodiphenyl ether

Synonym: PBDE-69, BDE-69, 1,3,5-tribromo-2-(30bromophenoxy)-benzene

Chemical Name: 2,3',4,6-tetrabromodiphenyl ether

CAS Registry No: 327185-09-1

Molecular Formula: $C_{12}H_6Br_4O$

Molecular Weight: 485.791

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

288.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.1 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00007 (calculated for tetraBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.35×10^{-4} – 2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

4.0×10^{-4} ; 3.20×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4757/(T/K) + 12.56$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.23; 10.04 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

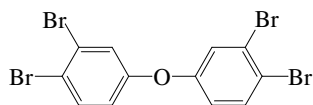
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.20 3,3',4,4'-Tetrabromodiphenyl ether (BDE-77)



Common Name: 3,3',4,4'-Tetrabromodiphenyl ether

Synonym: PBDE-77, BDE-77, 1,1'-xylbix[2,3-dibromophenoxy]-benzene

Chemical Name: 3,3',4,4'-tetrabromodiphenyl ether

CAS Registry No: 93703-48-1

Molecular Formula: $C_{12}H_6Br_4O$

Molecular Weight: 485.791

Melting Point ($^{\circ}C$):

96.7–98 (Tittlemier et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

288.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

95.3 (Wong et al. 2001)

98.7 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00007 (calculated for tetraBDE, Alcock et al. 1999)

0.006 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.35×10^{-4} – 2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

1.56×10^{-4} ; 1.20×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4977/(T/K) + 12.89$, (GC-RT correlation, Wong et al. 2001)

6.79×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5156/(T/K) + 13.13$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.2 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.96 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

10.87* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -5.69 + 4936/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

11.343, 10.762, 10.218, 9.709 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

11.218, 10.603, 10.097, 9.590 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

10.70; 10.46 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.20.1

Reported octanol-air partition coefficients of 3,3',4,4'-tetrabromodiphenyl ether (PBDE 77) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^{\circ}\text{C}$	log K_{OA}	$t/^{\circ}\text{C}$	log K_{OA}
QRSETP* model 3			
15	11.486	15	11.343
25	10.829	25	10.762
35	10.371	35	10.218
45	9.844	45	9.709
25	10.87	QRSETP model 5	
log $K_{OA} = A + B/(T/K)$		15	11.218
A	-5.69	25	10.639
B	4936	35	10.097
enthalpy of phase change		45	9.59
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 94.5$			

Quantitative relationships between structures, environmental temperatures and properties.

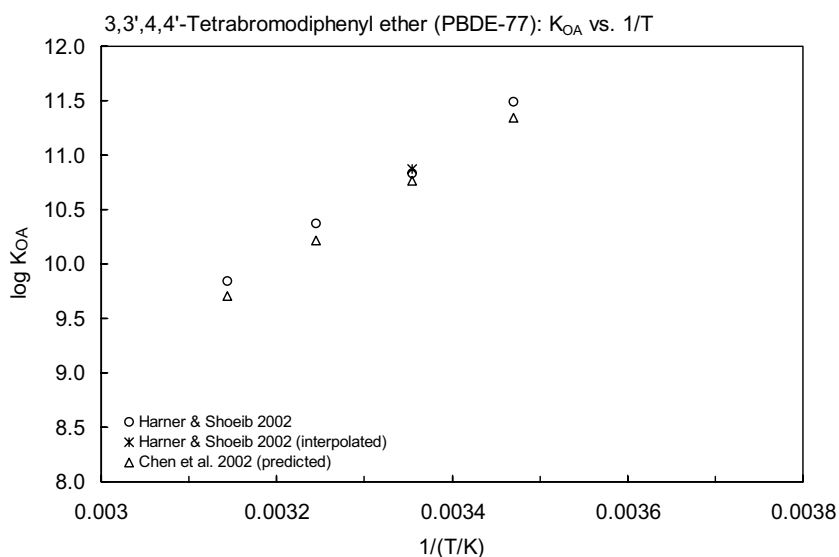
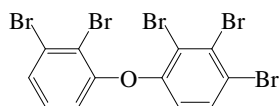


FIGURE 10.1.5.20.1 Logarithm of K_{OA} versus reciprocal temperature for 3,3',4,4'-tetrabromodiphenyl ether (PBDE-77).

10.1.5.21 2,2',3,3',4-Pentabromodiphenyl ether (BDE-82)



Common Name: 2,2',3,3',4-Pentabromodiphenyl ether

Synonym: PBDE-82, BDE-82, 1,2,3-tribromo-4-(2,3-dibromophenoxy)-benzene

Chemical Name: 2,2',3,3',4-pentabromodiphenyl ether

CAS Registry No: 327185-11-5

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

99.1 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for pentaBDE, Alcock et al. 1999)

6.47×10^{-5} ; 4.80×10^{-5} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -5175/(T/K) + 13.12$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

11.14; 10.86 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

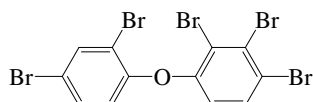
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.22 2,2',3,4,4'-Pentabromodiphenyl ether (BDE-85)



Common Name: 2,2',3,4,4'-Pentabromodiphenyl ether

Synonym: PBDE-85, BDE-85, 1,2,3-tribromo-4-(2,4-dibromophenoxy)-benzene

Chemical Name: 2,2',3,4,4'-pentabromodiphenyl ether

CAS Registry No: 182346-21-0

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

119–121 (Tittlemier et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

110.95 (Tittlemier & Tomy 2001)

110 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

0.006 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for pentaBDE, Alcock et al. 1999)

2.88×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -5795/(T/K) + 13.91$, (GC-RT correlation, Tittlemier & Tomy 2001)

2.81×10^{-5} (supercooled P_L , GC-RT correlation on a CPSil-8 column, Wong et al. 2001)

9.86×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5761/(T/K) + 14.43$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.11 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

7.03 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.66* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

12.312, 11.631, 11.118, 10.544 (15 , 25 , 35 , $45^{\circ}C$, generator column-GC/MS, Harner & Shoeib 2002)

$\log K_{OA} = -6.22 + 5331/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

12.131, 11.549, 11.006, 10.497 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

12.130, 11.551, 11.009, 10.502 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.22.1

Reported octanol-air partition coefficients of 2,2',3,4,4'-pentabromodiphenyl ether (PBDE 85) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
		QRSETP* model 3	
15	12.312	15	12.131
25	11.631	25	11.549
35	11.118	35	11.006
45	10.544	45	10.497
25	11.66	QRSETP model 5	
		15	12.13
log K _{OA} = A + B/(T/K)		25	11.551
A	-6.22	35	11.009
B	5331	45	10.502
enthalpy of phase change			
ΔH _{OA} /(kJ mol ⁻¹) = 102.0			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

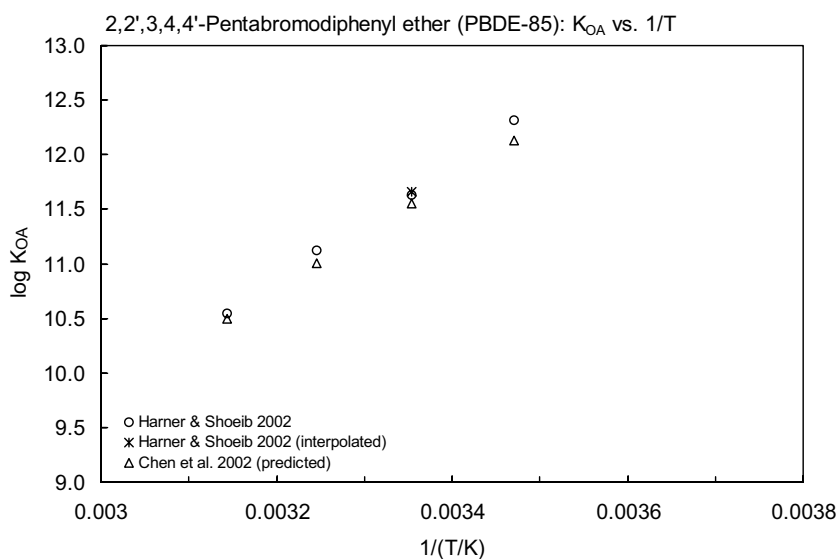
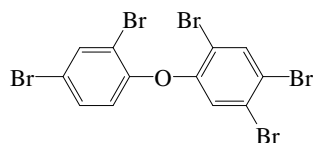


FIGURE 10.1.5.22.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',3,4,4'-pentabromodiphenyl ether (PBDE-85).

10.1.5.23 2,2',4,4',5-Pentabromodiphenyl ether (BDE-99)



Common Name: 2,2',4,4',5-Pentabromodiphenyl ether

Synonym: PBDE-99, BDE-99, 1,2,4-tribromo-5-(2,4-dibromophenoxy)-benzene

Chemical Name: 2,2',4,4',5-pentabromodiphenyl ether

CAS Registry No: 60348-60-9

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

90.5–94.5 (Tittlemier et al. 2002)

92.5 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

104.80 (Tittlemier & Tomy 2001)

100.2 (Wong et al. 2001)

108 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.215 (at mp $92.5^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

0.0094 (solid S_s , generator column-GC/ECD, Tittlemier et al. 2002)

0.0275, 0.0389 (supercooled S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for pentaBDE, Alcock et al. 1999)

1.26×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -5474/(T/K) + 13.47$, (GC-RT correlation, Tittlemier & Tomy 2001)

6.82×10^{-5} ; 5.0×10^{-5} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -5241/(T/K) + 13.41$, (GC-RT correlation, Wong et al. 2001)

1.76×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5339/(T/K) + 13.37$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

4.57×10^{-5} , 3.63×10^{-5} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.23 (calculated- P_L/C_L , Tittlemier et al. 2002)

0.530 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

- 6.81 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)
 7.13 (estimated, Tittlemier et al. 2002)
 6.61, 6.76 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.
 Additional data at other temperatures designated * are compiled at the end of this section:

- 11.31* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
 $\log K_{OA} = -4.64 + 4757/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
 12.067, 11.485, 10.942, 10.433 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
 12.002, 11.422, 10.881, 10.373 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
 11.28; 10.99 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
 11.31, 11.26 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (K_1 and K_2):

- $k_1 = 170 \text{ L d}^{-1} \text{ g}^{-1} \text{ dry wt}$; $k_2 = 0.123 \text{ d}^{-1}$ in blue mussels (Gustafsson et al. 1999)
 $k_1 = 0.066 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$; $k_2 = 0.022 \text{ d}^{-1}$ in Lake Höytiäinen sediment; $k_1 = 0.99 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$;
 $k_2 = 0.026 \text{ d}^{-1}$ in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)

Half-Lives in the Environment:

- Air: first order degradation $t_{1/2} = 467 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
 Surface water: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
 Ground water:
 Sediment: first order degradation $t_{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
 Soil: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
 Biota: depuration $t_{1/2} = 5.6 \text{ d}$ in blue mussels (Gustafsson et al. 1999);
 biphasic depuration kinetics observed in oligochaete tissues with $t_{1/2} = 10.5\text{--}47.5 \text{ h}$ in compartment A for sediment ingesting oligochaetes (Leppänen & Kukkonen 2004)

TABLE 10.1.5.23.1
Reported octanol-air partition coefficients of 2,2',4,4',5-pentabromodiphenyl ether (PBDE 99) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^\circ\text{C}$	$\log K_{OA}$	$t/^\circ\text{C}$	$\log K_{OA}$
		QRSETP* model 3	
15	11.847	15	12.067
25	11.321	25	11.485
35	10.887	35	10.942
45	10.258	45	10.433
25	11.31	QRSETP model 5	
		15	12.002
$\log K_{OA} = A + B/(T/K)$		25	11.422
A	-4.64	35	10.881
B	4757	45	10.373
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 91.1$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

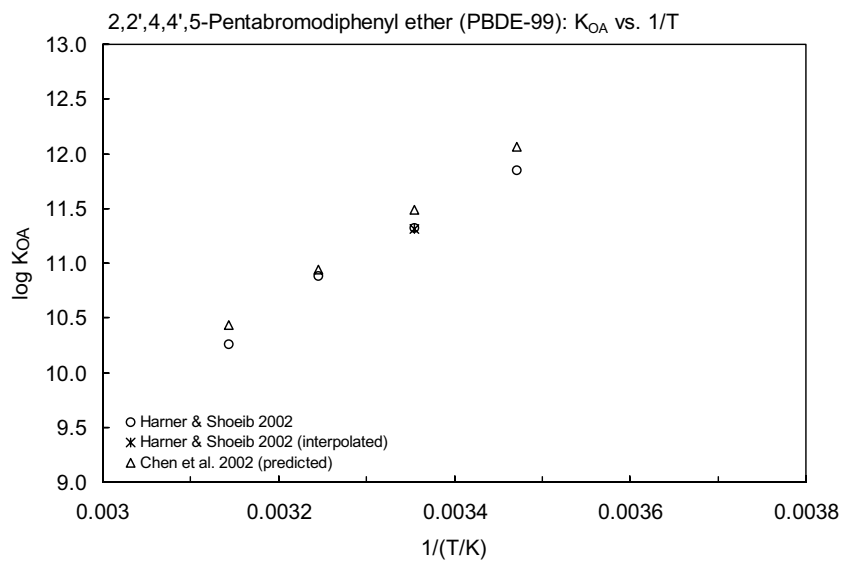
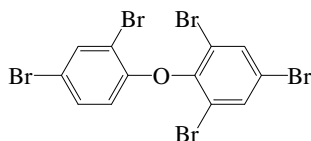


FIGURE 10.1.5.23.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4',5-pentabromodiphenyl ether (PBDE-99).

10.1.5.24 2,2',4,4',6-Pentabromodiphenyl ether (BDE-100)



Common Name: 2,2',4,4',6-Pentabromodiphenyl ether

Synonym: PBDE-100, 1,3,5-tribromo-2-(2,4-dibromophenoxy)-benzene

Chemical Name: 2,2',4,4',6-pentabromodiphenyl ether

CAS Registry No: 189084-64-8

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

102 (Tittlemier et al. 2002)

110 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

102 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.179 (at mp $100.5^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.040 (generator column-GC/ECD, Tittlemier et al. 2002)

0.0499, 0.0541 (supercooled S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

2.86×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5339/(T/K) + 13.37$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

3.99×10^{-5} , 3.68×10^{-5} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.069 (calculated- P_L/C_L , Tittlemier et al. 2002)

0.384 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.86 (estimated, Tittlemier et al. 2002)

6.51, 6.53 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.13* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -7.18 + 5459/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

11.721, 11.140, 10.596, 10.087 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

11.758, 11.179, 10.637, 10.130 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

11.20; 11.52 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

11.13, 11.02 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 357$ h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400$ h (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

TABLE 10.1.5.24.1

Reported octanol-air partition coefficients of 2,2',4,4',6-pentabromodiphenyl ether (PBDE 100) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^{\circ}\text{C}$	log K_{OA}	$t/^{\circ}\text{C}$	log K_{OA}
		QRSETP* model 3	
15	11.755	15	11.721
25	11.185	25	11.14
35	10.509	35	10.596
45	9.993	45	10.087
25	11.13	QRSETP model 5	
		15	11.758
		25	11.179
		35	10.637
		45	10.13
log $K_{OA} = A + B/(T/K)$			
A	-7.18		
B	5459		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 105.0$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

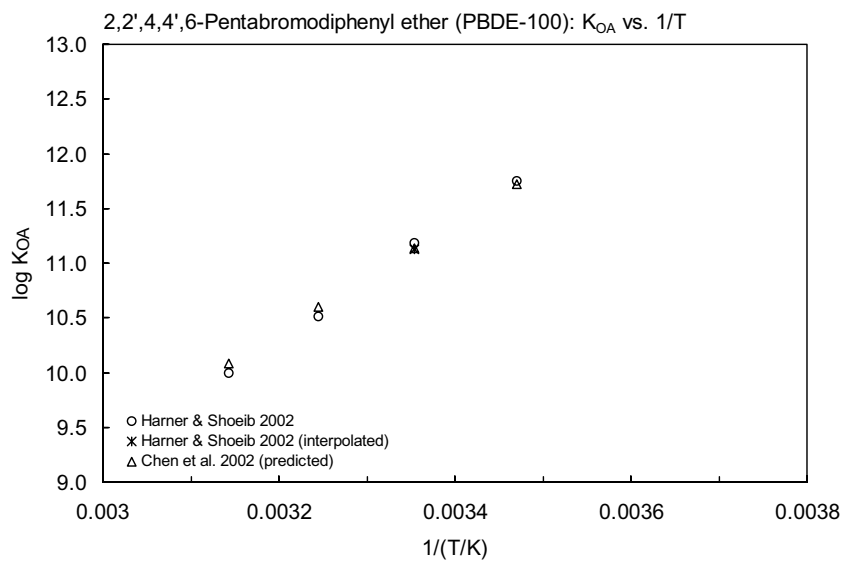
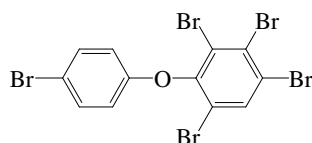


FIGURE 10.1.5.24.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4',6-pentabromodiphenyl ether (PBDE-100).

10.1.5.25 2,3,4,4',6-Pentabromodiphenyl ether (BDE-115)

Common Name: 2,3,4,4',6-Pentabromodiphenyl ether

Synonym: PBDE-115, BDE-115, 1,2,3,5-tetrabromo-4-(4-bromophenoxy)benzene

Chemical Name: 2,3,4,4',6-pentabromodiphenyl ether

CAS Registry No: 446254-78-0

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

101.8 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for penta-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for penta-BDE, Alcock et al. 1999)

3.02×10^{-5} ; 3.20×10^{-5} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -5219/(T/K) + 13.32$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$:

11.52; 11.20 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

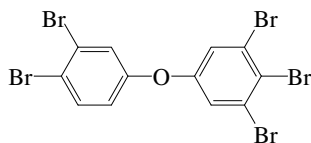
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.26 3,3',4,4',5-Pentabromodiphenyl ether (BDE-126)



Common Name: 3,3',4,4',5-Pentabromodiphenyl ether

Synonym: PBDE-126, BDE-126, 1,2,3-tribromo-5-(3,4-dibromophenoxy)-benzene

Chemical Name: 3,3',4,4',5-pentabromodiphenyl ether

CAS Registry No: 366791-32-4

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for penta-PBDEs, Alcock et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.97* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -8.41 + 6077/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

12.642, 12.001, 11.441, 10.611 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

12.544, 11.964, 11.423, 10.915 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.26.1

Reported octanol-air partition coefficients of 3,3',4,4',5-pentabromodiphenyl ether (PBDE 126) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
15	12.642	QRSETP* model 3	
25	12.001	15	12.574
35	11.441	25	11.992
45	10.611	35	11.449
25	11.97	45	10.939
		QRSETP model 5	
log K _{OA} = A + B/(T/K)		15	12.544
A	-8.41	25	11.964
B	6077	35	11.423
		45	10.915
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 116.0$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

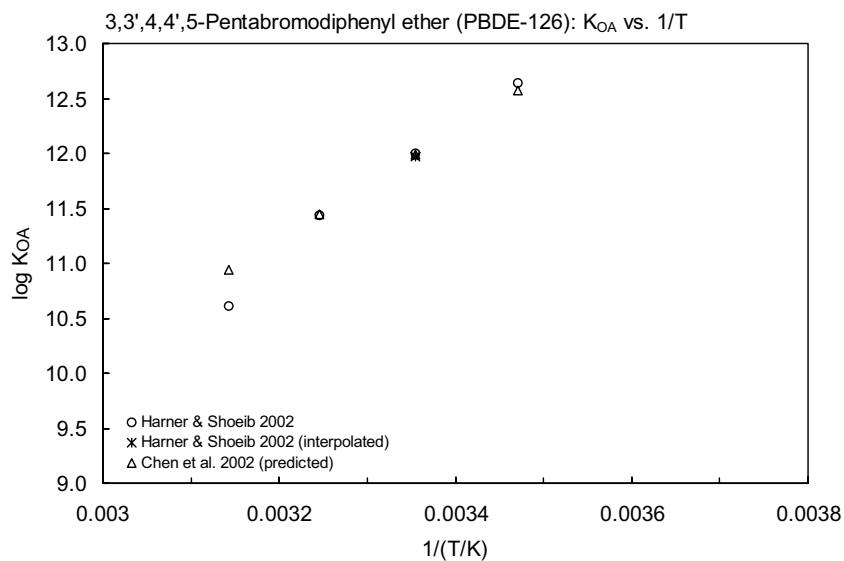
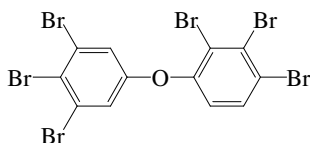


FIGURE 10.1.5.26.1 Logarithm of K_{OA} versus reciprocal temperature for 3,3',4,4',5-pentabromodiphenyl ether (PBDE-126).

10.1.5.27 2,3,3',4,4',5'-Hexabromodiphenyl ether (BDE-138)



Common Name: 2,3,3',4,4',5'-Hexabromodiphenyl ether

Synonym: PBDE-138, BDE-138, 1,2,3-tribromo-4-(2,4,5-tribromophenoxy)-benzene

Chemical Name: 2,3,3',4,4',5'-hexabromodiphenyl ether

CAS Registry No: 182677-30-1

Molecular Formula: $C_{12}H_4Br_6O$

Molecular Weight: 643.584

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

114.06 (Tittlemier & Tomy 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.08×10^{-6} (calculated for hexaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

9.44×10^{-6} – 4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.95–0.99 (estimated for hexa-BDE, Alcock et al. 1999)

1.51×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -5957/(T/K) + 14.17$, (GC-RT correlation, Tittlemier & Tomy 2001)

1.58×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -6191/(T/K) + 14.97$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

7.91 (estimated, Tittlemier et al. 2002)

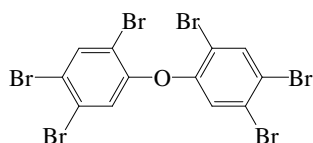
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.28. 2,2',4,4',5,5'-Hexabromodiphenyl ether (BDE-153)

Common Name: 2,2',4,4',5,5'-Hexabromodiphenyl ether

Synonym: PBDE-153, BDE-153, 1,1'-oxybis[2,4,5-tribromophenoxy]-benzene

Chemical Name: 2,2',3,3',5,5'-hexabromodiphenyl ether

CAS Registry No: 68631-49-2

Molecular Formula: $C_{12}H_4Br_6O$

Molecular Weight: 643.583

Melting Point ($^{\circ}C$):

160–163 (Tittlemier et al. 2002)

161.5 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

107.6 (Wong et al. 2001)

110 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.045 (calculated at mp $161.5^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.08×10^{-6} (calculated for hexaBDE, Alcock et al. 1999)

8.70×10^{-7} (Solid S_s , generator column-GC/ECD, Tittlemier et al. 2002)

0.0195, 0.0167 (supercooled S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

9.44×10^{-6} – 4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.95–0.99 (estimated for hexa-BDE, Alcock et al. 1999)

8.43×10^{-6} ; 5.80×10^{-8} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -5620/(T/K) + 13.78$, (GC-RT correlation, Wong et al. 2001)

2.09×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5763/(T/K) + 13.66$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

7.58×10^{-6} , 8.87×10^{-6} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.067 (calculated- P_L/C_L , Tittlemier et al. 2002)

0.342 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.86–7.93 (hexabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

7.39 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)

7.62 (estimated, Tittlemier et al. 2002)

7.13, 7.08 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.82* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -5.39 + 5131/(T/K)$, temp range 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)

12.708, 12.127, 11.583, 11.074 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)

12.556, 11.977, 11.435, 10.928 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

12.15; 11.78 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

11.82, 11.89 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 19 \text{ L d}^{-1} \text{ g}^{-1}$ dry wt. in blue mussels (Gustafsson et al. 1999)

$k_2 = 0.086 \text{ d}^{-1}$ in blue mussels (Gustafsson et al. 1999)

$k_2 = 0.051 \text{ d}^{-1}$ with $t_{1/2} = 13.6 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 1110 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota: depuration $t_{1/2} = 8.1 \text{ d}$ in blue mussels (Gustafsson et al. 1999);

$t_{1/2} = 13.6 \pm 9 \text{ d}$ in carp (Stapleton et al. 2004a)

depuration $t_{1/2} = 13.6 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.28.1

Reported octanol-air partition coefficients of 2,2',4,4',5,5'-hexabromodiphenyl ether (PBDE 153) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^\circ\text{C}$	$\log K_{OA}$	$t/^\circ\text{C}$	$\log K_{OA}$
		QRSETP* model 3	
15	12.318	15	12.708
25	11.86	25	12.127
35	11.569	35	11.583
45	10.534	45	11.074
25	11.82	QRSETP model 5	
		15	12.556
		25	11.977
		35	11.435
		45	10.928
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 98.2$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

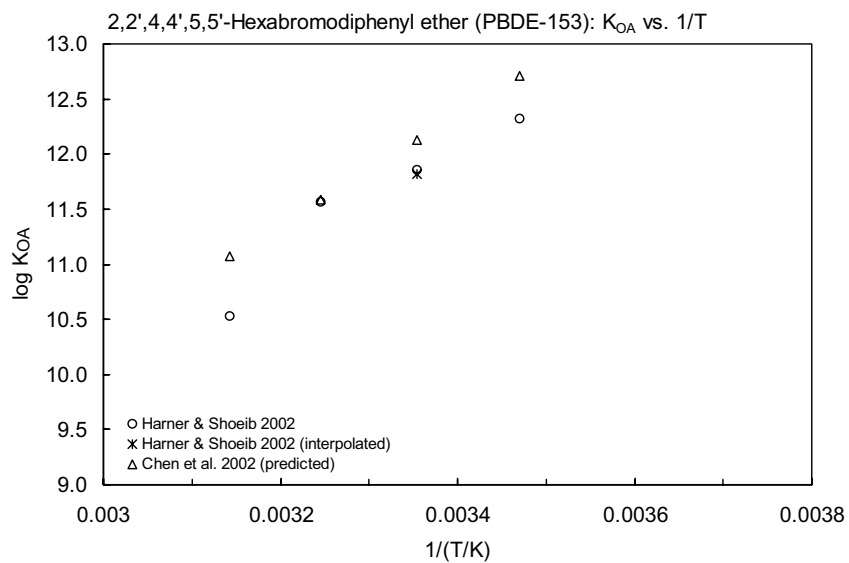
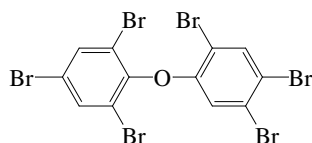


FIGURE 10.1.5.28.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4',5,5'-hexabromodiphenyl ether (PBDE-153).

10.1.5.29 2,2',4,4',5,6'-Hexabromodiphenyl ether (BDE-154)



Common Name: 2,2',4,4',5,6'-Hexabromodiphenyl ether

Synonym: PBDE-154, BDE-154, 1,3,5-tribromo-2-(2,4,5-tribromophenoxy)-benzene

Chemical Name: 2,2',4,4',5,6'-hexabromodiphenyl ether

CAS Registry No: 207122-15-4

Molecular Formula: $C_{12}H_4Br_6O$

Molecular Weight: 643.583

Melting Point ($^{\circ}C$):

131–132.5 (Tittlemier et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

113 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.08×10^{-6} (calculated for hexa-PBDEs, Alcock et al. 1999)

8.70×10^{-7} (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$):

9.44×10^{-6} – 4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.95–0.99 (estimated for hexa-PBDEs, Alcock et al. 1999)

3.80×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5900/(T/K) + 14.38$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.24 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

7.39 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section

11.92* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -4.62 + 4931/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

12.471, 11.890, 11.346, 10.837 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

12.361, 11.782, 11.240, 10.733 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 2.0 \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 35 \text{ d}$ in juvenile carp (Stapleton et al. 2004a)

Half-Lives in the Environment:

Biota: depuration $t_{1/2} = 35 \pm 18 \text{ d}$ in juvenile carp (Stapleton et al. 2004a)

TABLE 10.1.5.29.1

Reported octanol-air partition coefficients of 2,2',4,4',5,6'-hexabromodiphenyl ether (PBDE 154) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
QRSETP* model 3			
15	12.455	15	12.471
25	11.935	25	11.89
35	11.531	35	11.346
45	10.789	45	10.837
25	11.92	QRSETP model 5	
		15	12.361
		25	11.782
		35	11.24
		45	10.733
log $K_{OA} = A + B/(T/K)$			
A	-4.62		
B	4931		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 94.4$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

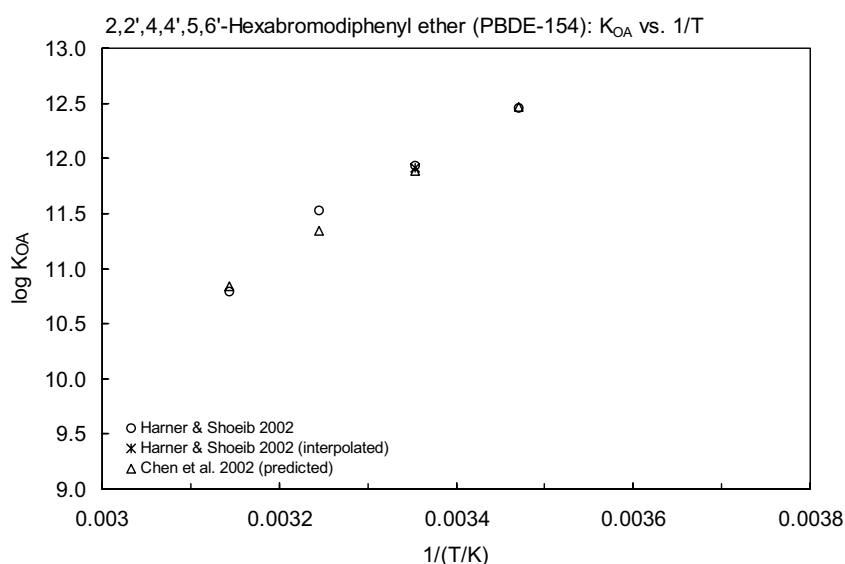
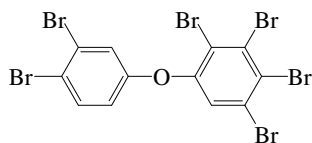


FIGURE 10.1.5.29.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4',5,6'-hexabromodiphenyl ether (PBDE-154).

10.1.5.30 2,3,3',4,4',5-Hexabromodiphenyl ether (BDE-156)



Common Name: 2,3,3',4,4',5-Hexabromodiphenyl ether

Synonym: PBDE-156, BDE-156, 1,2,3,4-tetrabromo-5-(3,4-dibromophenoxy)-benzene

Chemical Name: 2,3,3',4,4',5-hexabromodiphenyl ether

CAS Registry No: 405237-85-6

Molecular Formula: $C_{12}H_4Br_6O$

Molecular Weight: 643.583

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.08×10^{-6} (calculated for hexa-PBDEs, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

$9.44 \times 10^{-6} - 4.22 \times 10^{-6}$ (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.95–0.99 (estimated for hexa-PBDEs, Alcock et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.97* (generator column-GC/MS, measured range $15-45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -5.80 + 5298/(T/K)$, temp range: $15-45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

13.211, 12.630, 12.087, 11.577 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

13.150, 12.571, 12.029, 11.522 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.30.1

Reported octanol-air partition coefficients of 2,3,3',4,4',5'-hexabromodiphenyl ether (PBDE 156) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
QRSETP* model 3			
15	-	15	13.211
25	11.976	25	12.63
35	-	35	12.087
45	10.858	45	11.577
25	11.97	QRSETP model 5	
log K _{OA} = A + B/(T/K)		15	13.15
A	-5.80	25	12.571
B	5298	35	12.029
enthalpy of phase change		45	11.522
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 101.0$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

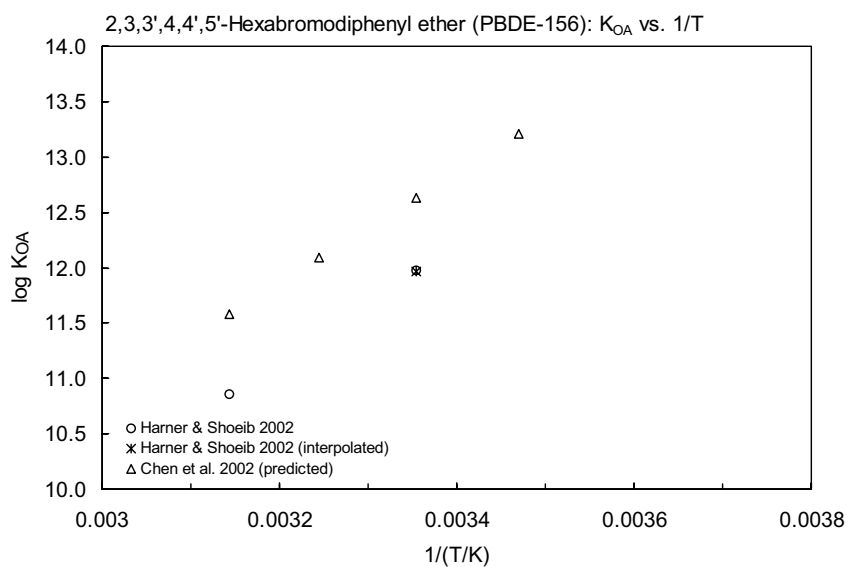
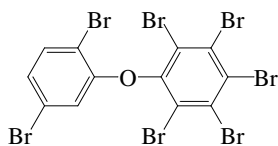


FIGURE 10.1.5.30.1 Logarithm of K_{OA} versus reciprocal temperature for 2,3,3',4,4',5'-hexabromodiphenyl ether (PBDE-156).

10.1.5.31 2,2',3,4,5,5',6-Heptabromodiphenyl ether (BDE-183)



Common Name: 2,2',3,4,5,5',6-Heptabromodiphenyl ether

Synonym: PBDE-183, BDE-183, 1,2,3,5-tetrabromo-4-(2,4,5-trobromophenoxy)-benzene

Chemical Name: 2,2',3,4,5,5',6-heptabromodiphenyl ether

CAS Registry No: 207122-16-5

Molecular Formula: $C_{12}H_3Br_7O$

Molecular Weight: 722.479

Melting Point ($^{\circ}C$):

171–173 (Tittlemier et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

358.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

118 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.035 (calculated at mp $172^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.50×10^{-6} (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

4.68×10^{-7} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -6185/(T/K) + 14.43$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0074 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.14 (quoted, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.96* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -3.71 + 4672/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

13.263, 12.681, 12.138, 11.628 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

13.206, 12.627, 12.085, 11.577 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: first-order degradation $t_{1/2} = 1540$ h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first-order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400$ h (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

TABLE 10.1.5.31.1

Reported octanol-air partition coefficients of 2,3,3',4,4',5'-hexabromodiphenyl ether (PBDE 183) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
15	-	15	13.263
25	11.964	25	12.681
35	11.477	35	12.138
45	10.978	45	11.628
25	11.96	QRSETP model 5	
log K _{OA} = A + B/(T/K)		15	13.206
A	-3.71	25	12.627
B	4672	35	12.085
		45	11.577
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 89.5$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

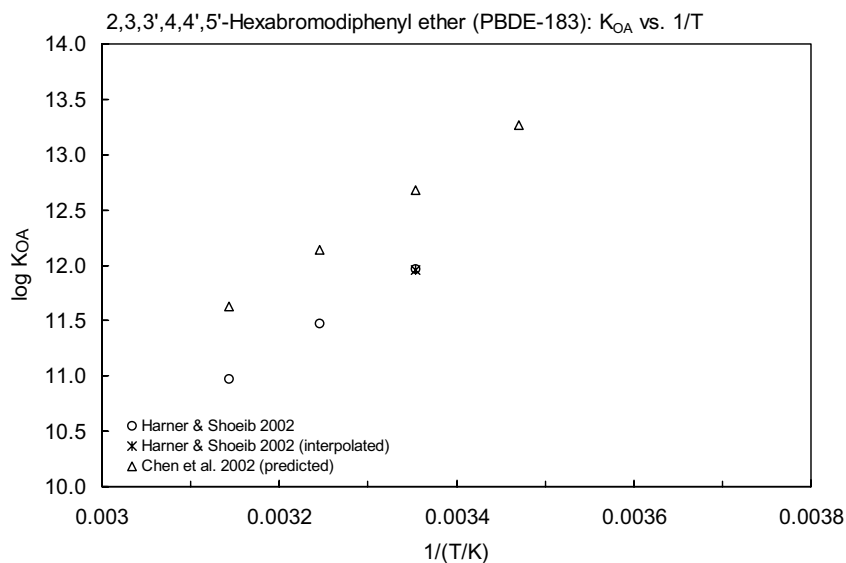
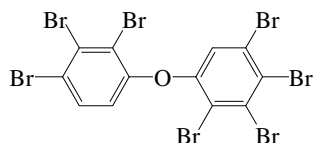


FIGURE 10.1.5.31.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',3,4,4',5',6-heptabromodiphenyl ether (PBDE-183).

10.1.5.32 2',3,3',4,4',5,6-Heptabromodiphenyl ether (BDE-190)



Common Name: 2',3,3',4,4',5,6-Heptabromodiphenyl ether

Synonym: PBDE-190, BDE-190, pentabromo-(3,4-dibromophenoxy)-benzene

Chemical Name: 2',3,3',4,4',5,6-heptabromodiphenyl ether

CAS Registry No: 189084-68-2

Molecular Formula: $C_{12}H_3Br_7O$

Molecular Weight: 722.479

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

358.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

121.15 (Tittlemier & Tomy 2001)

115.8 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ at $25^{\circ}C$ and reported temperature dependence equation):

2.34×10^{-7} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -6327/(T/K) + 14.60$, (GC-RT correlation, Tittlemier & Tomy 2001)

9.05×10^{-7} ; 5.70×10^{-7} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -6048/(T/K) + 14.24$, (GC-RT correlation, Wong et al. 2001)

2.82×10^{-7} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -6552/(T/K) + 15.44$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.36 (estimated, Tittlemier et al. 2002)

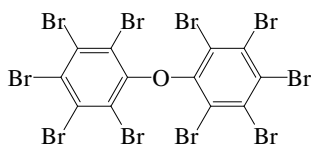
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.33 Decabromodiphenyl ether (BDE-209)

Common Name: Decabromodiphenyl ether

Synonym: PBDE-209, BDE-209, 1,1'-oxybis[2,3,4,5,6-pentabromo]-benzene, bis(pentabromophenyl)-ether, 102(E), 2,2',3,3',4,4',5,5',6,6'-decabromodiphenyl ether, Decabromobiphenyl oxide, decabromophenyl ether

Chemical Name: decabromodiphenyl ether

CAS Registry No: 1163-19-5

Molecular Formula: $C_{12}Br_{10}O$

Molecular Weight: 959.167

Melting Point ($^{\circ}C$):

302.5 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

428.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.17×10^{-9} (solid S_s , quoted lit., Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$):

2.95×10^{-9} (supercooled liquid P_L , estimated, Wania & Dugani 2003)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

9.97 (decabromodiphenyl ether, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

9.97 (quoted from Watanabe & Tatsukawa 1990, Pijnenburg et al. 1995)

9.97 (quoted, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{1/2} < 0.25$ h on silica gel, $t_{1/2} = 12$ h on sand, $t_{1/2} = 40$ – 60 h on sediment and $t_{1/2} = 150$ – 200 h in soil; for outdoors under sunlight "discontinuous": $t_{1/2} = 37$ h on sand and 80 h on sediment; for outdoor sunlight "continuous": $t_{1/2}(\text{calc}) = 13$ h on sand and $t_{1/2}(\text{calc}) = 30$ on sediment (Söderström et al. 2004)

Photooxidation:

Hydrolysis:

Biodegradation: anaerobic degradation decreased by 30% within 238 d corresponding to a pseudo-first-order $k = 1 \times 10^{-3} d^{-1}$ by sewage sludge collected from a mesophilic digester (Gerecke et al. 2005)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 1.4 \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 50 \text{ d}$ in juvenile carp (Stapleton et al. 2004)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 7620 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003); photolysis half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{1/2} = 40\text{--}60 \text{ h}$ on sediment; for outdoors under sunlight "discontinuous": $t_{1/2} = 80 \text{ h}$ on sediment; for outdoor sunlight "continuous": $t_{1/2}(\text{calc}) = 30$ on sediment (Södertröm et al. 2004)

Soil: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003); photolysis half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{1/2} = 12 \text{ h}$ on sand, and $150\text{--}200 \text{ h}$ in soil; for outdoors under sunlight "discontinuous": 37 h on sand; for outdoor sunlight "continuous": $t_{1/2}(\text{calc}) = 13 \text{ h}$ on sand (Södertröm et al. 2004)

Biota: depuration $t_{1/2} = 50 \pm 17 \text{ d}$ in juvenile carp (Stapleton et al. 2004)

10.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 10.2.1

Summary of physical properties of ethers and halogenated ethers

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/m ³ at 20°C	Molar volume, V _M cm ³ /mol	
								MW/ρ at 20°C	Le Bas
Aliphatic ethers:									
Dimethyl ether (Methyl ether)	115-10-6	(CH ₃) ₂ O	46.068	−141.5	−24.8	1	0.6689	68.87	60.9
Diethyl ether (Ethyl ether)	60-29-7	(C ₂ H ₅) ₂ O	74.121	−116.2	34.5	1	0.71361	103.87	106.1
Methyl <i>t</i> -butyl ether (MTBE)	1634-04-4	CH ₃ OC(CH ₃) ₃	88.148	−108.6	55	1	0.7404	119.05	127.5
Di- <i>n</i> -propyl ether	111-43-3	(C ₃ H ₇) ₂ O	102.174	−114.8	90.08	1	0.7466	136.85	151.6
Di-isopropyl ether	108-20-3	((CH ₃) ₂ CH) ₂ O	102.174	−85.4	68.4	1	0.73	139.96	151.6
Butyl ethyl ether	628-81-9	(C ₄ H ₉)O(C ₂ H ₅)	102.174	−124	92.3	1	0.7495	136.32	150.5
Di- <i>n</i> -butyl ether	142-96-1	(C ₄ H ₉) ₂ O	130.228	−95.2	140.28	1	0.7684	169.48	196
1,2-Propylene oxide	75-56-9	C ₃ H ₆ O	58.079	−111.9	35	1			69.7
Furan	110-00-9	C ₄ H ₄ O	68.074	−85.61	31.5	1	0.9378	72.59	73.5
2-Methylfuran	534-22-5	C ₅ H ₆ O	82.101	−91.3	64.7	1	0.9132	89.90	95.7
Tetrahydrofuran	109-99-9	C ₄ H ₈ O	72.106	−108.44	65	1	0.8892	81.09	88.3
Tetrahydropyran	142-68-7	C ₅ H ₁₀ O	86.132	−49.1	88	1	0.8814	97.72	107
1,4-Dioxane	123-91-1	C ₄ H ₈ O ₂	88.106	11.85	101.5	1	1.0336	85.24	92
Halogenated ethers:									
Epichlorohydrin	106-89-8	C ₃ H ₅ ClO	92.524	−26	118	1	1.18066	78.37	90.6
Chloromethyl methyl ether	107-30-2	ClCH ₂ -O-CH ₃	80.513	−103.5	59.5	1	1.0703	75.22	81.8
Bis(2-chloromethyl)ether	542-88-1	C ₂ H ₄ Cl ₂ O	114.958	−41.5	106	1			102.7
Bis(2-chloroethyl)ether	111-44-4	(ClC ₂ H ₄) ₂ O	143.012	−51.9	178.5	1	1.2192	117.30	147.9
Bis(2-chloroisopropyl)ether	108-60-1	(ClC ₃ H ₆) ₂ O	171.064	−97	187	1	1.11	154.11	193.4
2-Chloroethyl vinyl ether	110-75-8	ClC ₂ H ₄ -O-C ₂ H ₃	106.551	−70	108	1	1.0475	101.72	119.6
Bis(2-chloroethoxy)methane	111-91-1	(ClC ₂ H ₄) ₂ O ₂ CH ₂	173.037		215	1			180.0
Aromatic ethers:									
Anisole (Methoxybenzene)	100-66-3	(C ₆ H ₅)O(CH ₃)	108.138	−37.13	153.7	1	0.994	108.79	127.3
2-Chloroanisole	766-51-8	C ₇ H ₇ ClO	142.583	−26.8	198.5	1	1.1911	119.71	148.2
3-Chloroanisole	2845-89-8	C ₇ H ₇ ClO	142.583		193.5				148.2
4-Chloroanisole	227881	C ₇ H ₇ ClO	142.583	< −18	197.5	1	1.201	118.72	148.2
2,3-Dichloroanisole	1984-59-4	C ₇ H ₆ Cl ₂ O	177.028	32		0.854			169.1
2,6-Dichloroanisole	1984-65-2	C ₇ H ₆ Cl ₂ O	177.028	10		1			169.1

(Continued)

TABLE 10.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/m ³ at 20°C	Molar volume, V_M cm ³ /mol	
								MW/ ρ at 20°C	Le Bas
2,3,4-Trichloroanisole	54135-80-7	C ₇ H ₅ Cl ₃ O	211.473	70		0.362			190.0
2,4,6-Trichloroanisole	87-40-1	C ₇ H ₅ Cl ₃ O	211.473	61.5	241	0.438			190.0
2,3,4,5-Tetrachloroanisole	938-86-3	C ₇ H ₄ Cl ₄ O	245.918	88		0.241			210.9
2,3,5,6-Tetrachloroanisole	6936-40-9	C ₇ H ₄ Cl ₄ O	245.918	84		0.264			210.9
Veratrole (1,2-Dimethoxybenzene)	91-16-7	C ₈ H ₁₀ O ₂	138.164	22.5	206	1			158.6
4,5-Dichloroveratrole	2772-46-5	C ₈ H ₈ Cl ₂ O ₂	207.054	83		0.270			200.4
3,4,5-Trichloroveratrole	16766-29-3	C ₈ H ₇ Cl ₃ O ₂	241.499	66		0.396			221.3
Tetrachloroveratrole	944-61-6	C ₈ H ₆ Cl ₄ O ₂	275.944	90		0.230			242.2
Phenetole (Ethoxybenzene)	103-73-1	(C ₆ H ₅)O(C ₂ H ₅)	122.164	-29.43	169.81	1	0.9651	126.58	150.3
Benzyl ethyl ether	539-30-0	C ₆ H ₅ CH ₂ OC ₂ H ₅	136.190		186	1	0.949	143.51	172.5
Styrene oxide	96-09-3	C ₈ H ₈ O	120.149	-35.6	194.1	1	1.0500	114.43	136.1
Diphenyl ether	101-84-8	C ₁₂ H ₁₀ O	170.206	26.87	258	0.959	1.0748	158.36	195.6

* Assuming $\Delta S_{\text{fus}} = 56$ J/mol K.

TABLE 10.2.2

Summary of selected physical-chemical properties of ethers and halogenated ethers at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol) calculated P/C
	Vapor pressure		Solubility			log K _{OW}	
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)		
Aliphatic ethers:							
Dimethyl ether (Methyl ether)	600000	600000	353000	7662	7662	0.1	13.22*
Diethyl ether (Ethyl ether)	71600	71600	60500	816.2	816.2	0.89	87.72
Methyl <i>t</i> -butyl ether (MTBE)	33500	33500	42000	476.5	476.5	0.94	70.31
Di- <i>n</i> -propyl ether	8334	8334	3306	32.35	32.35	2.03	257.6
Di-isopropyl ether	20000	20000	7900	77.31	77.31	1.52	258.7
Butylethyl ether	8200	8200	6500	63.61	63.61	2.03	128.9
Di- <i>n</i> -butyl ether	850	850	230	1.766	1.776	3.21	481.3
1,2-Propylene oxide	71000	71000	476000	8196	8196	0.03	8.663
Furan	80000	80000	10000	146.9	146.9	1.34	544.6
Tetrahydrofuran	21600	21600	miscible				
Tetrahydropyran	9536	9536	85700	995.0	995.0	0.82	9.584
1,4-Dioxane	5000	5000	miscible			0.27	
Halogenated ethers:							
Epichlorohydrin	2400	2400	65800	771.2	711.2	0.30	3.37
Chloromethyl methyl ether	24900	24900	decompose				
Bis(chloromethyl)ether	4000	4000	22000	191.4	191.4	0.38	20.90
Bis(2-chloroethyl)ether	206	206	10200	71.32	71.32	1.12	2.888
Bis(2-chloroisopropyl)ether	104	104	1700	9.938	9.938	2.58	10.46
2-Chloroethyl vinyl ether	3566	3566	15000	140.8	140.8	1.28	25.33
Bis(2-chloroethoxy)methane	21.6	21.6	81000	468.1	468.1	1.26	0.0461
Aromatic ethers:							
Anisole (Methoxybenzene)	472	472	1600	14.80	14.80	2.11	31.90
2-Chloroanisole			490	3.436	3.436	2.50	
3-Chloroanisole			235	1.648		2.60	
4-Chloroanisole			237	1.662	1.662	2.70	
2,3-Dichloroanisole			86.9	0.4909	0.5748	3.24	
2,6-Dichloroanisole			13.12	0.0741	0.0741	3.14	

(Continued)

TABLE 10.2.2 (Continued)

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol) calculated P/C
	Vapor pressure		Solubility			log K _{OW}	
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)		
2,3,4-Trichloroanisole			10.8	0.0511	0.1411	4.03	
2,4,6-Trichloroanisole			13.2	0.0624	0.1425	4.02	
2,3,4,5-Tetrachloroanisole			1.35	0.0055	0.0228	4.50	
2,3,5,6-Tetrachloroanisole			1.82	0.0074	0.0280	4.40	
Veratrole (1,2-Dimethoxybenzene)			6690	48.42	48.42	2.18	
4,5-Dichloroveratrole			72	0.2477	1.2879	3.11	
3,4,5-Trichloroveratrole			10.3	0.0426	0.1077	4.01	
Tetrachloroveratrole			1.59	0.0058	0.0250	4.86	
Phenetole (Ethoxybenzene)	204	204	569	4.658	4.658	2.68	43.80
Benzyl ethyl ether	100	100				2.64	
Styrene oxide	40	40	2800	23.30	23.0	1.61	1.716
Diphenyl ether	2.93	3.05	18.7	0.1099	0.1146	4.21	26.67

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H (Pa·m³/mol) = 101325 Pa/C^S mol/m³.

TABLE 10.2.3

Suggested half-life classes of ethers and halogenated ethers in various environmental compartments at 25°C

Compound	Air class	Water* class	Soil class	Sediment class
Aliphatic ethers:				
Dimethyl ether (Methyl ether)	2	5	5	6
Diethyl ether (Ethyl ether)	2	5	5	6
Methyl <i>t</i> -butyl ether (MTBE)	2	5	5	6
Di- <i>n</i> -propyl ether	2	5	5	6
1,2-Propylene oxide	2	4	5	6
Furan	2	4	5	6
Tetrahydrofuran	2	4	5	6
1,4-Dioxane	2	4	5	6
Halogenated ethers:				
Chloromethyl methyl ether	2	5	5	6
Bis(chloromethyl)ether	2	5	5	6
Bis(2-chloroethyl)ether	2	5	5	6
Bis(2-chloroisopropyl)ether	2	5	5	6
2-Chloroethyl vinyl ether	2	5	5	6
Bis(2-chloroethoxy)methane	2	5	5	6
Aromatic ethers:				
Anisole (Methoxybenzene)	2	5	5	6
Styrene oxide	2	4	5	6
Diphenyl ether	2	5	5	6

* Certain ethers will have much shorter half-lives because of hydrolysis with singlet oxygen, and biodegradation; this half-life class is conservatively assigned, see [Chapter 1](#) for a discussion.

where,

	Class	Mean half-life (h)	Range (h)
1		5	< 10
2		17 (~ 1 d)	10–30
3		55 (~ 2 d)	30–100
4		170 (~ 1 week)	100–300
5		550 (~ 3 weeks)	300–1,000
6		1700 (~ 2 months)	1,000–3,000
7		5500 (~ 8 months)	3,000–10,000
8		17000 (~ 2 years)	10,000–30,000
9		55000 (~ 6 years)	> 30,000

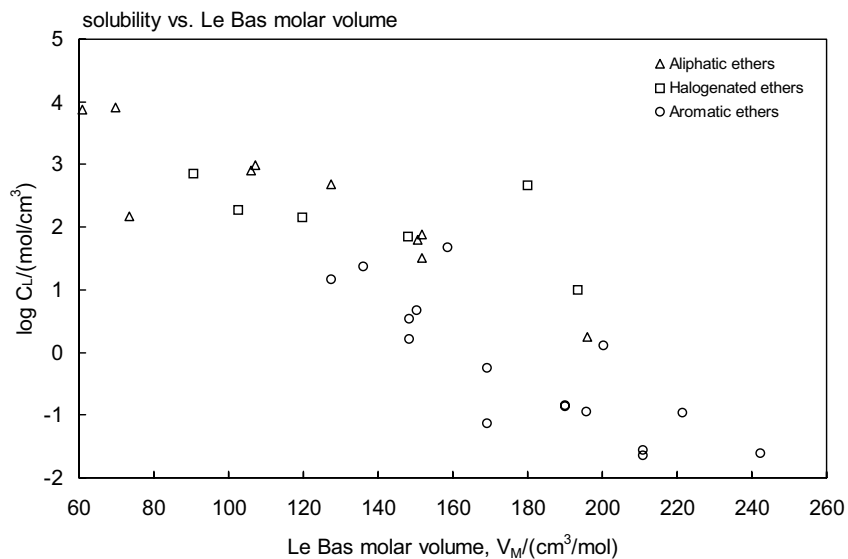


FIGURE 10.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for ethers.

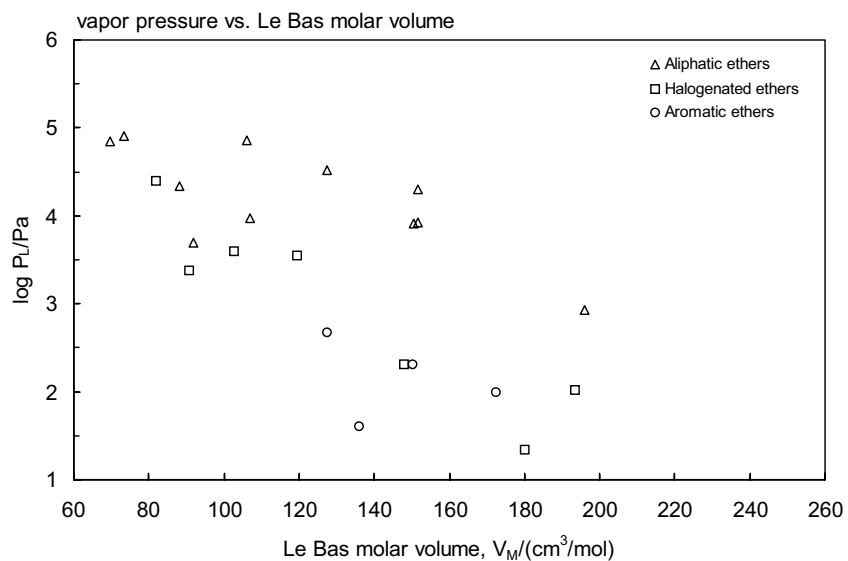


FIGURE 10.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for ethers.

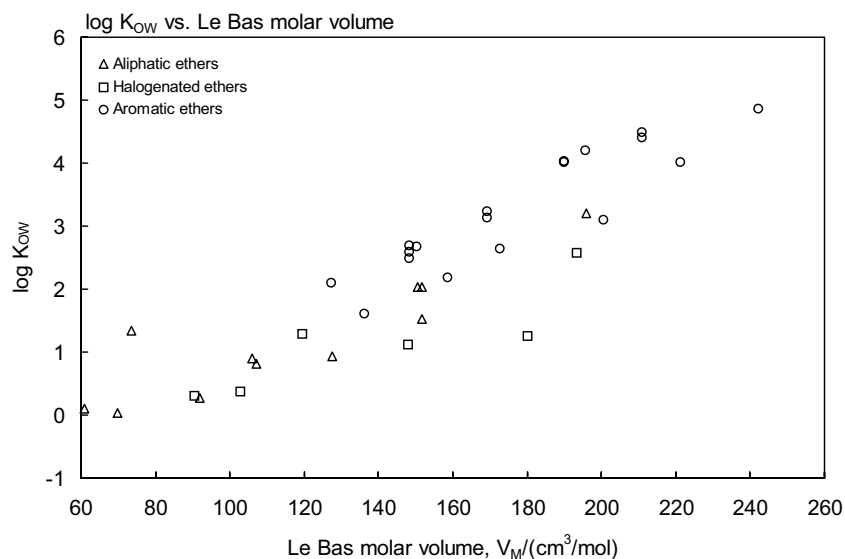


FIGURE 10.2.3 Octanol-water partition coefficient versus Le Bas molar volume for ethers.

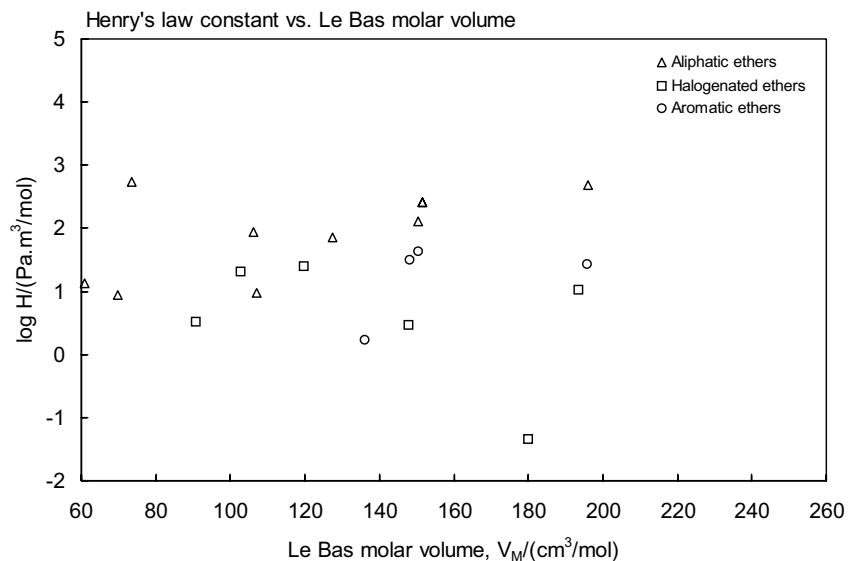


FIGURE 10.2.4 Henry's law constant versus Le Bas molar volume for ethers.

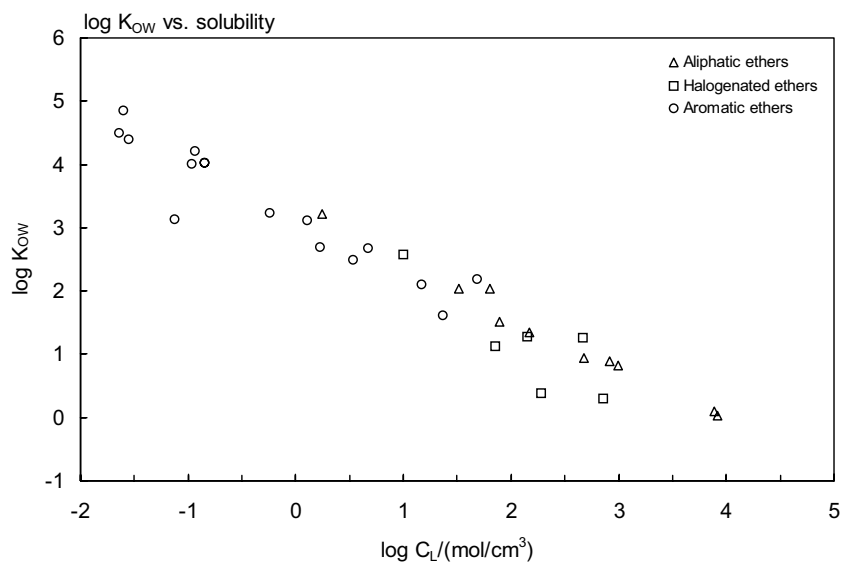


FIGURE 10.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for ethers.

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11 Alcohols

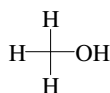
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11.1 LIST OF CHEMICALS AND DATA COMPILATIONS

11.1.1 ALCOHOLS

11.1.1.1 Methanol



Common Name: Methanol

Synonym: methyl alcohol, carbinol, wood alcohol, wood spirit

CAS Registry No: 67-56-1

Molecular Formula: CH₃OH

Molecular Weight: 32.042

Melting Point (°C):

−97.53 (Lide 2003)

Boiling Point (°C):

64.6 (Lide 2003)

Density (g/cm³ at 20°C):

0.7914 (Weast 1982–83)

Molar Volume (cm³/mol):

42.5 (exptl. at normal bp, Lee et al. 1972; quoted, Reid et al. 1977)

40.6 (calculated-density, Rohrschneider 1973)

37.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Dean 1985; Howard 1990)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

16210* (interpolated-regression of tabulated data, temp range −44.0 to 64.7°C, Stull 1947)

16937* (comparative ebulliometry, measured range 15–83.7°C, Ambrose & Sprake 1970)

log (P/Pa) = 7.18411 − 1569.492/(T/K − 34.613); restricted temp range 15–39°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 7.20519 − 1581.933/(T/K − 33.439); temp range 15–83.7°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

16927 (vapor-liquid equilibrium VLE data, Polák & Lu 1972)

log (P/mmHg) = [−0.2185 × 8978.8/(T/K)] + 8.639821; temp range −44 to 224°C (Antoine eq., Weast 1972–73)

16958* (static method, measured range 288.15–337.65 K, Gibbard & Creek 1974)

12260, 21330 (20°C, 30°C, Verschueren 1983)

16960 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 7.24693 − 1806.615/(241.833 + t/°C); temp range 1.72–63.38°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 7.20660 − 1582.698/(239.765 + t/°C); temp range 14–79.63°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

log (P/kPa) = 7.023029 − 1595.671/(240.905 + t/°C), temp range 15–65°C (Antoine eq. derived from exptl data of Gibbard & Creek 1974, Boublik et al. 1984)

16670 (interpolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.89750 − 1474.08/(229.13 + t/°C); temp range −14 to 65°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.97328 − 1515.14/(232.85 + t/°C); temp range 64–110°C (Antoine eq., Dean 1985, 1992)

16937 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 7.20519 - 1581.993/(175.47 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P_L/\text{kPa}) = 7.4182 - 1710.2/(-22.25 + T/\text{K})$; temp range 175–273 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.25164 - 1608.39/(-31.07 + T/\text{K})$; temp range 274–337 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.09489 - 1521.23/(-39.18 + T/\text{K})$; temp range 338–487 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.86277 - 1105.884/(-64.272 + T/\text{K})$; temp range 188–228 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.44355 - 1712.316/(-22.61 + T/\text{K})$; temp range 224–290 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.26415 - 1615.59/(-30.437 + T/\text{K})$; temp range 285–345 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.14736 - 1544.804/(-37.235 + T/\text{K})$; temp range 335–376 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.27466 - 1641.542/(-25.789 + T/\text{K})$; temp range 373–458 K (Antoine eq.-VIII, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 45.6171 - 3.2447 \times 10^3/(T/\text{K}) - 13.988 \cdot \log(T/\text{K}) + 6.6365 \times 10^{-3} \cdot (T/\text{K}) - 1.0507 \times 10^{-13} \cdot (T/\text{K})^2$;
 temp range 175–513 K (vapor pressure eq., Yaws 1994)
 35341 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designed * are compiled at the end of this section):

0.446 (partial pressure-isotenoscope, Butler et al. 1935)
 0.444 (entrainment method-GC, Burnett 1963)
 0.472 (exptl., Hine & Mookerjee 1975)
 0.367, 0.319 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
 0.45* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 0.451 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 0.704 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.451 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 0.620 (gas stripping-GC, Altschuh et al. 1999)
 0.506 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{\text{AW}} = 8.969 - 5206.8/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
 0.334 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 3.444 - 2142/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 1.239* (40°C, headspace-GC, measured range 40–65°C, Teja et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

-0.82 (shake flask-CR, Collander 1951)
 -0.66 (shake flask-GC, Hansch & Anderson 1967)
 -0.77 ± 0.02 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
 -0.52 (shake flask-RC, Cornford 1982)
 -0.70 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
 -0.64, -0.63 (quoted, calculated-TSA, Iwase et al. 1985)
 -0.71 (shake flask-GC at pH 7.0, Riebesehl & Tomlinson 1986)
 -0.74 (recommended, Sangster 1989, 1993)
 -0.77 (recommended value, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ as 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.98* (20.29°C, from GC determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
 2.84 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

4.45	(alga <i>Chlorella fusca</i> , wet wt. basis, Geyer et al. 1984)
4.45	(alga <i>Chlorella fusca</i> , calculated- K_{OW} , Geyer et al. 1984)
< 1.0	(golden ide, after 3 d, Freitag et al. 1985)
4.46	(algae, after 1 d, Freitag et al. 1985)
2.67	(activated sludge, after 5 d, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC} :

-0.23	(calculated-MCI χ , Gerstl & Helling 1987)
0.44	(soil, quoted exptl., Meylan et al. 1992)
-0.36	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
-1.08	(calculated- K_{OW} , Kollig 1993)
0.44	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 5.3$ h and 2.6 d for a model river 1-m deep and an environmental pond (Lyman et al. 1982; selected, Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} ; for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = (5.7 \pm 0.6) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ or $9.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)

$k_{OH} = (1.06 \pm 0.10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

$k_{OH} = (1.00 \pm 0.10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)

$k_{OH} = 5.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k \sim 0.024 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with O_3 in water at pH 2-5 and 20-23°C (Hoigné & Bader 1983)

$k_{OH} = 0.76 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K in air (Meier et al. 1985; quoted, Atkinson 1985)

$k_{OH}(\text{calc}) = 6.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 9.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 0.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Zellner & Lorenz 1984; quoted, Carlier et al. 1986)

$k_{OH}(\text{exptl}) = 0.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (8.61 \pm 0.47) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240-440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{NO_3} < 6.0 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (flash photolysis-absorption technique (Wallington et al. 1987; selected, Atkinson 1991)

$k(\text{aq.}) = 1.60 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987b)

$k_{OH}(\text{exptl})^* = 8.61 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240-440 (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 8.61 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.60 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 9.32 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (9.0 \pm 0.9) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (1.0 \pm 0.23) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 4.05 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: $t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 1$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

estimated $t_{1/2} = 17.8$ d in ambient atmosphere (Howard 1990);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994);

calculated lifetimes of 12 d and 1.0 yr for reactions with OH radical, NO₃ radical, respectively (Atkinson 2000).

Surface water: $t_{1/2}$ (aerobic) = 1 d, $t_{1/2}$ (anaerobic) = 1 d in natural waters (Capel & Larson 1995)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.1.1

Reported vapor pressures of methanol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
ln P = A – B/T/K) – C/(T/K)² + D/(T/K)³		(5)					
Stull 1947		Ambrose & Sprake 1970		Gibbard & Creek 1974			
summary of literature data		comparative ebulliometry		static method-manometer			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/kPa	T/K	P/kPa
–44.0	133.3	14.899	9815	288.1506	9.8844	323.1420	55.5900
–25.3	666.6	19.236	12468	288.1508	9.8858	323.1460	55.5996
–16.2	1333	23.323	15519	288.1511	9.8889	323.1490	55.5972
–6.0	2666	27.083	18858	288.1516	9.8867	328.1436	68.8187
5.0	5333	29.911	21769	293.1361	13.0023	328.1442	68.8158
12.1	7999	32.885	25206	293.1443	13.0119	328.1476	68.8450
21.2	13332	35.858	29128	293.1507	13.0109	328.1517	84.5907
34.8	26664	40.637	36493	293.1628	13.0228	333.1417	84.5859
49.9	53329	45.407	45347	298.1478	16.9558	333.1466	84.5940
64.7	101325	48.876	52883	298.1500	16.9562	333.1468	84.5859
		53.315	64036	298.1505	16.9578	333.1471	84.5940
mp/°C	–97.8	56.428	72975	298.1517	16.9584	337.6462	101.2523
		60.814	87345	303.1427	21.8743	337.6456	101.2526
		63.784	98330	303.1464	21.8782	337.6514	101.2742
		64.717	101998	303.1494	21.8823	vapor pressure eq.	
		68.403	117714	303.1503	21.8859		
		71.770	133741	308.1459	27.9763	eq. 5	P/kPa
		75.683	154640	308.1509	27.9844	A	15.6129944
		79.626	178306	308.1521	27.9871	10³B	2.8459280
		83.678	205653	313.1500	35.4685	10⁵C	3.743415457
				313.1504	35.4695	10⁷D	2.188669628
		Antoine eq. for full range		313.1504	35.4714		
		eq. 3	P/Pa	313.1520	35.4654		
		A	7.20519	318.1475	44.5814		
		B	–1581.93	318.1477	44.5799		
		C	–33.439	318.1483	44.5829		
				318.1506	44.5833		
		data also fitted to Cragoe equation, eq. 5 see ref.					

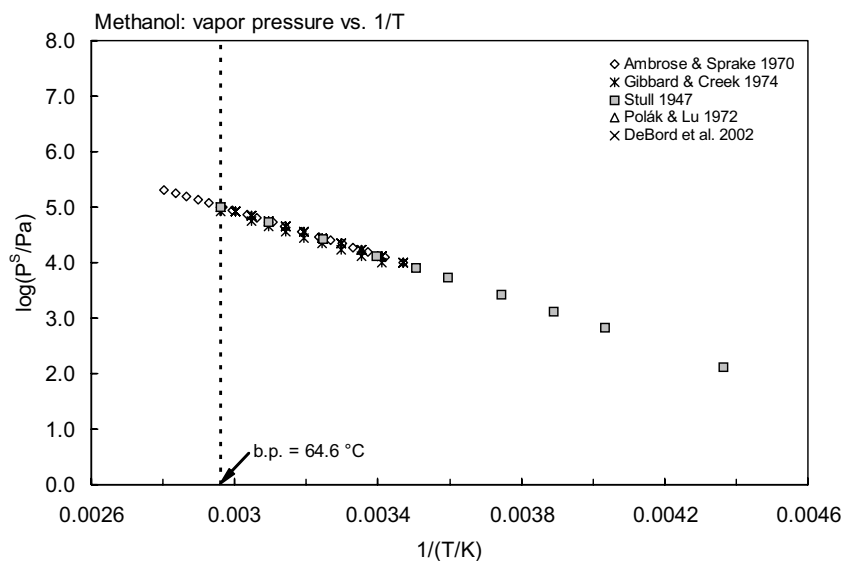


FIGURE 11.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methanol.

TABLE 11.1.1.1.2

Reported Henry's law constants and octanol-air partition coefficients of methanol at various temperatures

Henry's law constant		log K_{OA}			
Snider & Dawson 1985		Teja et al. 2001		Gruber et al. 1997	
gas stripping-GC		headspace-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OA}
0	0.0908	40	1.239	20.29	2.98
25	0.4507	50	2.066	30.3	2.76
		60	3.656	40.4	2.56
		65	4.526	50.28	2.40
enthalpy of transfer:					
$\Delta H/(\text{kJ mol}^{-1}) = 41.0$					

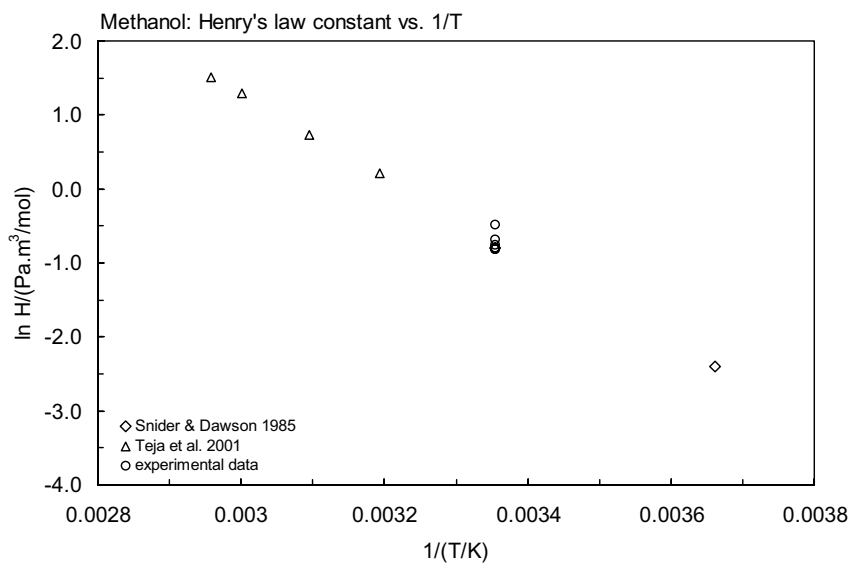


FIGURE 11.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for methanol.

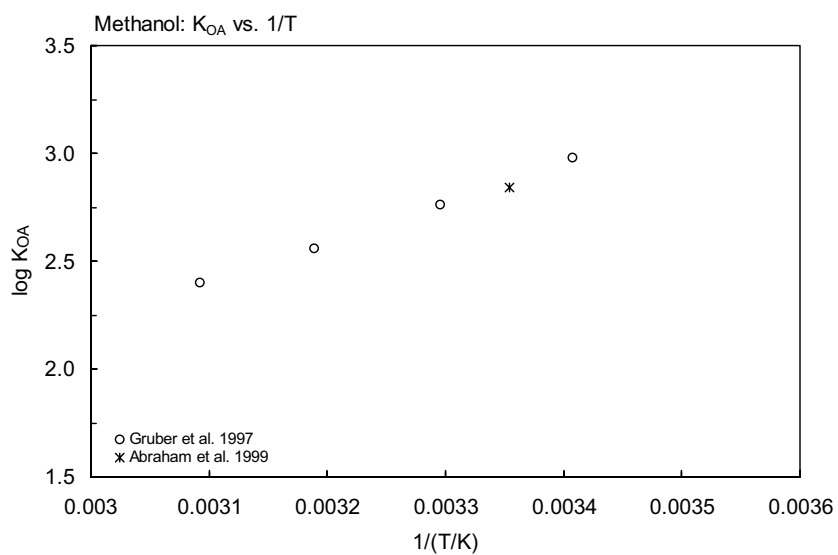


FIGURE 11.1.1.1.3 Logarithm of K_{OA} versus reciprocal temperature for methanol.

11.1.1.2 Ethanol



Common Name: Ethanol

Synonym: ethyl alcohol, methylcarbinol

Chemical Name: ethanol, ethyl alcohol

CAS Registry No: 64-17-5

Molecular Formula: $\text{CH}_3\text{CH}_2\text{OH}$

Molecular Weight: 46.068

Melting Point ($^{\circ}\text{C}$):

-114.14 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

78.29 (Lide 2003)

Density (g/cm^3 at 20°C):

0.78933, 0.78505 (20°C , 25°C , Dreisbach & Martin 1949)

0.7893 (Weast 1982–83)

Molar Volume (cm^3/mol):

58.6 (calculated-density, Rohrschneider 1973)

59.2 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

15.9 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.02 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7314, 7581* (24.4 , 24.8°C , measured range 12.80 – 78.0°C , Kahlbaum 1883)

6906* (22.7°C , static method, measured range 22.7 – 78°C , Smyth & Engel 1929)

7599 (gas saturation/air-bubbling method, Washburn & Handorf 1935)

39345* (vapor-liquid equilibrium VLE data, measured range 35 – 60°C , Scatchard & Raymond 1938)

7538* (interpolated-regression tabulated data, temp range -31.3 to 78.4°C , Stull 1947)

1593, 7869, 29456 (0 , 25 , 50°C , static method, vapor-liquid equilibrium VLE data, Kretschmer et al. 1948)

7869* (static method, measured range 0 – 78.553°C , Kretschmer & Wiebe 1949)

$\log(P/\text{mmHg}) = 8.11576 - 1595.76/(t/^{\circ}\text{C} + 226.5)$; temp range 0 – 78.553°C , Kretschmer & Wiebe 1949)

$\log(P/\text{mmHg}) = 8.24169 - 1652.6/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

7870* (comparative ebulliometry, measured range 19.622 – 93.5°C , Ambrose & Sprake 1970)

$\log(P/\text{Pa}) = 7.16879 - 1552.601/(T/\text{K} - 50.731)$; restricted temp range 19.6 – 43.2°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log(P/\text{Pa}) = 7.24739 - 1599.039/(T/\text{K} - 46.391)$; temp range 19.6 – 93.5°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

7865 (vapor-liquid equilibrium VLE data, Polák & Lu 1972)

$\log(P/\text{mmHg}) = [-0.2185 \times 9673.6/(T/\text{K})] + 8.827392$; temp range -31.3 – 242°C (Antoine eq., Weast 1972–73)

5852, 6665, 9998 (20 , 25 , 30°C , Verschuereen 1983)

8060 (calculated-Antoine eq., Boublik et al. 1984)

- $\log (P/\text{kPa}) = 7.24222 - 1595.811/(226.448 + t/^{\circ}\text{C})$; temp range 19.62–93.48°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 4.11678 - 323.237/(74.916 + t/^{\circ}\text{C})$; temp range 12.8–78.2°C (Antoine eq. from reported exptl. data of Kahlbaum 1883, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 7.31243 - 1630.868/(229.581 + t/^{\circ}\text{C})$; temp range 0–78.55°C (Antoine eq. from reported exptl. data of Kretschmer & Wiebe 1949, Boublik et al. 1984)
 7968 (calculated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 8.32109 - 1718.10/(237.52 + t/^{\circ}\text{C})$; temp range –2 to 100°C (Antoine eq., Dean 1985, 1992)
 7870 (Riddick et al. 1986)
 $\log (P/\text{kPa}) = 7.16879 - 1552.601/(222.419 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P_L/\text{kPa}) = 7.15946 - 1547.464/(-51.177 + T/\text{K})$; temp range 320–359 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.23347 - 1591.28/(-47.056 + T/\text{K})$, temp range: 292–367 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.9391 - 2381.5/(T/\text{K})$; temp range 210–271 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.5224 - 2299/(T/\text{K})$; temp range 193–223 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.16386 - 1550.006/(-50.941 + T/\text{K})$; temp range 320–359 K, (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.27664 - 1615.127/(-45.012 + T/\text{K})$; temp range 292–353 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.95131 - 1423.668/(-63.568 + T/\text{K})$; temp range 349–374 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 23.8442 - 2.8642 \times 10^3/(T/\text{K}) - 5.0474 \cdot \log(T/\text{K}) + 3.7448 \times 10^{-11} \cdot (T/\text{K}) + 2.7361 \times 10^{-5} \cdot (T/\text{K})^2$;
 temp range 159–516 K (vapor pressure eq., Yaws 1994)
 17819 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.520 (partial pressure-isoteniscope, Butler et al. 1935)
 0.0118 (partial vapor pressure, concn.-GC, Burnett & Swoboda 1962)
 0.4660 (entrainment method-GC, Burnett 1963)
 0.637 (exptl.-calculated C_w/C_A , Hine & Mookerjee 1975)
 0.495, 0.472 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.527* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 0.530 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 0.637 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 0.823 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.70 (correlated-molecular structure, Russell et al. 1992)
 0.542 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 0.593 (solid-phase microextraction SPME-GC, Bartelt 1997)
 0.744 (gas stripping-GC, Altschuh et al. 1999)
 0.568 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{AW} = 10.173 - 5531.6/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
 0.361 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 5.576 - 2757/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.32 (shake flask-CR, Collander 1951)
 –0.16 (Leo et al. 1969; Hansch & Dunn III 1972)
 –0.30 (shake flask-GC, Dillingham et al. 1973)
 –0.31 ± 0.02 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
 –0.22, –0.20 (calculated-f const., Rekker 1977)
 –0.18 (shake flask-RC, Cornford 1982)

-0.20	(shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
-0.30	(recommended, Sangster 1989, 1993)
-0.25	(thermometric titration, Fujiwara et al. 1991)
-0.29	(calculated-activity coeff. γ from UNIFAC, Dallos et al. 1993)
-0.31, -0.22	(recommended value; value at pH 7.2, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.34*	(20.29°C, from GC determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
3.20	(head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

-1.63	(calculated as per Mackay 1982, Schultz et al. 1990)
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Sorption Partition Coefficient, $\log K_{OC}$:

0.09	(calculated- MCI χ , Gerstl & Helling 1987)
0.20	(soil, exptl., Meylan et al. 1992)
-0.14	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
0.20	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 6$ d from water (estimated, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k = 0.01 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 8 \times 10^5$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (1.8 \pm 0.2) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ or $3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)

$k = < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen in aquatic systems at 25°C with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; Mill 1982)

$k_{OH} = 2 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at 25°C in the atmosphere with $t_{1/2} = 2.8$ d (Hendry & Kenley 1979)

$k_{OH} = (3.74 \pm 0.37) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Overend & Paraskevopoulos 1978)

$k_{OH} = 1.8 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k_{OH} = (2.62 \pm 0.36) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)

$k_{OH} = 1.75 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Meier et al. 1985)

$k(aq.) = (0.37 \pm 0.04) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with O_3 in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Zellner & Lorenz 1984; quoted, Carlier et al. 1986)

$k_{OH}(calc) = 3.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(obs.) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}(exptl) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(calc) = 3.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (33.3 \pm 2.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{NO_3} < 9.0 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (flash photolysis-absorption technique, Wallington et al. 1987; quoted, Atkinson 1991)

$k_{OH}^* = 3.33 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 3.33 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k(soln) = 3.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}}^* = 3.27 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}} = (3.04 \pm 0.25) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{\text{OH}} = (3.46 \pm 0.52) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k(\text{aq.}) = 0.51 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.2, $k = 0.72 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.3, and $k = 0.77 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8.1 for direct reaction with ozone in water at 21°C with $t_{1/2} = 18 \text{ h}$ at pH 7 (Yao & Haag 1991)

$k_{\text{OH}}(\text{calc}) = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Heukelekian & Rand 1955; Malaney & Gerhold 1969; selected, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$k = 0.043\text{--}0.055 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

$t_{1/2} \sim 5.9 \text{ d}$ to 4.0 d estimated in the atmosphere (Graedel 1978; quoted, Howard 1990), based on the reaction with a OH radical concentration of $8 \times 10^5 \text{ molecules/cm}^3$ (Campbell 1976; Lyman et al. 1982; quoted, Howard 1990);

photooxidation $t_{1/2} = 12.2\text{--}122 \text{ h}$, based on measured rate constant for the reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);

calculated lifetimes of 3.5 d and 26 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water: photooxidation $t_{1/2} = 334 \text{ d}$ –36.6 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; selected, Howard et al. 1991); measured rate constants of $0.51 \text{ M}^{-1} \text{ s}^{-1}$, $0.72 \text{ M}^{-1} \text{ s}^{-1}$, $0.77 \text{ M}^{-1} \text{ s}^{-1}$, at pH 7.2, 7.3, 8.1, respectively, for direct reaction with ozone in water at 21°C , with $t_{1/2} = 18 \text{ h}$ at pH 7 (Yao & Haag 1991).

Groundwater: $t_{1/2} = 48\text{--}336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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TABLE 11.1.1.2.1

Reported vapor pressures of ethanol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^\circ\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^\circ\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log(T/K) \quad (4)$$

Kahlbaum 1883		Scatchard & Raymond 1938		Kretschmer & Wiebe 1949		Ambrose & Sprake 1970	
Ber. 16, 2476 (1883)		vapor-liquid equilibrium		static method, VLE data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.80	2733	35	13703	0.0	1593	19.622	5726
17.4	4114	40	17877	25.0	7869	23.633	7269
21.0	5509	45	23033	34.988	13736	25.722	8205
24.4	7314	50	29488	44.994	23058	28.157	9430
24.8	7581	55	37312	50.0	29456	33.334	12566

(Continued)

TABLE 11.1.1.2.2
Reported Henry’s law constants and octanol-water partition coefficients of ethanol at various temperatures

Henry’s law constant		log K _{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det’d activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
0	0.0688	20.29	3.34
25	0.5274	30.3	3.10
		40.4	2.87
		50.28	2.69

enthalpy of transfer:
 $\Delta H/(\text{kJ mol}^{-1}) = 54.392$

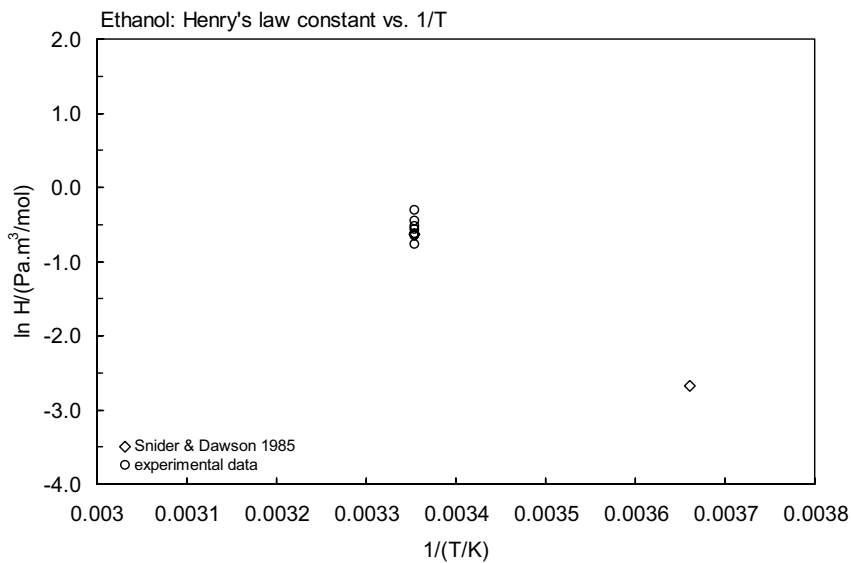


FIGURE 11.1.1.2.2 Logarithm of Henry’s law constant versus reciprocal temperature for ethanol.

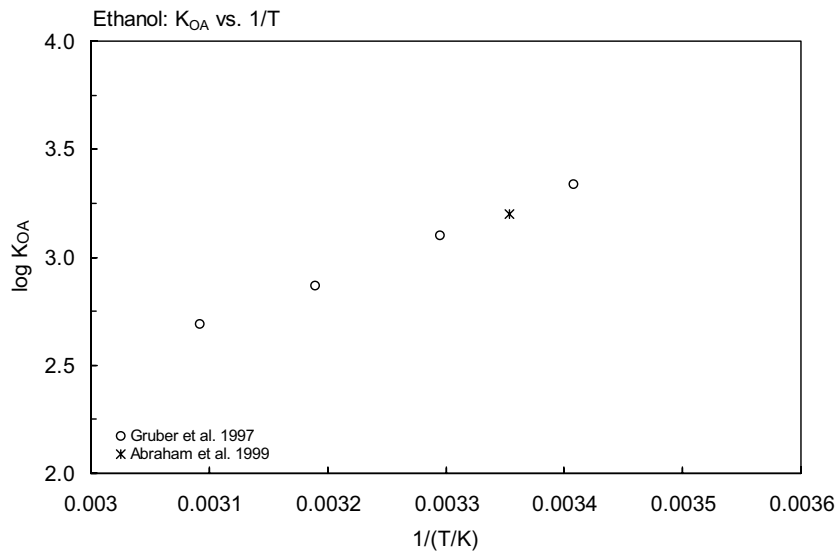
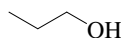


FIGURE 11.1.1.2.3 Logarithm of K_{OA} versus reciprocal temperature for ethanol.

11.1.1.3 Propanol (*n*-Propyl alcohol)

Common Name: Propanol

Synonym: propyl alcohol, 1-propanol, *n*-propyl alcohol

Chemical Name: propanol, propyl alcohol, *n*-propyl alcohol

CAS Registry No: 71-23-8

Molecular Formula: C₃H₈O, CH₃CH₂CH₂OH

Molecular Weight: 60.095

Melting Point (°C):

−124.39 (Lide 2003)

Boiling Point (°C):

97.2 (Lide 2003)

Density (g/cm³ at 20°C):

0.8035 (Weast 1982–83)

0.8037 (Dean 1985)

Molar Volume (cm³/mol):

75.1 (calculated-density, Rohrschneider 1973)

81.4 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK:

19.4 (pK_s, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.372 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

> 3.1 × 10⁶ (Booth & Everson 1948)

miscible (Dean 1985; Riddick et al. 1986, Yaws et al. 1990))

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2844 (saturated vapor density-gas saturation, Puck & Wise 1946)

2594* (interpolated-regression of tabulated data, temp range −15 to 97.8°C, Stull 1947)

10990* (48.14°C, measured range 48.14–97.1°C, Brown & Smith 1959)

2720* (ebulliometry-differential thermal analysis, measured range 19.3–97.3°C, Kemme & Kreps 1969)

log (P/mmHg) = 8.18894 − 1690.864/(221.346 + t/°C); temp range 19.3–97.3°C, or pressure range 14.7–758.5 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

2798* (comparative ebulliometry, measured range 60.2–104.5°C, Ambrose & Sprake 1970)

log (P/Pa) = 6.74390 − 1365.579/(T/K − 82.093); restricted temp range 60.2–81.2°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 6.87613 − 1441.705/(T/K − 74.291); temp range 60.2–104.5°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/mmHg) = [−0.2185 × 10421.1/(T/K)] + 8.937293; temp range −15 to 250°C (Antoine eq., Weast 1972–73)

2744 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.97878 − 1497.734/(204.094 + t/°C); temp range 48.14–94.36°C (Antoine eq. from reported exptl. data of Brown & Smith 1959, Boublik et al. 1984)

log (P/kPa) = 6.87065 − 1438.587/(198.552 + t/°C); temp range 60.2–104.6°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

2780 (interpolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.84767 − 1499.21/(204.64 + t/°C); temp range 2–120°C (Antoine eq., Dean 1985, 1992)

2798 (Riddick et al. 1986)

log (P/kPa) = 6.87613 − 1441.705/(198.859 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

- $\log (P_L/\text{kPa}) = 6.86874 - 1437.906/(-74.621 + T/\text{K})$; temp range 333–378 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.74195 - 1364.911/(-82.114 + T/\text{K})$; temp range 356–378 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.7592 - 2506/(T/\text{K})$; temp range 200–228 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.74403 - 1366.08/(-81.994 + T/\text{K})$; temp range 356–376 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.87377 - 1440.743/(-74.344 + T/\text{K})$; temp range 333–376 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.58415 - 1273.365/(-92.178 + T/\text{K})$; temp range 369–407 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 31.5155 - 3.457 \times 10^3/(T/\text{K}) - 7.5235 \cdot \log (T/\text{K}) - 4.287 \times 10^{-11} \cdot (T/\text{K}) + 1.3029 \times 10^{-7} \cdot (T/\text{K})^2$;
 temp range 124–537 K (vapor pressure eq., Yaws 1994)
 6939 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)
 9470 (45.43°C, vapor-liquid equilibrium VLE data, measured range 45.43–58.9°C, Pasanen et al. 2004)
 5876 (37.02°C, ebulliometric method, measured range 310.17–356.7 K, Lubomska & Malanowski 2004)
 $\log (P/\text{kPa}) = 7.219284 - 1629.492/[(T/\text{K}) - 57.556]$; temp range 310.17–356.7 K (Antoine eq., ebulliometric method, Lubomska & Malanowski 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.694 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 0.620 (entrainment method-GC, Burnett 1963)
 0.683 (exptl., Hine & Mookerjee 1975)
 0.699; 0.710 (calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
 0.751* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 0.683 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 0.925 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.683, 0.942 (quoted, correlated-molecular structure, Russell et al. 1992)
 0.715 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 1.034 (solid-phase microextraction SPME-GC, Bartelt 1997)
 0.372 (wetted-wall column-GC, Altschuh et al. 1999)
 0.802 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{\text{AW}} = 11.830 - 5923.2/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
 0.490 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 6.955 - 3123/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.34 (shake flask-GC, Hansch & Anderson 1967)
 0.30 (shake flask-GC, Dillingham et al. 1973)
 0.25 ± 0.01 (shake flask-GC, Leo et al. 1975)
 0.29 (Hansch & Leo 1979)
 0.32 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 0.25 (recommended, Sangster 1989)
 0.25 (recommended value, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.85* (20.29°C, from GC determined γ^∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
 3.20 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.069 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

0.37	(calculated-MCI χ , Gerstl & Helling 1987)
0.48	(soil, quoted exptl., Meylan et al. 1992)
0.12	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
0.48	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated * data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (2.3 \pm 0.2) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for the oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 2 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 2.8$ d (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{OH} = (5.33 \pm 0.53) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

$k = (0.37 \pm 0.04) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{exptl}) = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 5.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = (5.34 \pm 0.29) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{OH} = 5.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 4.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 5.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (5.64 \pm 0.48) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (5.50 \pm 0.44) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 6.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation $71.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water:

Groundwater:

Sediment:

Soil:

Biota

TABLE 11.1.1.3.1
Reported vapor pressures of propanol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log P = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Brown & Smith 1959		Kemme & Kreps 1969		Ambrose & Sprake 1970	
summary of literature data				differential thermal analysis		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
ebulliometry							
–15.0	133.1	48.14	10990	19.3	1960	60.168	20438
5.0	666.6	48.16	10996	19.8	1987	65.599	26579
14.7	1333	48.18	11018	24.5	2720	70.255	33024
25.3	2666	54.52	15405	30.3	3920	74.507	40001
36.4	5333	61.51	21851	30.3	3933	78.022	46676
43.5	7999	65.80	26867	35.2	5293	81.174	53435
52.8	13332	70.09	32831	41.3	7519	83.931	59974
66.8	26664	74.56	40177	48.1	10839	86.490	66638
82.0	53329	81.11	53379	55.4	16052	88.856	73334
97.8	101325	97.08	101358	65.7	26584	91.026	79952
mp/°C	–127	97.09	101331	74.6	39997	93.143	86877
		97.10	101393	86.6	66461	94.955	93192
		86.0	65456	97.3	101125	96.837	100132
		91.13	80472			97.595	103031
		94.36	91342	Antoine eq.		98.513	106666
				eq. 2	P/mmHg	100.155	113408
		A	8.18894	101.666	119903		
		B	1690.864	103.166	126648		
		C	221.346	104.515	133259		
				ΔH _v /(kJ mol ^{–1})			
				at bp	56.066		

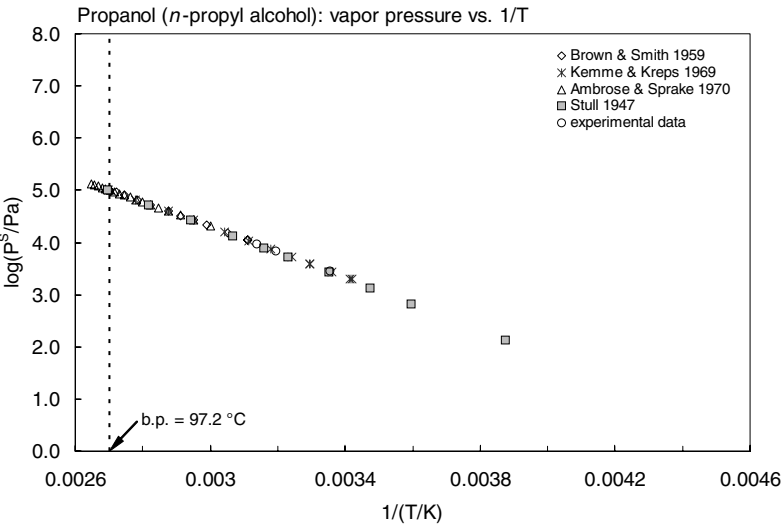


FIGURE 11.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for propanol.

TABLE 11.1.1.3.2

Reported Henry's law constants and octanol-air partition coefficients of propanol at various temperatures

Henry's law constant		log K _{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
0	0.0757	20.29	3.85
25	0.7512	30.3	3.56
		40.4	3.33
		50.28	3.11
enthalpy of transfer: $\Delta H/(\text{kJ mol}^{-1}) = 58.576$			

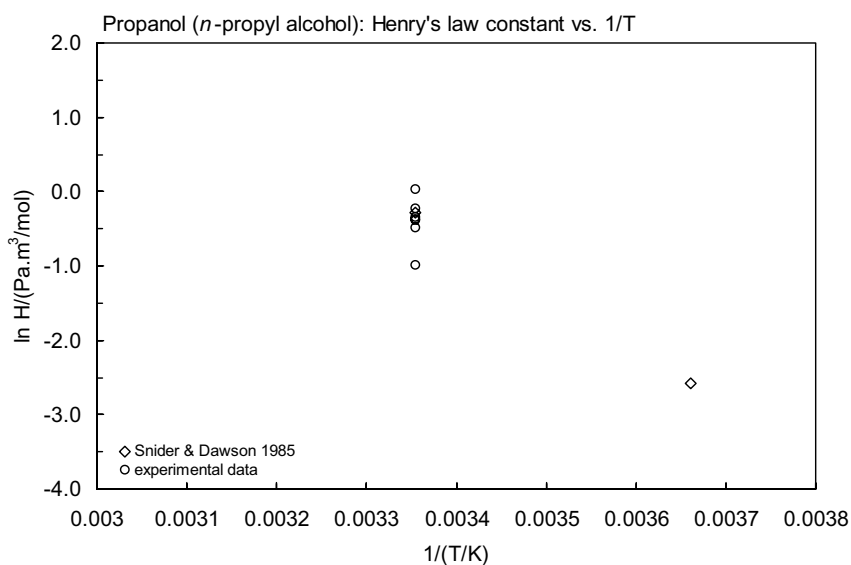
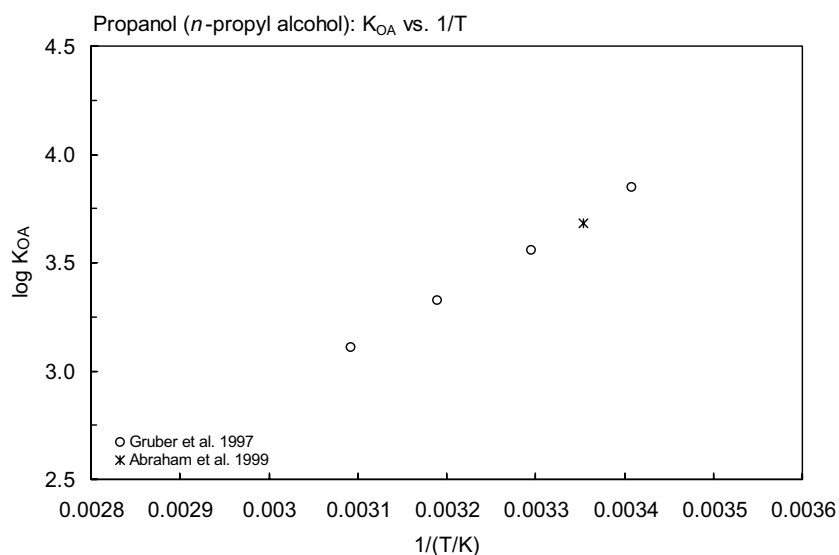


FIGURE 11.1.1.3.2 Logarithm of Henry's law constant versus reciprocal temperature for propanol.

FIGURE 11.1.1.3.3 Logarithm of K_{OA} versus reciprocal temperature for propanol.

11.1.1.4 Isopropanol (*i*-Propyl alcohol)

Common Name: Isopropanol

Synonym: isopropyl alcohol, 2-propanol, *i*-propyl alcohol, dimethylcarbinol, *sec*-propylalcohol, perspirit, petrohol, avantine, IPA

Chemical Name: isopropanol, isopropyl alcohol, *i*-propyl alcohol

CAS Registry No: 67-63-0

Molecular Formula: C_3H_8O , $CH_3(CH_3)CHOH$

Molecular Weight: 60.095

Melting Point ($^{\circ}C$):

−87.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

82.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7812 ($25^{\circ}C$, Butler et al. 1935)

0.7855 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

76.8 (calculated-density, Rohrschneider 1973)

81.4 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

17.1 (Serjeant & Dempsey 1979; Howard 1990)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.406 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

$> 3.1 \times 10^6$ (Booth & Everson 1948)

miscible (Dean 1985; Riddick et al. 1986; Howard 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5866* (static method-isoteniscope, measured 0 – $90^{\circ}C$, Parks & Barton 1928)

5700* (interpolated-regression of tabulated data, temp range -26.1 to $82.5^{\circ}C$, Stull 1947)

5775* (comparative ebulliometry, measured range 52.323 – $89.261^{\circ}C$, Ambrose & Sprake 1970)

$\log(P/Pa) = 6.73896 - 1290.345/(T/K - 82.778)$; restricted temp range 52.3 – $71.1^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log(P/Pa) = 6.86618 - 1360.131/(T/K - 75.558)$; temp range 52.3 – $89.3^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log(P/mmHg) = [-0.2185 \times 10063.5/(T/K)] + 7.805751$; temp range -91 to $160^{\circ}C$ (Antoine eq., Weast 1972–73) 4266, 7588 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

5070; 5700 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.86634 - 1360.183/(197.593 + t/^{\circ}C)$; temp range 52.3 – $89.26^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

$\log(P/kPa) = 6.358 - 1082.462/(166.482 + t/^{\circ}C)$; temp range 81.61 – $147.6^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6021 (calculated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 8.11778 - 1580.92/(219.61 + t/^{\circ}C)$; temp range 0 – $101^{\circ}C$ (Antoine eq., Dean 1985, 1992)

5775 (Riddick et al. 1986)

$\log(P/kPa) = 6.86618 - 1360.131/(126.36 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.86087 - 1357.514/(-75.786 + T/\text{K})$; temp range 325–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.72348 - 1282.26/(-83.591 + T/\text{K})$; temp range 347–363 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 9.681 - 2626/(T/\text{K})$; temp range 195–228 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.73782 - 1290.039/(-82.771 + T/\text{K})$; temp range 347–363 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.86451 - 1359.473/(-75.592 + T/\text{K})$; temp range 325–363 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.61939 - 1225.439/(-89.774 + T/\text{K})$; temp range 350–383 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 38.2363 - 3.5513 \times 10^3/(T/\text{K}) - 10.031 \cdot \log(T/\text{K}) - 3.474 \times 10^{-10} \cdot (T/\text{K}) + 1.7367 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 185–508 K (vapor pressure eq., Yaws 1994)
 13806 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.814 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 0.820 (exptl., Hine & Mookerjee 1975)
 1.159, 0.710 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
 0.80* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 1.131 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 3.16* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 $\ln (1/K_{AW}) = -10.6 + 5413/(T/\text{K})$; temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
 0.820, 0.715 (quoted, correlated-molecular structure, Russell et al. 1992)
 1.091 (gas stripping-GC, Altschuh et al. 1999)
 5.55 (EPICS-GC, Ayuttaya et al. 2001)
 0.521 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 5.576 - 2757/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 2.186 – 0.666 (27°C, equilibrium headspace-GC, solute concn 12.31–125.08 mg/L, measured range 300–315 K, Cheng et al. 2003)
 2.186* (27°C, equilibrium headspace-GC, measured range 27–42°C, Cheng et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.14 (Leo et al. 1969; Hansch & Dunn III 1972)
 0.05 (shake flask-GC, Dillingham et al. 1973)
 0.05 (Hansch & Leo 1985)
 0.14 (HPLC- k' correlation, Funasaki et al. 1986)
 0.55 (UNIFAC activity coefficient, Banerjee & Howard 1988)
 0.05 (recommended, Sangster 1989, 1993)
 0.05 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.54* (20.29°C, from GC determined γ^∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
 3.38 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: the estimated $t_{1/2} \sim 3.6$ d for evaporation from water 1 m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 197$ d to 22 yr in water, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 4.1 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 1.3$ d (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{OH} = (5.48 \pm 0.55) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(296 \pm 2) \text{ K}$ (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

$k_{OH} = 4.3 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k = (1.9 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2-6 and 20-23°C (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 6.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{exptl}) = 6.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{OH}(\text{calc}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (5.81 \pm 0.34) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240-440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{NO_3} < 2.3 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (flash photolysis-absorption technique, Wallington et al. 1987; quoted, Atkinson 1991)

$k(\text{aq.}) = 3.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987b)

$k_{OH}(\text{exptl})^* = 5.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240-440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 5.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 3.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 5.21 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (5.69 \pm 1.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (5.78 \pm 0.753) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 2.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

$k = 52.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$, average rate of biodegradation based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}$ (aq. aerobic) = 24-168 h, based on unacclimated aerobic aqueous screening test data (Gellman & Heukelekian 1955; Heukelekian & Rand 1955; Price et al. 1974; Takemoto et al. 1981; Wagner 1976; selected, Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 96-672 h, based on estimated aerobic aqueous biodegradation half-life and unacclimated anaerobic aqueous screening test data (Hou et al. 1983; Sonoda & Seiko 1968; Speece 1983; selected, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 6.2\text{--}72$ h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985, 1987; quoted, Howard 1990; selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 197$ d to 22 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991);

$t_{1/2} = 26$ –168 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48$ –336 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24$ –168 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 11.1.1.4.1

Reported vapor pressures of isopropanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)			
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)			
$\log P = A - B/(C + T/K)$	(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)					
Parks & Barton 1928	Stull 1947	Ambrose & Sprake 1970				
static method/isoteniscope	summary of literature data	comparative ebulliometry				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	
0	1187	−26.1	133.1	52.323	26540	
5	1613	−7.00	666.6	56.779	33044	
10	2266	2.40	1333	60.798	40017	
15	3173	12.7	2666	64.091	46612	
20	4320	23.8	5333	67.087	53371	
25	5866	30.5	7999	69.704	59931	
30	7879	39.5	13332	72.131	66601	
35	10519	53.0	26664	74.372	73286	
40	14079	67.8	53329	76.454	79997	
45	18239	82.5	101325	78.431	86822	
50	23571			80.160	93175	
55	30318	mp/°C	−85.8	81.931	100078	
60	38464			82.958	104266	
65	48409			85.090	113416	
70	60635			86.550	120046	
75	74847			87.992	126573	
80	92232			89.261	133218	
85	112737					
90	136082					
$\Delta H_v/(\text{kJ mol}^{-1}) =$						
at 25°C	44.43					
at bp	40.166					

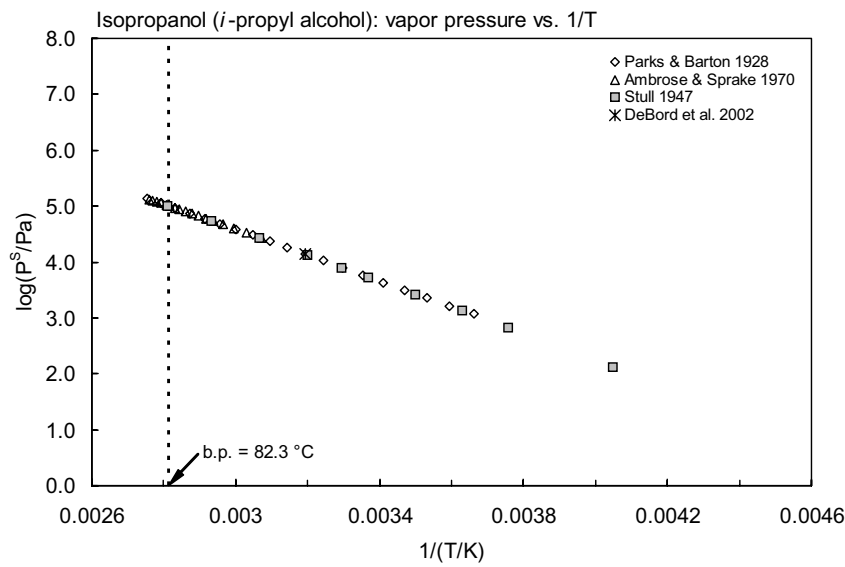


FIGURE 11.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for isopropanol.

TABLE 11.1.1.4.2
Reported Henry’s law constants and octanol-air partition coefficients of isopropanol at various temperatures

Henry’s law constant				log K _{OA}			
Snider & Dawson 1985		Kolb et al. 1992		Cheng et al. 2003		Gruber et al. 1997	
gas stripping-GC		equilibrium headspace-GC		equilibrium headspace-GC		GC det’d activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
0	0.0811	40	3.16	27	2.186	20.29	3.54
25	0.800	60	9.68	32	2.51	30.3	3.27
		70	15.94	37	3.35	40.4	3.04
		80	25.09	42	4.24	50.28	2.85
enthalpy of transfer: ΔH/(kJ mol ⁻¹) = 58.576		$\ln (1/K_{AW}) = A - B/(T/K)$					
		1/K _{AW}					
		A -10.6					
		B -5413					

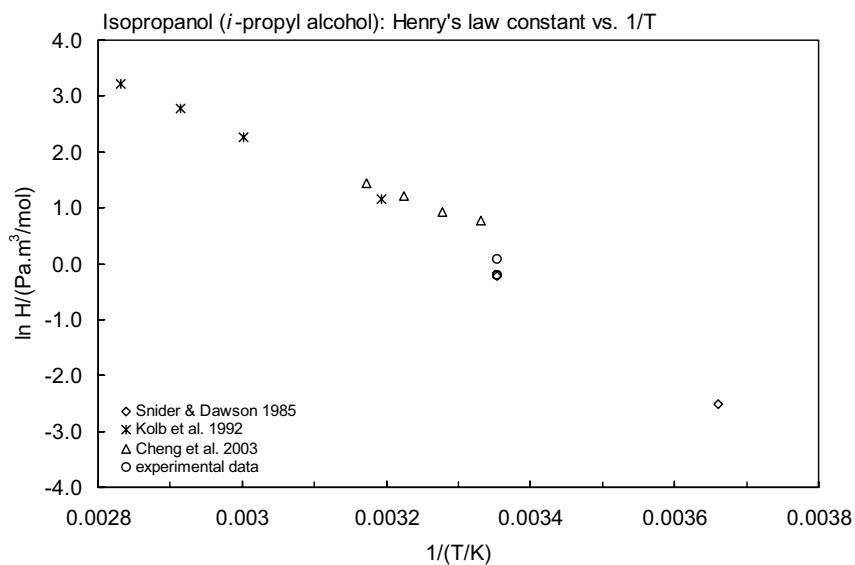


FIGURE 11.1.1.4.2 Logarithm of Henry's law constant versus reciprocal temperature for isopropanol.

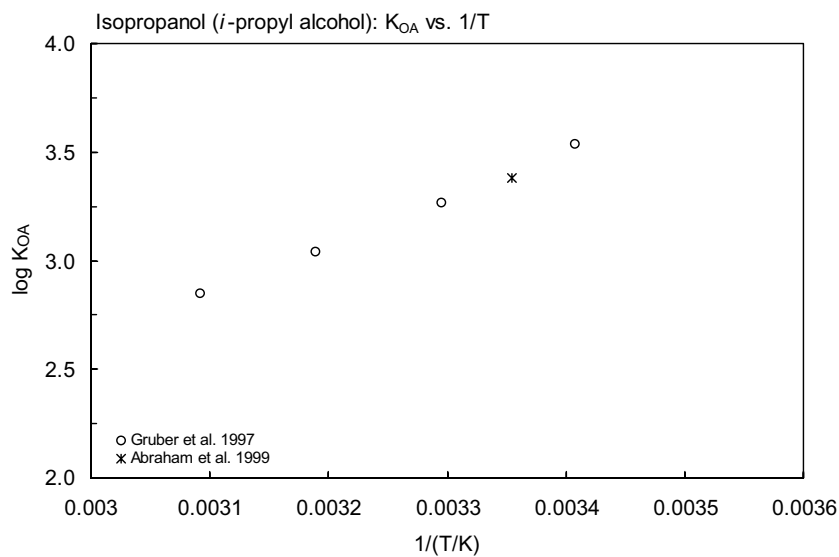
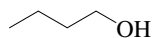


FIGURE 11.1.1.4.3 Logarithm of K_{OA} versus reciprocal temperature for isopropanol.

11.1.1.5 *n*-Butanol (*n*-Butyl alcohol)Common Name: *n*-ButanolSynonym: 1-butanol, *n*-butyl alcohol, *n*-propylcarbinolChemical Name: *n*-butyl alcohol, 1-butanol

CAS Registry No: 71-36-3

Molecular Formula: C₄H₁₀O, CH₃CH₂CH₂CH₂OH

Molecular Weight: 74.121

Melting Point (°C):

-88.6 (Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):

117.73 (Lide 2003)

Density (g/cm³ at 20°C):

0.80593 (25°C, Butler et al. 1935)

0.80980 (Weast 1982–83)

0.80956, 0.80575 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

91.7 (calculated-density, Rohrschneider 1973)

103.6 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a:

20.89 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.37 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

68120, 79000* (18, 20°C, shake flask-turbidity, Fühner 1924)

73500* (volumetric method, Hill & Malisoff 1926)

64000* (20°C, synthetic method, Jones 1929)

70800* (30°C, vapor liquid equilibrium, measured range 0–105°C, Mueller et al. 1931)

74500 (gravimetric method, Stockhart & Hull 1931)

73180 (24.85°C, shake flask-interferometer, Butler et al. 1933)

73100 (shake flask-cloud point, Butler et al. 1933)

70000 (26°C, synthetic method, Othmer et al. 1945)

73320 (shake flask-residue volume, Booth & Everson 1948)

74100 (shake flask-interferometry, Hansen et al. 1949)

73000 (shake flask-interferometry, quoted from Butler et al. 1933, Donahue & Bartell 1952)

75850 (estimated, McGowan 1954)

78700 (26.7°C, shake flask-turbidity, Skrzec & Murphy 1954)

74000 (surface tension, Kinoshita et al. 1958)

70000 (titration, Petriris & Geankopolis 1959)

75600* (20°C, synthetic method, measured range 0–125°C, von Erichsen 1962)

77800 (shake flask-GC, Korenman et al. 1974, 1975)

74000* (shake flask-colorimetric analysis, De Santis et al. 1976)

70000* (29.8°C, shake flask-refractometry, measured range 29.8–124.6°C, Aoki & Moriyoshi 1978)

63300 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

77000 (Verschuereen 1983; Howard 1990)

74000* (recommended, IUPAC solubility series, temp range 10–110°C, Barton 1984)

74500 (selected, Riddick et al. 1986)

80300*	(20°C, shake flask-GC/TC, measured range 0–90.8°C, Stephenson & Stuart 1986)
74600	(selected, Yaws et al. 1990)
65720	(shake flask-GC, Li et al. 1992)
71230	(shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

800*	(24.0°C, static method, measured range 15.1–117.6°C, Kahlbaum 1898)
904*	(24.98°C, modified isoteniscope method, measured range 24.98–101.16°C, Butler et al. 1935)
$\log (P/\text{mmHg}) = 40.2105 - 4100/(T/K) - 10.35 \cdot \log (T/K)$; temp range 25–110°C (isoteniscope measurements, Butler et al. 1935)	
819	(saturated vapor density-gas saturation, Puck & Wise 1946)
667*	(20°C, summary of literature data, temp range –1.20 to 117°C, Stull 1947)
$\log (P/\text{mmHg}) = 8.27488 - 1873.9/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)	
10274*	(64.56°C, measured range 64.56–117.56°C, Brown & Smith 1959)
820	(calculated-Antoine eq., Reid & Sherwood 1966)
733*	(22.6°C, ebulliometry-differential thermal analysis, measured range 22.6–117.8°C, Kemme & Kreps 1969)
$\log (P/\text{mmHg}) = 7.42117 - 1351.555/(179.810 + t/^\circ\text{C})$; temp range 22.6–117.8°C, or pressure range 5.5–766 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)	
910*	(comparative ebulliometry, measured range 78.558–125.686°C, Ambrose & Sprake 1970)
$\log (P/\text{Pa}) = 6.41435 - 1262.767/(T/K - 104.445)$; restricted temp range 78.558–100.74°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)	
$\log (P/\text{Pa}) = 6.54743 - 1338.769/(T/K - 96.108)$; temp range 78.558–125.686°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)	
864	(Hoy 1970)
948*	(298.11 K, measured range 283.10–323.12 K, Geiseler et al. 1973)
$\log (P/\text{mmHg}) = [-0.2185 \times 10970.5/(T/K)] + 8.929597$; temp range –1.2 to 277°C (Antoine eq., Weast 1972–73)	
868*	(24.96°C, vapor-liquid equilibrium data, temp range 281.1–323.12 K, Gmehling et al. 1982)
586, 1333	(20°C, 30°C, quoted, Verschueren 1983)
890	(interpolated-Antoine eq., Boublik et al. 1984)
$\log (P/\text{kPa}) = 6.54068 - 1335.018/(176.654 + t/^\circ\text{C})$; temp range 78.56–125.7°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)	
$\log (P/\text{kPa}) = 6.71950 - 1428.939/(185.552 + t/^\circ\text{C})$; temp range 41.5–108.8°C (Antoine eq. from reported exptl. data Kahlbaum 1898, Boublik et al. 1984)	
$\log (P/\text{kPa}) = 6.66896 - 1405.473/(183.866 + t/^\circ\text{C})$; temp range 64.5–117.56°C (Antoine eq. from reported exptl. data of Brown & Smith 1959, Boublik et al. 1984)	
$\log (P/\text{kPa}) = 6.7666 - 1460.309/(189.211 + t/^\circ\text{C})$; temp range 22.6–117.8°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)	
936	(Daubert & Danner 1985)
824	(interpolated-Antoine eq., Dean 1985)
$\log (P/\text{mmHg}) = 7.47680 - 1362.39/(178.77 + t/^\circ\text{C})$; temp range 15–131°C (Antoine eq., Dean 1985, 1992)	
910	(selected, Riddick et al. 1986)
$\log (P/\text{kPa}) = 6.54743 - 1338.769/(177.042 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)	
$\log (P_L/\text{kPa}) = 6.41661 - 1264.515/(-104.202 + T/K)$; temp range 376–399 K (Antoine eq.-I, Stephenson & Malanowski 1987)	
$\log (P_L/\text{kPa}) = 6.54172 - 1336.026/(-96.348 + T/K)$; temp range 323–413 K (Antoine eq.-II, Stephenson & Malanowski 1987)	
$\log (P_L/\text{kPa}) = 7.05559 - 1738.4/(-46.544 + T/K)$, temp range: 413–550 K, (Antoine eq.-III, Stephenson & Malanowski 1987)	
$\log (P_L/\text{kPa}) = 8.9241 - 2697/(T/K)$; temp range 209–251 K (Antoine eq.-IV, Stephenson & Malanowski 1987)	
$\log (P_L/\text{kPa}) = 6.41594 - 1264.106/(-104.251 + T/K)$; temp range 376–397 K (Antoine eq.-V, Stephenson & Malanowski 1987)	
$\log (P_L/\text{kPa}) = 6.54723 - 1339.093/(-96.03 + T/K)$; temp range 351–397 K (Antoine eq.-VI, Stephenson & Malanowski 1987)	

- 905* (298.11 K, static method-Hg manometer, measured range 283.10–323.12 K, Gracia et al. 1992)
 998 (calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 39.6673 - 4.0017 \times 10^3/(T/K) - 10.295 \cdot \log(T/K) - 3.2572 \times 10^{-10} \cdot (T/K) + 8.6672 \times 10^{-7} \cdot (T/K)^2$;
 temp range 184–563 K (vapor pressure eq., Yaws 1994)
 933* (static method-manometer, measured range 278.15–323.15 K, Garriga et al. 2002)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.866 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 0.731 (entrainment method-GC, Burnett 1963)
 0.892 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
 0.860; 0.964; 1.057 (exptl.; calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.80* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 0.860 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 4.024* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 $\ln(K_{\text{AW}}) = -10.2 + 5234/(T/K)$; temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
 0.880 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 0.868 (wetted-wall column-GC, Altschuh et al. 1999)
 1.214 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{\text{AW}} = 12.141 - 5982.0/(T/K)$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
 0.53 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 6.600 - 3009/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.83 (shake flask-CR, Collander 1951)
 0.84 (calculated- π constant, Hansch et al. 1968)
 0.88 (Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Leo 1985)
 0.84, 0.86; 0.84 (calculated-fragment const.; calculated- π constant, Rekker 1977)
 0.89 (Hansch & Leo 1979)
 0.955 (HPLC-RV/RT correlation, Yonezawa & Urushigawa 1979)
 1.02 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
 0.80 (calculated by Rekker's method, Hanai et al. 1981)
 0.79 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 0.76 (calculated from measured activity coeff. γ , Wasik et al. 1981)
 0.93 (shake flask-RC, Cornford 1982)
 0.80 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 0.87 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 0.79 (generator column-GC, Schantz & Martire 1987)
 0.80 (calculated from measured activity coeff., γ , Schantz & Martire 1987)
 0.87 (calculated- γ from UNIFAC, Banerjee & Howard 1988)
 0.823, 0.84 (calculated-CLOGP, calculated-M.O. indices, Bodor et al. 1989)
 0.84 (recommended, Sangster 1989, 1993)
 0.87 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)
 0.89 (calculated-UNIFAC activity coeff., Dallos et al. 1993)
 0.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 4.19 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- −0.439 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.85	(calculated- K_{OW} , Lyman et al. 1982)
0.64	(calculated-MCI χ , Gerstl & Helling 1987)
0.50	(soil, quoted exptl., Meylan et al. 1992)
0.39	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
0.50	(calculated- K_{OW} , Kollig 1993)
0.50	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate $k = 2.538 \times 10^{-4} \text{ mol m}^{-2} \text{ h}^{-1}$ was determined by gravimetric method with an air flow rate $k = (50 \pm 1) \text{ L h}^{-1}$ at $20 \pm 0.1^\circ\text{C}$ (Gückel et al. 1973);
estimated half-lives, $t_{1/2} \sim 2.4 \text{ h}$ in streams, $t_{1/2} \sim 3.9 \text{ h}$ in rivers and $t_{1/2} \sim 125.9 \text{ h}$ in lakes (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k = 2.2 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with $1 \times 10^{-17} \text{ M}$ hydroxyl radical in water with $t_{1/2} \sim 1 \text{ yr}$ (Anbar & Neta 1967; quoted, Howard 1990)

photooxidation $t_{1/2} = 2602\text{--}104000 \text{ h}$ in water, based on measured rate constant for reaction with OH radical in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991)

$k_{OH} = 6.8 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)

photooxidation $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$t_{1/2} = 6.5 \text{ h}$ for the vapor phase reaction with photochemically produced NO radical in the atmosphere (Dilling et al. 1976; quoted, Howard 1990)

$k_{OH} = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k = 0.58 \pm 0.06 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0-6.0 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 6.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 7.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

photooxidation $t_{1/2} = 8.8\text{--}87.7 \text{ h}$ in air, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

estimated half-life of 2.3 d for the vapor phase reaction with photochemically produced OH radical in the atmosphere (GEMS 1986; quoted, Howard 1990)

$k_{OH}(\text{exptl}) = 7.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{OH}(\text{calc}) = 6.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = (8.31 \pm 0.63) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{OH}(\text{exptl}) = 8.31 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k(\text{soln}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987b)

$k_{OH} = 8.31 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = (7.2 - 8.31) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292-296 K (review, Atkinson 1989)

$k_{OH} = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1990)

$k_{OH} = (7.80 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (8.56 \pm 0.70) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 8.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168 \text{ h}$, based on unacclimated freshwater grab sample data (Hammerton 1955) and aqueous screening test data (Bridie et al. 1979; selected, Howard et al. 1991);

$k = 84.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$, average rate of biodegradation based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}$ (aq. anaerobic) = 96–1296 h, based on acclimated screening test data (Chou et al. 1979; selected, Howard et al. 1991) and aqueous aerobic biodegradation half-life (Howard et al. 1991);

k (calc) = $(0.959 \pm 0.063) \times 10^2 \text{ h}^{-1}$ by activated sludge (Yonezawa & Urushigawa 1979)

$k = 0.035\text{--}0.046 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 6.5 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976);

$t_{1/2}$ (calc) = 1.2 d for the atmospheric reaction with $1 \times 10^{-6} \text{ molecules/cm}^3$ of OH radical (Howard 1990);

photooxidation $t_{1/2} = 8.8\text{--}87.7 \text{ h}$, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; selected Howard et al. 1991).

Surface water: $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated freshwater grab sample data (Hammerton 1955; selected, Howard et al. 1991) and aqueous screening test data (Bridie et al. 1979; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 2602\text{--}104000 \text{ h}$, based on measured rate constant for reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991);

estimated volatilization half-lives, $t_{1/2} = 2.4 \text{ h}$ in streams, $t_{1/2} = 3.9 \text{ h}$ in rivers and $t_{1/2} = 125.9 \text{ h}$ in lakes (Lyman et al. 1982; quoted, Howard 1990).

Groundwater: $t_{1/2} = 48\text{--}1296 \text{ h}$, based on estimated aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 11.1.1.5.1

Reported aqueous solubilities of 1-butanol at various temperatures

1.

Fühner 1924		Hill & Malisoff 1926		Jones 1929		Mueller et al. 1931	
synthetic method		volumetric method		synthetic method		vapor liquid equilibrium	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	104500	5	95500	0	91000	0	95500
10	90000	10	89100	20.0	64000	15	83000
20	79000	15	82100	40.0	60300	30	70800
30	71000	20	78100	60.0	60000	45	65000
40	65500	25	73500	65.0	60300	60	65200
50	63500	30	70800	80.0	64000	75	68000
60	63500	35	68300	100.0	82000	90	78000
70	65500	40	66000	107.72	97900	105	98000
80	70000	50	64600	110.0	102000		
90	78000	60	65200	120.0	147000		
100	90500	70	67300				
110	10900	80	68900				
		97.9	87400				
		114.5	127300				
		116.9	134600				
		123.3	197300				
		125.15	304400				

(Continued)

TABLE 11.1.1.5.1 (Continued)

2.

von Erichsen 1952		Aoki & Moriyoshi 1978		Barton 1984		Stephenson & Stuart 1986	
synthetic method		shake flask-refractometry		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
at 1atm							
0	103200	29.8	70000	0	104000	0	103300
10	86800	49.6	69000	5	96000	9.6	89800
20	75600	59.5	75000	10	89000	20.0	80300
30	70600	69.5	67000	15	82000	30.8	70700
40	67200	89.5	75000	20	78000	40.1	67700
50	65500	99.3	95000	25	74000	50.0	65400
69	65200	106.9	106000	30	71000	60.1	63500
70	66700	109.8	110000	35	68000	70.2	67300
80	69000	118.1	145000	40	66000	80.1	70400
90	75000	119.1	172000	50	64000	90.8	72600
100	88200	122.1	182000	60	65000		
110	110500	122.7	189000	70	67000		
120	154500	123.9	218000	75	69000		
125	235000	124.3	247000	80	70000		
		124.6	279000	85	73000		
				90	77000		
				95	83000		
				100	91000		
				105	100000		
				110	111000		
				115	130000		
De Santis et al. 1976							
shake flask-colorimetry							
20	80000						
30	79400						
40	66000						

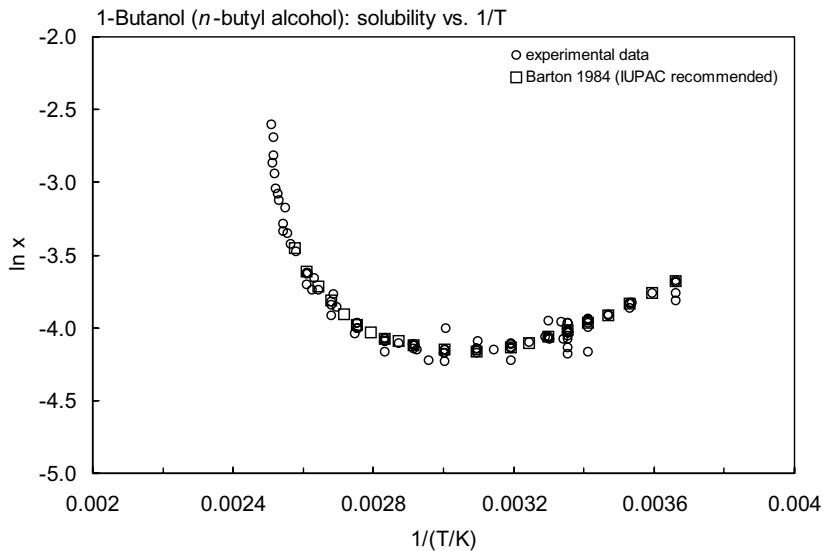


FIGURE 11.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-butanol.

TABLE 11.1.1.5.2

Reported vapor pressures of 1-butanol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & \ln P = A - B/\{(T/K) - C\} & (3a) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Kahlbaum 1898		Butler et al. 1935		Stull 1947		Brown & Smith 1959	
static method		isoteniscope method		summary of literature data			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
41.5	2866	24.98	904	-1.20	133.3	64.56	10274
44.3	3200	40.0	1276	20.0	666.6	64.74	10371
46.2	3466	45.03	1800	30.2	1333	70.15	13668
48.6	4133	50.08	4593	41.5	2666	75.39	17692
50.1	4400	60.11	8091	53.4	5333	79.00	20982
52.0	5066	70.29	13732	60.3	7999	79.02	21022
55.0	5999	80.58	22465	70.1	13332	89.14	33160
60.2	7999	90.83	35544	84.3	26664	97.33	46859
64.3	9999	101.16	77140	100.8	53329	103.3	59548
69.8	13332			117.5	101325	108.23	72038
78.1	19998	bp/°C	117.71			113.26	86855
84.3	26664	D ²⁵	0.8059	mp/°C	-79.9	117.56	131371
89.4	33330						
93.7	39997	eq. 4	P/mmHg				
97.4	46663	A	40.2105				
100.0	53329	B	4100				
103.7	59995	C	10.35				
106.3	66661						
108.8	73327	$\Delta H_v(\text{kJ mol}^{-1}) = 52.84$ at 25°C					

2.

Kemme & Kreps 1969		Ambrose & Sprake 1970		Geiseler et al. 1973		Gmehling et al. 1982	
differential thermal analysis		comparative ebulliometry		Z. Phys. Chem. 254, 261		V-L equil. data collection	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
22.6	733.3	78.558	20413	283.10	309	283.10	269
30.9	1373	84.243	26518	288.13	457	288.13	405
36.2	1973	89.212	33045	293.12	663	293.12	599
40.7	2613	93.662	39973	298.11	948	298.11	868
48.2	4133	97.357	46601	303.11	1335	303.11	1241
52.4	5280	100.743	53450	308.10	1856	308.10	1744
58.3	7373	103.636	59932	313.08	2545	313.08	2416
65.8	10852	106.367	66630	318.11	3457	318.11	3309
73.5	16185	108.884	73332	323.12	4640	323.12	4473
85.1	27731	111.162	79856				
93.8	40463	113.429	86807	ref. from	Gracia 1989		
196.5	67594	115.324	92996				

(Continued)

TABLE 11.1.1.5.2 (Continued)

Kempe & Kreps 1969		Ambrose & Sprake 1970		Geiseler et al. 1973		Gmehling et al. 1982	
differential thermal analysis		comparative ebulliometry		Z. Phys. Chem. 254, 261		V-L equil. data collection	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
117.8	102125	117.413	100142				
		119.193	106702				
Antoine eq.		120.939	113410				
eq. 2	P/mmHg	122.564	119943				
A	7.42117	124.115	126625				
B	1351.864	125.686	133323				
C	179.810						

3.

Gracia et al. 1992		Garriga et al. 2002	
static method-Hg manometer		static method-manometer	
T/K	P/Pa	T/K	P/Pa
283.10	265	278.15	192
288.13	411	283.15	230
293.12	613	288.15	453
298.11	905	293.15	635
303.11	1315	298.15	933
308.10	1831	303.15	1315
313.08	2522	308.15	1827
318.11	3420	313.15	2518
323.12	4600	318.15	3429
		323.15	4586
Antoine eq.			
eq. 3a	P/kPa		
A	12.12863		
B	2039.057		
C	132.925		

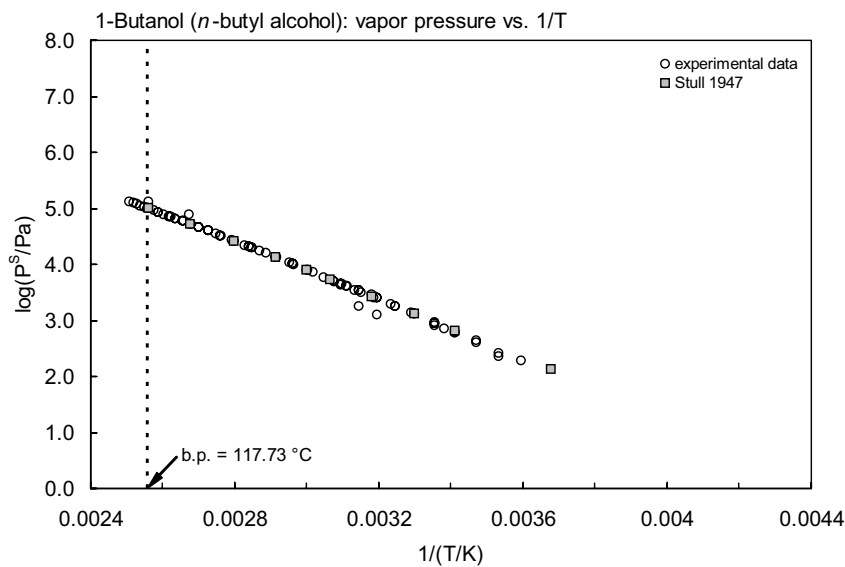


FIGURE 11.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 1-butanol.

TABLE 11.1.1.5.3
Reported Henry’s law constants of 1-butanol at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$
$$\ln (1/K_{AW}) = A - B/(T/K)$$
$$\ln (k_H/\text{atm}) = A - B/(T/K)$$
$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$
$$\log (1/K_{AW}) = A - B/(T/K)$$
$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

$$(1)$$
$$(2)$$
$$(3)$$
$$(4)$$
$$(5)$$

$$(1a)$$
$$(2a)$$
$$(4a)$$

Snider & Dawson 1985		Kolb et al. 1992	
gas stripping-GC		equilibrium headspace-GC	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
0	0.0873	40	4.024
25	0.800	60	11.64
		70	19.81
		80	29.69
enthalpy of transfer: ΔH/(kJ mol ⁻¹) = 58.576		eq. 2a	1/K _{AW}
		A	-10.2
		B	5234

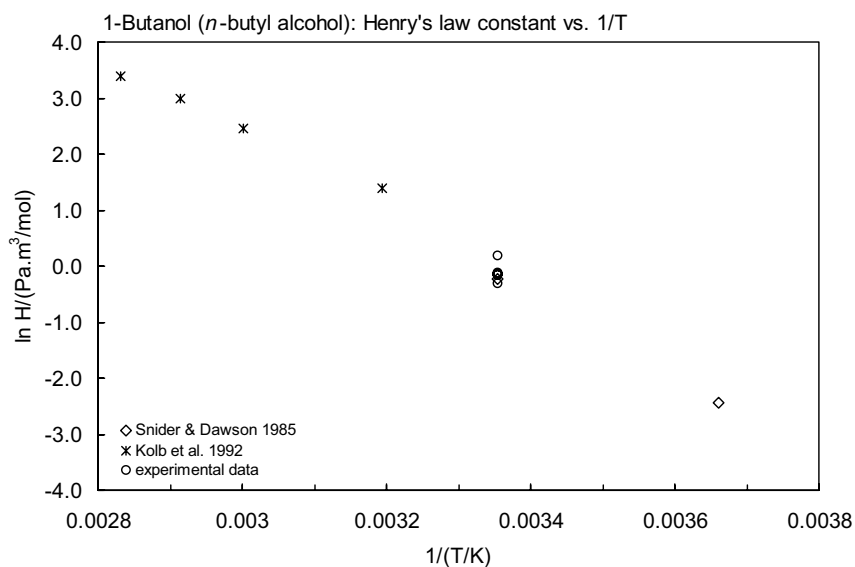
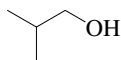


FIGURE 11.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for 1-butanol.

11.1.1.6 Isobutanol (*i*-Butyl alcohol)

Common Name: Isobutanol

Synonym: isobutyl alcohol, 2-methyl-1-propanol, *i*-butyl alcohol

Chemical Name: isobutanol, isobutyl alcohol, 2-methyl-1-propanol

CAS Registry No: 78-83-1

Molecular Formula: $C_4H_{10}O$, $(CH_3)_2CHCH_2OH$

Molecular Weight: 74.121

Melting Point ($^{\circ}C$):

−101.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

1087.89 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8018 (Weast 1982–83)

0.8016, 0.7978 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.5 ($20^{\circ}C$, calculated-density)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.32 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

100140 ($18^{\circ}C$, shake flask-turbidity, Fühner 1924)

85000 ($20^{\circ}C$, Seidell 1941)

75600 (shake flask-interferometry, Donahue & Bartell 1952)

94000 (shake flask-colorimetric, De Santis et al. 1976)

95000 ($18^{\circ}C$, Verschueren 1983)

76270 (IUPAC recommended, Barton 1984)

100000 (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1541* ($24.98^{\circ}C$, modified isoteniscope method, measured range 25 – $90^{\circ}C$, Butler et al. 1935)

$\log (P/mmHg) = 43.5513 - 4185/(T/K) - 11.50 \cdot \log (T/K)$; temp range 25 – $100^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

1648 (interpolated-regression of tabulated data, Stull 1947)

1333* ($21.7^{\circ}C$, summary of literature data, temp range -9.0 to $108^{\circ}C$, Stull 1947)

1527* (comparative ebulliometry, measured range 343.044 – $388.733\ K$, Ambrose & Sprake 1970)

$\log (P/Pa) = 6.35383 - 1194.628/(T/K - 106.291)$; restricted temp range 343 – $367.4\ K$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log (P/Pa) = 6.50091 - 1275.197/(T/K - 97.363)$; temp range 343 – $388.8\ K$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log (P/mmHg) = [-0.2185 \times 10936.0/(T/K)] + 9.1138032$; temp range -9.0 to $241^{\circ}C$ (Antoine eq., Weast 1972–73)

1527 (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.50091 - 1295.197/(t/^{\circ}C + 175.787)$, temp range not specified (Riddick et al. 1986)

$\log (P_L/kPa) = 6.34528 - 1190.463/(-106.712 + T/K)$; temp range 369 – $389\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.49241 - 1271.027/(-97.758 + T/\text{K})$; temp range 313–411 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.05055 - 1511.48/(-81.634 + T/\text{K})$; temp range 381–524 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 9.8507 - 2875/(T/\text{K})$; temp range 202–243 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.34606 - 1190.8481/(-106.673 + T/\text{K})$; temp range 369–389 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.50104 - 1275.669/(-97.269 + T/\text{K})$; temp range 342–389 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.27047 - 1147.676/(-111.933 + T/\text{K})$; temp range 383–416 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 109.2803 - 6.306 \times 10^3/(T/\text{K}) - 36.947 \cdot \log(T/\text{K}) + 1.4462 \times 10^{-2} \cdot (T/\text{K}) - 3.948 \times 10^{-13} \cdot (T/\text{K})^2$;
 temp range 165–548 K (vapor pressure eq., Yaws 1994)
 1500 (selected, Mackay et al. 1992, 1995)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

1.20 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 1.214 (exptl.- C_W/C_A , Hine & Mookerjee 1975)
 1.159, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.992 (headspace-GC, Snider & Dawson 1985)
 1.186 (calculated-MCI χ , Nirmalakhandan & Speece 1988b)
 1.84 (solid-phase microextraction SPME-GC, Bartelt 1997)
 2.73 (gas stripping-GC, Shiu & Mackay 1997)
 0.892 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.83 (shake flask-CR, Collander 1951)
 0.61 (calculated- π constant, Hansch et al. 1968)
 0.64 (Leo et al. 1969)
 0.65 (from Hansch & Dunn III unpublished result, Leo et al. 1971)
 0.76 (shake flask-GC, Dillingham et al. 1973)
 0.76 (shake flask, Hansch & Leo 1985; 1987)
 0.76 (recommended, Sangster 1989, 1993)
 0.76 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.80 (calculated-measured γ^∞ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2}(\text{calc}) = 79.7$ h for evaporation from a model river of 1-m deep with a current of 3 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982; selected, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 201$ d to 22 yr in water, based on measured rate for the reaction with OH radical in water (Anbar & Neta 1967; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 0.24$ –2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

photooxidation $t_{1/2} = 9.96\text{--}99.6$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis:

Biodegradation: biodegradation rate constant $k = 0.015\text{--}0.020$ h⁻¹ in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986)

$t_{1/2}$ (aq. aerobic) = 43–173 h, based on river die-away data for one sample of water from one river (Hammerton 1955; selected, Howard et al. 1991)

$t_{1/2}$ (aq. anaerobic) = 172–692 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation half-life of 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radicals, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976); photodecomposition $t_{1/2} = 3.5$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976); photooxidation $t_{1/2} = 9.96\text{--}99.6$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 201$ d to 22 yr, based on measured rate for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; quoted, Howard et al. 1991); $t_{1/2} = 43\text{--}173$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 86\text{--}346$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 43\text{--}173$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

biota:

TABLE 11.1.1.6.1

Reported vapor pressures of isobutanol at various temperatures and the coefficients for the equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Butler et al. 1935		Stull 1947		Ambrose & Sparke 1970	
isoteniscope method		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
24.98	1541	−9.0	133.3	343.044	20457
40.0	2196	11.0	666.6	348.552	26554
45.03	2985	21.7	1333	353.357	33057
50.08	7415	32.4	2666	357.674	39994
60.11	12778	44.1	5333	361.213	46532
70.29	21292	51.7	7999	364.531	53442
80.58	34184	61.5	13332	367.356	59959
90.83	53036	75.9	26664	369.965	66546
		91.4	53329	372.439	73326
bp/°C	82.39	108.0	101325	374.696	79983
D ²⁵	0.7812			376.846	86765

(Continued)

TABLE 11.1.1.6.1 (Continued)

Butler et al. 1935		Stull 1947		Ambrose & Sparke 1970	
isoteniscope method		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
		mp/°C	−108	378.739	93121
eq. 4	P/mmHg			380.718	100153
A	43.5513			382.476	106746
B	4185			384.166	113.417
C	11.50			385.775	120072
ΔH_v /(kJ mol ^{−1}) = 51.63				387.252	126441
at 25°C				388.773	133283

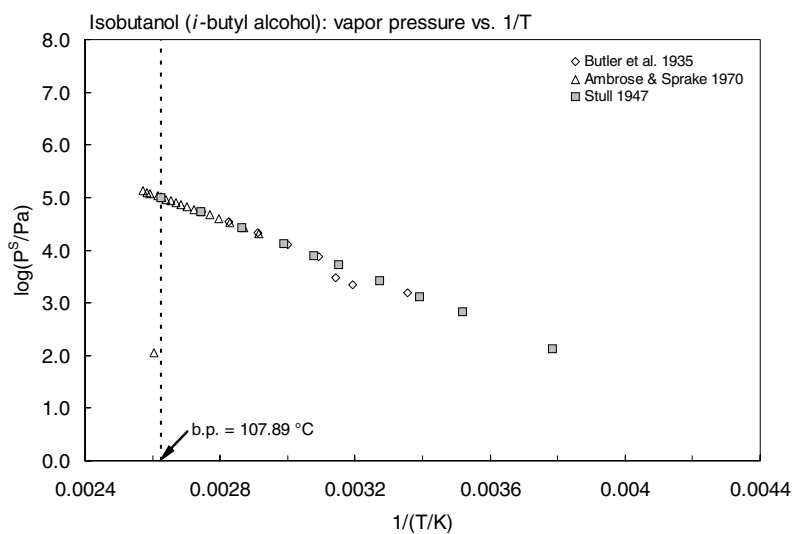
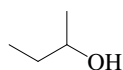


FIGURE 11.1.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for isobutanol.

11.1.1.7 *sec*-Butyl alcohol

Common Name: *sec*-Butyl alcohol

Synonym: 2-butyl alcohol, 2-butanol, methylethylcarbinol

Chemical Name: 2-butanol, *sec*-butyl alcohol

CAS Registry No: 78-92-2

Molecular Formula: $C_4H_{10}O$, $CH_3CH_2CHOHCH_3$

Molecular Weight: 74.121

Melting Point ($^{\circ}C$):

−88.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

99.51 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8063 (Weast 1982–83)

0.8065, 0.8024 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

91.9 ($20^{\circ}C$, calculated-density)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

200000 ($20^{\circ}C$, synthetic method, Jones 1929)

185000 ($20^{\circ}C$, shake flask, Evans 1936)

198000* ($20^{\circ}C$, shake flask-refractometer, measured range 20 – $85^{\circ}C$, Morachevskii & Popovich 1965)

177000, 165000 (25 , $35^{\circ}C$, shake flask-titration, Ratouis & Dodé 1965)

202000* ($20^{\circ}C$, equilibrium pressure cell/shake flask-refractometric method, measured range 10 – $110^{\circ}C$, pressure range 1 – 800 atm, Moriyoshi et al. 1975)

225000 (shake flask-colorimetric analysis, De Santis et al. 1976)

130000 (shake flask-refractometric method, Becke & Quitzch 1977)

187000* (equilibrium pressure vessel/shake flask-GC, measured range 265 – $372 K$, pressure range 0.1 – 75 MPa, Bozdog & Lamb 1983)

181000* (recommended, IUPAC solubility series, temp range 10 – $110^{\circ}C$, Barton 1984)

196000* ($20^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.2^{\circ}C$, Stephenson & Stuart 1986)

175340* ($25.28^{\circ}C$, shake flask-laser scattering technique, measured range 276.94 – $386.6 K$, Ochi et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2286* (modified isoteniscope method, measured range 25 – $91^{\circ}C$. Butler et al. 1935)

$\log (P/mmHg) = 43.4800 - 4110/(T/K) - 11.50 \cdot \log (T/K)$; temp range 25 – $90^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

2266* (interpolated-regression of tabulated data, temp range -12.2 to $99.5^{\circ}C$, Stull 1947)

33031* ($73.392^{\circ}C$, ebulliometry, measured range 73.392 – $107.146^{\circ}C$, Biddiscombe et al. 1954)

10610* ($49.730^{\circ}C$, measured range 49.730 – $99.410^{\circ}C$, Brown et al. 1969)

2317* (comparative ebulliometry, measured range 67.723 – $107.743^{\circ}C$, Ambrose & Sprake 1970)

$\log (P/Pa) = 6.26852 - 1126.667/(T/K - 108.361)$; restricted temp range 67.7 – $83.34^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log (P/Pa) = 6.86618 - 1360.131/(T/K - 75.558)$; temp range 67.723 – $107.743^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

2357 (Hoy 1970)

$\log(P/\text{mmHg}) = [-0.2185 \times 10712.3/(T/K)] + 9.096778$; temp range -12.2 – 251°C (Antoine eq., Weast 1972–73)
1600, 3200 (20°C, 30°C, Verschuereen 1983)

2200, 2190, 2275 (extrapolated-Antoine equations, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.35079 - 1169.924/(169.731 + t/^\circ\text{C})$; temp range 67.7 – 107.14°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.32690 - 1157.363/(168.32 + t/^\circ\text{C})$; temp range 72.39 – 107.15°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1954, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.47826 - 1235.4/(176.82 + t/^\circ\text{C})$; temp range 49.73 – 99.41°C (Antoine eq. from reported exptl. data of Brown et al. 1969, Boublik et al. 1984)

2438 (calculated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 7.47431 - 1314.31/(186.55 + t/^\circ\text{C})$; temp range 25 to 120°C (Antoine eq., Dean 1985, 1992)

2317 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.35457 - 1171.893/(t/^\circ\text{C} + 169.955)$, temp range not specified (Riddick et al. 1986)

$\log(P_L/\text{kPa}) = 6.26823 - 1126.887/(-108.291 + T/K)$; temp range 359 – 381 K (Antoine eq-I., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.34976 - 1169.754/(-103.388 + T/K)$; temp range 3039 – 403 K (Antoine eq-II., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.74369 - 735.87/(-176.795 + T/K)$; temp range 372 – 5241 K (Antoine eq-III., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 7.50959 - 1751.931/(-52.906 + T/K)$; temp range 210 – 303 K (Antoine eq-IV., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.2663 - 1125.853/(-108.414 + T/K)$; temp range 359 – 380 K (Antoine eq-V., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.35314 - 1171.484/(-103.199 + T/K)$; temp range 340 – 379 K (Antoine eq-VI., Stephenson & Malanowski 1987)

2440, 997 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 49.4476 - 4.2487 \times 10^3/(T/K) - 13.793 \cdot \log(T/K) + 6.2736 \times 10^{-11} \cdot (T/K) + 2.1988 \times 10^{-6} \cdot (T/K)^2$;
temp range 158 – 536 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.040 (measured partial pressure/mole fraction x at dilute concn, Butler 1935)

1.033 (exptl., Hine & Mookerjee 1975)

1.60, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.918* (headspace-GC, measured range 0 – 25°C , Snider & Dawson 1985)

1.107 (calculated-MCI χ , Nirmalakhandan & Speece 1988b)

0.604 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 6.734 - 3031/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.61 (shake flask-GC, Hansch & Anderson 1967; Hansch et al. 1968)

0.74, 0.64 (calculated-f const., calculated- π const., Rekker 1977)

0.81 (HPLC-RT correlation, Yonezawa & Urushigawa 1979)

0.87 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

0.65 (recommended, Sangster 1989)

0.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.99* (20.29°C , from GC determined γ^∞ in octanol, measured range 20.29 – 50.28°C , Gruber et al. 1997)

3.80 (calculated from determined γ^∞ in octanol and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 129$ d to 23 yr, based on measured rate for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 0.24$ – 2.4 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 4.1 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for at 25°C with $t_{1/2} = 1.3$ d (Hendry & Kenley 1979; quoted, Mill 1982)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 24$ – 168 h, based on river die-away studies (Hammerton 1955; selected, Howard et al. 1991) and aqueous anaerobic $t_{1/2} = 96$ – 672 h, based on estimated aqueous aerobic biodegradation half-life (selected, Howard et al. 1991);

average rate of biodegradation $k_B = 55.0 \text{ (mg COD g}^{-1} \text{ h}^{-1})$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.24$ – 2.4 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 4.0$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976);

photooxidation $t_{1/2} = 7.2$ – 72 h, based on measured rate constant for the reaction with OH radical in air (Edney & Corse 1986; selected, Howard et al. 1991);

calculated lifetimes of 1.3 d and 17 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000)

Surface water: $t_{1/2} = 24$ – 168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48$ – 336 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24$ – 168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 11.1.1.7.1

Reported aqueous solubilities of sec-butyl alcohol at various temperatures

1.

Morachevskii & Popovich '65		Moriyoshi et al. 1975		Bozdag & Lamb 1983		Barton 1984	
shake flask-refractometry		shake flask-refractometry		equil. pressure cell-GC		IUPAC recommended	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
			at 1 atm		at 0.1 MPa		
20	198000	10	239000	–8	271000	10	239000
40	146000	20	202000	–6	266000	20	199000
60	140000	27	179000	–4	266000	25	181000
80	140000	40	149000	–3	263000	30	175000

(Continued)

TABLE 11.1.1.7.1 (Continued)

Morachevskii & Popovich '65		Moriyoshi et al. 1975		Bozdag & Lamb 1983		Barton 1984	
shake flask-refractometry		shake flask-refractometry		equil. pressure cell-GC		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
85	150000	50	132000	0	264000	35	163000
		60	128000	2	256000	40	155000
		70	129000	5	249000	50	140000
		80	138000	10	232000	60	142000
		90	155000	15	228000	70	138000
		100	183000	20	203000	80	143000
		110	239000	25	187000	90	158000
				30	171000	100	186000
						110	239000
		measured range 283–378 K pressure range 1–800 atm full list of data see ref.		measured range 265–372 K pressure range 0.1–75 MPa full list of data see ref.			

2.

Stephenson & Stuart 1986		Ochi et al. 1996			
shake flask-GC/TC		laser scattering technique			
t/°C	S/g·m ⁻³	T/K	mole frac. x	T/K	mole frac. x
0	260000	276.94	0.0738	362.51	0.0406
10	235000	278.13	0.0725	364.96	0.0421
20	196000	279.96	0.0705	370.41	0.0459
29.9	170000	284.94	0.0642	376.89	0.0530
40	151000	289.08	0.0590	379.76	0.0573
50	140000	290.58	0.0571	381.25	0.0621
60.3	134000	292.18	0.0553	383.23	0.0680
70.1	133000	295.15	0.0522	384.39	0.0751
80.1	136000	298.43	0.0491	385.63	0.0820
90.2	145000	301.48	0.0471	386.04	0.0908
		305.14	0.0452	386.23	0.0965
		309.16	0.0421	386.58	0.1050
		311.88	0.0406	386.65*	0.1151
		314.10	0.0393	*the upper critical solution point	
		321.88	0.0371		
		324.99	0.0361		
		332.50	0.0342		
		340.01	0.0342		
		349.30	0.0361		
		352.25	0.0371		
		360.81	0.0393		

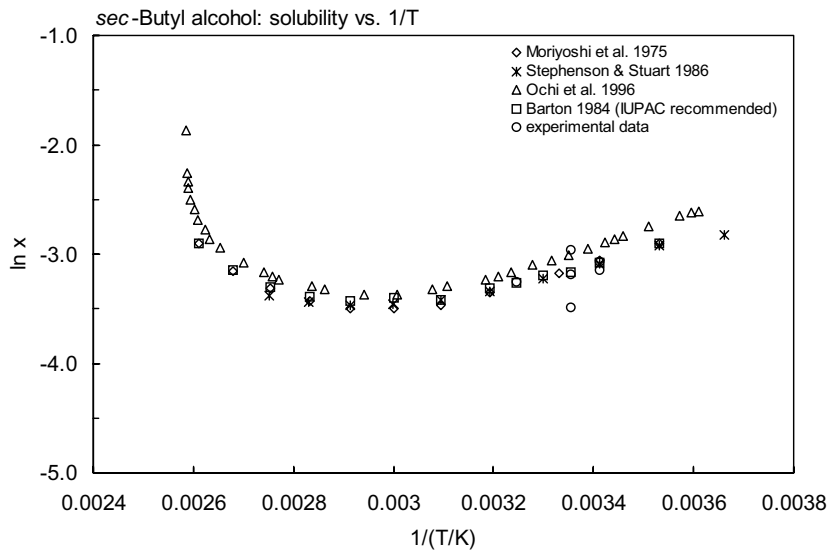


FIGURE 11.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for sec-butyl alcohol.

TABLE 11.1.1.7.2
Reported vapor pressures of sec-butyl alcohol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)

log P = A – B/(C + t/°C)

log P = A – B/(C + T/K)

log P = A – B/(T/K) – C·log (T/K)

(1)

(2)

(3)

(4)

ln P = A – B/(T/K)

ln P = A – B/(C + t/°C)

(1a)

(2a)

1.

Butler et al. 1935		Stull 1947		Biddiscombe et al. 1954		Brown et al. 1969	
isoteniscope method		summary of literature data		ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	2286	–12.2	133.3	73.392	33031	49.730	10610
40.0	3272	7.20	666.6	76.600	39942	54.050	13402
45.03	4440	16.9	1333	80.131	46616	57.740	16271
50.08	10764	27.3	2666	83.340	53447	62.020	20198
60.12	18452	38.1	5333	86.112	39983	67.498	16382
70.3	29878	45.2	7999	88.693	66641	72.180	32861
80.59	47356	54.1	13332	91.068	73266	76.970	40792
90.84	72407	67.9	26664	93.303	80010	83.060	53067
		83.9	53329	95.394	86761	88.450	66274
bp/°C	99.95	99.5	101325	97.252	93093	94.160	83033
D ²⁵	0.8029			99.201	100155	99.410	101321
		mp/°C	–114.7	100.931	106774		
eq. 4	P/mmHg			120.611	113533		
A	43.4800			104.186	120168		
B	4110			105.647	126596		
C	11.50			107.146	133.471		
ΔH _v /(kJ mol ^{–1}) = 50.21							
at 25°C							

(Continued)

TABLE 11.1.1.7.2 (Continued)

2.

Ambrose & Sprake 1970

comparative ebulliometry

t/°C	P/Pa
67.723	26556
72.392	33031
76.601	39942
80.131	46616
83.340	53447
86.111	59984
88.693	66641
91.067	73284
93.303	81010
95.394	86759
97.253	93095
99.201	100154
100.931	106775
102.611	113530
104.186	120167
105.647	126593
107.143	133470

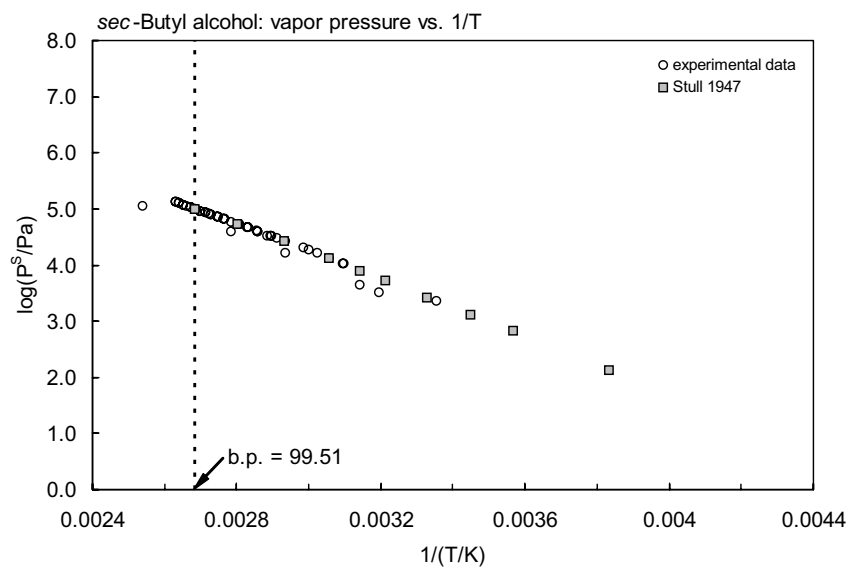


FIGURE 11.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for sec-butyl alcohol.

TABLE 11.1.1.7.3
Reported Henry’s law constants and octanol-air partition coefficients of *sec*-butyl alcohol at various temperatures

Henry’s law constant		log K _{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det’d activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
0	0.0987	20.29	3.98
25	0.9180	30.3	3.68
		40.4	3.44
		50.28	3.22
enthalpy of transfer: ΔH/(kJ mol ⁻¹) = 58.576			

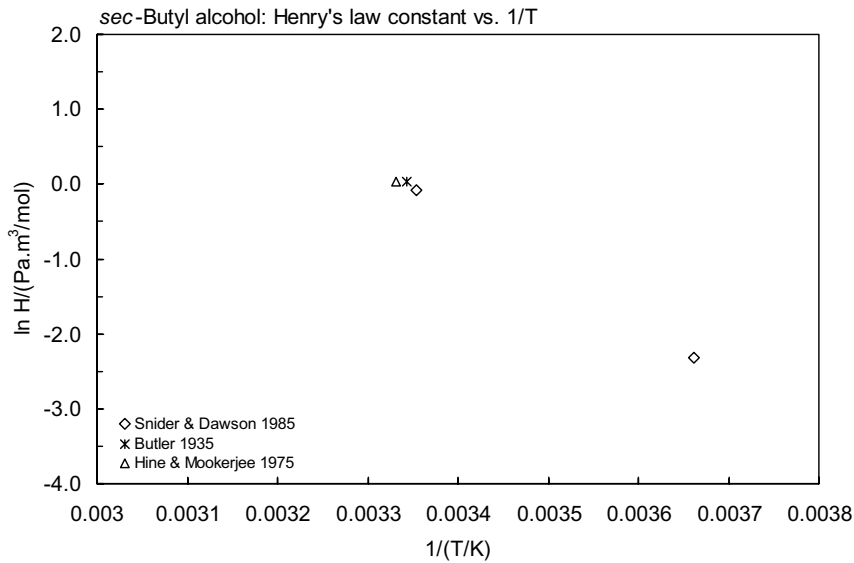


FIGURE 11.1.1.7.3 Logarithm of Henry’s law constant versus reciprocal temperature for *sec*-butyl alcohol.

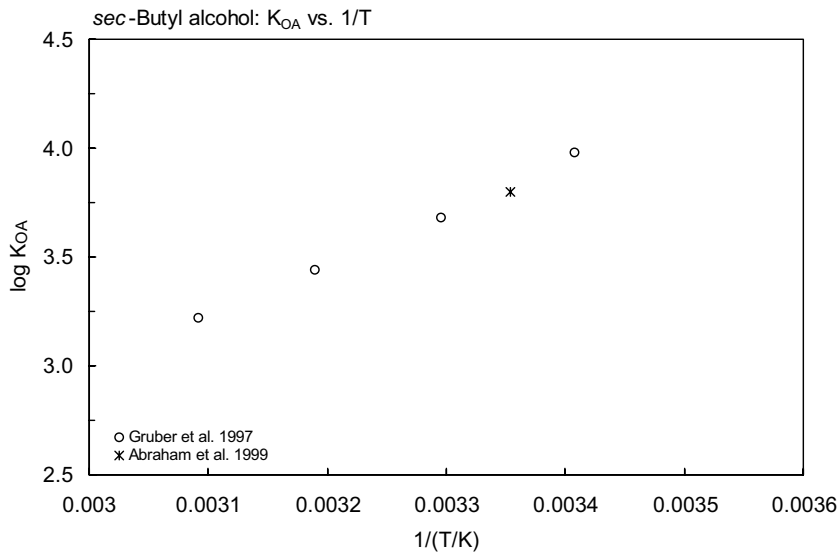


FIGURE 11.1.1.7.4 Logarithm of K_{OA} versus reciprocal temperature for *sec*-butyl alcohol.

11.1.1.8 *tert*-Butyl alcohol

Common Name: *tert*-Butyl alcohol

Synonym: 3-butanol, *t*-butyl alcohol, 2-methyl-2-propanol, trimethylcarbinol,

Chemical Name: *t*-butanol, *t*-butyl alcohol, 2-methyl-2-propanol

CAS Registry No: 75-65-0

Molecular Formula: C₄H₁₀O, (CH₃)₃COH

Molecular Weight: 74.121

Melting Point (°C):

25.69 (Lide 2003)

Boiling Point (°C):

82.4 (Lide 2003)

Density (g/cm³ at 20°C):

0.78581, 0.78086 (20°C, 25°C, Dreisbach & Martin 1949)

0.7883 (Weast 1982–83)

0.7858 (Dean 1985)

0.7812 (25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

94.2 (calculated-density, Rohrschneider 1973)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.64 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

22.76, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Palit 1947; Riddick et al. 1986)

miscible (Barton 1984; Dean 1985; Howard 1990; Yaws et al. 1990)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5600* (static method/isoteniscope, measured range 20–90°C, Parks & Barton 1928)

5654* (24.98°C, modified isoteniscope method, measured range 30–80°C, Butler et al. 1935)

log (P/mmHg) = 43.2834 – 3935/(T/K) – 11.50·log (T/K); temp range 30–80°C (isoteniscope measurements, Butler et al. 1935)

5019* (interpolated-regression of tabulated data, temp range –20.4 to 82.9°C, Stull 1947)

log (P/mmHg) = 8.24380 – 1675.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

16500* (43.34°C, measured range 43.34–82.41°C, Dreisbach & Shrader 1949)

5637* (comparative ebulliometry, measured range 329.946–362.710 K, Ambrose & Sprake 1970)

log (P/Pa) = 6.24072 – 1049.320/(T/K – 107.724); restricted temp range 329.946–345.288 K (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 6.35648 – 1107.060/(T/K – 101.048); temp range 329.946–362.71 K (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/mmHg) = [–0.2185 × 10413.2/(T/K)] + 9.193472; temp range –20.4 to 222.5°C (Antoine eq., Weast 1972–73)

5600 (Verschueren 1983; Howard et al. 1986)

5637 (selected, Riddick et al. 1986)

log (P/kPa) = 6.35648 – 1107.060/(t/°C + 172.102) temp not specified (Riddick et al. 1986)

log (P_L/kPa) = 6.22619 – 1042.416/(–108.5 + T/K); temp range 347–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)

- $\log (P_L/\text{kPa}) = 6.35045 - 1104.341/(-101.315 + T/\text{K})$; temp range 299–375 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.27388 - 989.74/(-124.966 + T/\text{K})$; temp range 356–480 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.23125 - 1044.891/(-108.211 + T/\text{K})$, temp range: 347–363 K, (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.35498 - 1106.556/(-101.071 + T/\text{K})$; temp range 329–363 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.09542 - 975.944/(-116.864 + T/\text{K})$; temp range 357–461 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 1008, 5600 (calculated-solvatochromic parameters, quoted lit., Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 71.8181 - 4.9966 \times 10^3/(T/\text{K}) - 21.805 \cdot \log(T/\text{K}) + 1.9238 \times 10^{-8} \cdot (T/\text{K}) + 5.8247 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 299–506 K (vapor pressure eq., Yaws 1994)
 5610* (static method-manometer, measured range 298.15–323.15 K, Garriga et al. 2002)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1.210 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 1.214 (exptl., Hine & Mookerjee 1975)
 1.057, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 1.460* (25°C headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 1.426 (calculated-MCI χ , Nirmalakhandan & Speece 1988b)
 0.917 (wetted-wall column-GC, Altschuh et al. 1999)
 0.907 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 8.467 - 3488/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.37 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1969)
 0.59 (HPLC-RT correlation, Yonezawa & Urushigawa 1979)
 0.35 (Hansch & Leo 1985)
 0.40 (calculated-solvatochromic parameters, Taft et al. 1985)
 0.39 (HPLC- k' correlation, Funasaki et al. 1986)
 0.34 (shake flask, Log P Database, Hansch & Leo 1987)
 0.35 (recommended, Sangster 1989)
 0.34 (calculated-UNIFAC activity coefficient, Dallos et al. 1993)
 0.35 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 3.50 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.46 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.57 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated half-lives, $t_{1/2} = 51.6$ h in streams, $t_{1/2} = 65.37$ h in rivers and $t_{1/2} = 3104.3$ h in lakes were estimated by using Henry's law constant and assuming the wind velocity to be 3 m/s, the current velocities of the streams, rivers, and lakes 2, 1, and 0.01 m/s with depths of lakes 50 m and that of the streams and lakes 1 m deep (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 771 \text{ d to } 64500 \text{ yr}$, based on measured rate for the reaction with hydroxyl radical in water (Howard et al. 1991)

photooxidation $t_{1/2} > 9.9 \text{ d}$ (Darnall et al. 1976)

$k \sim 0.003 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2–6 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}}(\text{calc}) = 6.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 59\text{--}590 \text{ h}$, based on measured rate for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

$k_{\text{OH}}(\text{calc}) = 5.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{exptl}) = 1.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = (1.08 \pm 0.11) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{\text{OH}} = 1.07 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}}^* = 1.07 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 243–440 K (flash photolysis-resonance fluorescence, Wallington 1988c)

$k_{\text{OH}}^* = 1.12 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k(\text{aq.}) = 0.01 \text{ M}^{-1} \text{ s}^{-1}$ at pH 2.3, $k = 0.45 \text{ M}^{-1} \text{ s}^{-1}$ at pH 2.2, $k = 0.46 \text{ M}^{-1} \text{ s}^{-1}$ at pH 5.2 for direct reaction with ozone in water and 20°C, with $t_{1/2} = 390 \text{ d}$ at pH 7 (Yao & Haag 1991).

$k_{\text{OH}}(\text{calc}) = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation $30.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}(\text{aq. aerobic}) = 677\text{--}4320 \text{ h}$, based on river die-away studies; $t_{1/2}(\text{aq. anaerobic}) = 2400\text{--}12000 \text{ h}$, based on degradation rates in microcosm studies simulating anaerobic aquifers (Howard et al. 1991).

$t_{1/2}(\text{aerobic}) = 28 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 100 \text{ d}$ in natural waters (Capel & Larson 1995)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} > 9.9 \text{ d}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 34.5 \text{ h}$ for 10 ppm in the air reacted with 5 ppm NO (Dilling et al. 1976);

photooxidation $t_{1/2} = 59\text{--}590 \text{ h}$, based on measured rate for the reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);

$t_{1/2} \sim 1.09 \text{ month}$ for the vapor phase reaction with photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1990).

Surface water: $t_{1/2} \sim 8.8 \text{ yr}$, based on rate constant $k = 2.5 \times 10^8 \text{ L/mol}\cdot\text{s}$ for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; quoted, Howard 1990);

$t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

measured rate constant $k = 0.001 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.3 and 20°C, with $t_{1/2} = 390 \text{ d}$ at pH 7 (Yao & Haag 1991)

$t_{1/2}(\text{aerobic}) = 28 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 100 \text{ d}$ in natural waters (Capel & Larson 1995)

Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 360\text{--}4800 \text{ h}$, based on soil microcosm studies (Howard et al. 1991).

Biota:

TABLE 11.1.1.8.1

Reported vapor pressures of *tert*-butyl alcohol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Parks & Barton 1928		Butler et al. 1935		Stull 1947		Garriga et al. 2002	
static method/isoteniscope		isoteniscope method		summary of literature data		static method-manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	4080	24.98	5654*	–20.4	133.3	25	5610
25	5600	40.0	7753	–3.0	666.6	30	7685
30	7586	45.03	10423	5.5	1333	35	10347
35	10172	50.08	23705	14.3	2666	40	13787
40	13639	60.12	38850	24.5	5333	45	18143
45	17839	70.3	61648	31.0	7999	50	23578
50	23238	75.43	72927	39.8	13332	Ambrose & Sprake 1970 comparative ebulliometry	
55	29891	80.59	100112	52.7	26664		
60	38024		*solid	68.0	53329	T/K	P/Pa
65	47756	bp/°C	82.75	82.9	101325	329.946	33123
70	59635					333.931	40058
75	73754	eq. 4	P/mmHg	mp/°C	25.3	337.204	46623
80	90579	A	43.2834			340.225	53431
85	110164	B	3935			342.857	60007
90	132816	C	11.59			347.448	73160
ΔH _v /(kJ mol ^{–1}) = at 25°C 45.56 at bp 39.66		ΔH _v /(kJ mol ^{–1}) = 46.86 at 25°C		Dreisbach & Shrader 1949		347.448	73160
				ebulliometry		351.659	86911
				t/°C	P/Pa	355.146	99932
				43.34	16500	358.422	113545
				61.82	42066	362.710	133505
				72.49	67661	full list of data see ref.	
				82.41	101325		

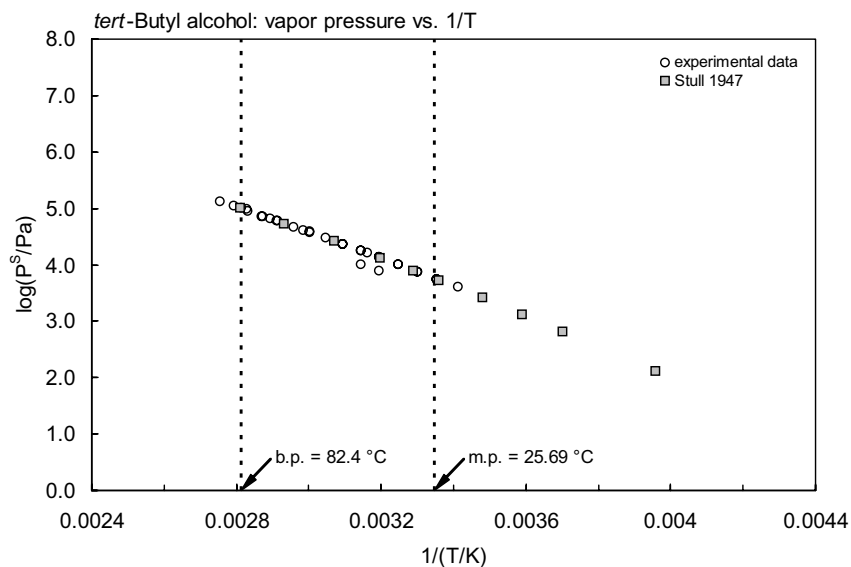


FIGURE 11.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for *tert*-butyl alcohol.

TABLE 11.1.1.8.2

Reported Henry's law constants of *tert*-butyl alcohol at various temperatures

Snider & Dawson 1985

gas stripping-GC

t/°C	H/(Pa m ³ /mol)
0	0.1135
25	1.4581

enthalpy of transfer:
 $\Delta H/(\text{kJ mol}^{-1}) = 66.944$

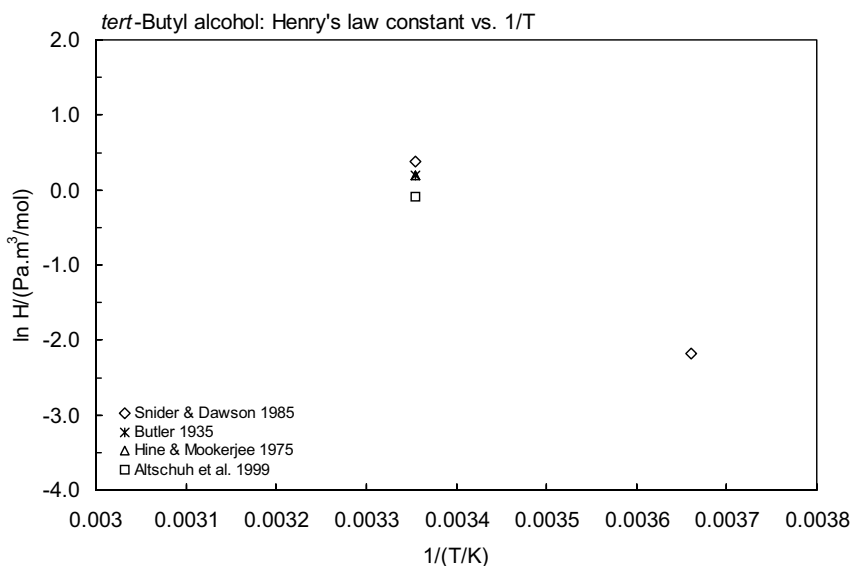
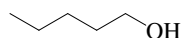


FIGURE 11.1.1.8.2 Logarithm of Henry's law constant versus reciprocal temperature for *tert*-butyl alcohol.

11.1.1.9 1-Pentanol (*n*-Amyl alcohol)

Common Name: 1-Pentanol

Synonym: amyl alcohol, *n*-butylcarbinol, 1-pentanol, *n*-pentyl alcohol, pentyl alcohol

Chemical Name: *n*-amyl alcohol, *n*-pentyl alcohol, 1-pentanol

CAS Registry No: 71-41-0

Molecular Formula: $C_5H_{12}O$, $CH_3CH_2CH_2CH_2CH_2OH$

Molecular Weight: 88.148

Melting Point ($^{\circ}C$):

−77.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

137.98 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.81253 ($25^{\circ}C$, Butler et al. 1935)

0.8144 (Weast 1982–83)

0.81445, 0.81080 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

108.0 (calculated-density, Lande & Banerjee 1981)

125.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

20.81 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.5 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

22080 (shake flask-interferometer, Butler et al. 1933)

21900* (volumetric method, measured range 20 – $30^{\circ}C$, Ginnings & Baum 1937)

22100 ($20^{\circ}C$, surface tension, Addison 1945)

23600 ($20^{\circ}C$, Seidell 1941)

27570 (shake flask-residue volume, Booth & Everson 1948)

15230 ($20^{\circ}C$, shake flask-turbidity, Laddha & Smith 1948)

25400 (shake flask-interferometry, Hansen et al. 1949)

23500* ($20^{\circ}C$, synthetic method, measured range 0 – $180^{\circ}C$, von Erichsen 1952)

22000 (shake flask-titration, Crittenden & Hixon 1954)

22140 (estimated, McGowan 1954)

22000 (surface tension, Kinoshita et al. 1958)

23800 (shake flask-GC, Korenman 1974, 1975)

21950 (Riddick & Bunger 1955)

18800 (shake flask-GC, Evans et al. 1978)

11720 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

22000* (recommended best value, IUPAC Solubility Data Series, temp range 0 – $180^{\circ}C$, Barton 1984)

22500* ($20.2^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.7^{\circ}C$, Stephenson et al. 1984)

20190 (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

333* ($25^{\circ}C$, extrapolated-modified isoteniscope method, measured range 60 – $131^{\circ}C$, Butler et al. 1935)

- $\log (P/\text{mmHg}) = 46.4925 - 4580/(T/K) - 12.42 \cdot \log (T/K)$; temp range 60–131°C (isoteniscope measurements, Butler et al. 1935)
- 349* (interpolated-regression of tabulated data, temp range 13.6–138°C, Stull 1947)
- 286* (extrapolated-ebulliometry, measured range 33.9–138°C, Kemme & Kreps 1969)
- 573.3* (33.9°C, ebulliometry-differential thermal analysis, measured range 33.9–138°C, Kemme & Kreps 1969)
- $\log (P/\text{mmHg}) = 7.55787 - 1492.549/(181.529 + t/^{\circ}\text{C})$; temp range 33.9–138°C, or pressure range 4.3–765.4 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
- 293* (comparative ebulliometry, measured range 74.763–156°C, Ambrose & Sprake 1970)
- $\log (P/\text{Pa}) = 6.13796 - 1190.412/(T/K - 123.055)$; restricted temp range 74.763–128.665°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- $\log (P/\text{Pa}) = 6.30306 - 1286.333/(T/K - 111.843)$; temp range 74.763–128.665°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- 313 (calculated-Antoine eq., Riddick & Bunger 1970)
- $\log (P/\text{mmHg}) = [-0.2185 \times 12495.5/(T/K)] + 9.574342$; temp range 13.6–137.8°C (Antoine eq., Weast 1972–73)
- 189 (20°C, extrapolated-Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
- 373 (20°C, Verschueren 1983)
- 172, 250 (extrapolated-Antoine equations., Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.00024 - 1103.91/(138.221 + t/^{\circ}\text{C})$; temp range 165–240.65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.31559 - 1292.273/(161.837 + t/^{\circ}\text{C})$; temp range 74.5–156°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
- 313 (extrapolated-Antoine eq., Dean 1985)
- $\log (P/\text{mmHg}) = 7.17758 - 1314.56/(168.11 + t/^{\circ}\text{C})$; temp range 37–138°C (Antoine eq., Dean 1985, 1992)
- 293 (selected, Riddick et al. 1986)
- $\log (P/\text{kPa}) = 6.30306 - 1286.333/(t/^{\circ}\text{C} + 161.307)$, temp range not specified (Riddick et al. 1986)
- $\log (P_L/\text{kPa}) = 6.14668 - 1195.924/(-122.348 + T/K)$; temp range 388–420 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.30990 - 1290.23/(-111.419 + T/K)$; temp range 347–429 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.1490 - 1197.233/(-122.194 + T/K)$; temp range 388–420 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.3975 - 1337.613/(-106.567 + T/K)$; temp range 326–411 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.28069 - 1277.413/(-112.34 + T/K)$; temp range 408–441 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
- $\log (P/\text{mmHg}) = 71.2535 - 5.4977 \times 10^3/(T/K) - 21.366 \cdot \log(T/K) + 3.8108 \times 10^{-10} \cdot (T/K) + 5.0339 \times 10^{-6} \cdot (T/K)^2$; temp range 196–586 K (vapor pressure eq., Yaws 1994)
- 891 (40°C, vapor-liquid equilibrium VLE data, Rhodes et al. 1997)

Henry's Law Constant (Pa m³/mol):

- 1.324 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
- 1.271 (exptl., Hine & Mookerjee 1975)
- 1.426, 1.60 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 1.04 (calculated-P/C, Mackay & Yuen 1983)
- 1.017 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
- 1.271 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 1.236 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
- 1.60 (correlated-molecular structure, Russell et al. 1992)
- 1.186 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
- 1.057 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
- $\ln K_{AW} = 14.233 - 6559.6/(T/K)$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.40 (from Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Dunn III 1972)

- 1.37, 1.38; 1.34 (calculated-fragment const.; calculated- π constant, Rekker 1977)
 1.44, 1.48 (HPLC-RV/RT correlation, Yonezawa & Urushigawa 1979)
 1.53 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 1.33 (HPLC-RT correlation, D'Amboise & Hanai 1982)
 1.56 (shake flask, Log P Database, Hansch & Leo 1987)
 1.49 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 1.53 (generator column-GC, Schantz & Martire 1987)
 1.55 (calculated from measured γ , Schantz & Martire 1987)
 1.51 (recommended value, Sangster 1989, 1993)
 1.41 (shake flask-GC, Fujiwara et al. 1991)
 1.56 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 4.69 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 0.241 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.93 (calculated-MCI χ , Gerstl & Helling 1987)
 0.70 (soil, quoted exptl., Meylan et al. 1992)
 0.65 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 0.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate of $6.92 \times 10^{-5} \text{ mol cm}^{-2} \text{ h}^{-1}$ was determined by gravimetric method with an air flow rate of $(50 \pm 1) \text{ L h}^{-1}$ at $20 \pm 0.1^\circ\text{C}$ (Gückel et al. 1973).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH}(\text{exptl}) = 1.08 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k = 6.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in aqueous solution at 298 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987)

$k_{OH} = 1.08 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 10.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (review, Atkinson 1989)

$k_{OH} = (12.0 \pm 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (10.5 \pm 1.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 9.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.9.1

Reported aqueous solubilities of 1-pentanol at various temperatures

Ginnings & Baum 1937		von Erichsen 1952		Barton 1984		Stephenson et al. 1984	
volumetric method		synthetic method		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	23600	0	30500	0	31000	0	23100
25	21900	10	27000	10	27000	10.2	25900
30	20300	20	23500	20	23100	20.2	22500
		30	21000	25	22000	30.6	20200
		40	19000	30	20400	40.2	18700
		50	18000	40	20000	50.0	18300
		60	18000	50	18000	60.3	18300
		70	18500	60	18000	70.0	19500
		80	19000	70	19000	80.0	19900
		90	20000	80	19000	90.7	22100
		100	22500	90	20000		
		110	26000	100	23000		
		120	30000	110	26000		
		130	35500	120	30000		
		140	43000	130	36000		
		150	53500	140	43000		
		160	69000	150	54000		
		170	95500	160	69000		
		180	175000	170	96000		
				180	175000		

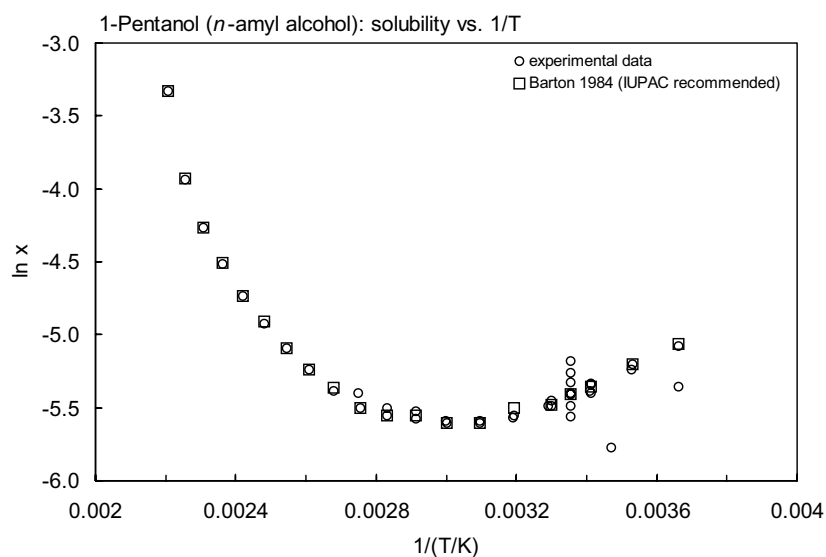
FIGURE 11.1.1.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-pentanol.

TABLE 11.1.1.9.2
Reported vapor pressures of 1-pentanol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Butler et al. 1935		Stull 1947		Kemme & Kreps 1969		Ambrose & Sprake 1970	
isoteniscope method		summary of literature data		differential thermal analysis		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	333.3	13.6	133.3	33.9	573.3	74.763	7175
60.12	3468	34.7	666.6	45.6	1267	83.542	11204
70.3	6153	44.9	1333	52.6	2027	87.571	13615
80.59	10364	55.8	2666	56.7	2640	90.768	15825
90.84	16772	68.0	5333	63.6	3920	95.514	19660
101.17	26398	75.5	7999	69.3	5426	101.629	25714
110.2	38250	85.8	13332	74.9	7306	106.362	31393
120.56	56542	102.0	26664	83.1	11026	110.658	37413
130.89	81580	119.8	53329	90.7	15879	115.564	45399
		137.8	101325	102.4	26664	119.681	53129
bp/°C	137.75			112.3	40263	124.099	62576
D ²⁵	0.8125	mp/°C	-	125.8	66941	128.665	73706
				138.0	102045	133.309	86610
eq. 4	P/mmHg					136.688	97054
A	46.4925			Antoine eq.		138.514	103110
B	4580			eq. 2	P/mmHg	142.435	117105
C	11.42			A	7.55787	146.598	133550
				B	1492.549	151.332	154379
				C	181.529	155.977	177156
ΔH _v /(kJ mol ⁻¹) = 56.90 at 25°C							
						Antoine eq. for full range	
						eq. 3	P/mmHg
						A	6.30306
						B	1286.333
						C	111.843
						Data also fitted to Cragoe equation, see ref.	

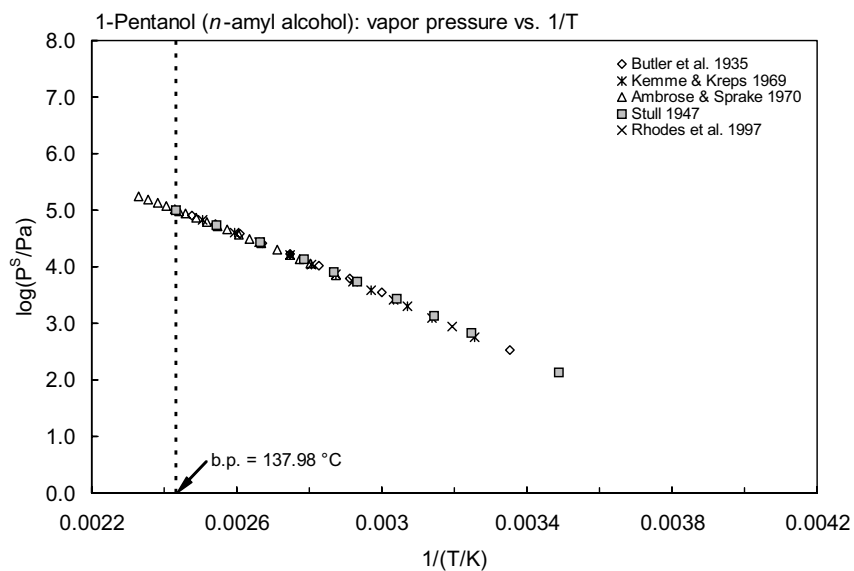
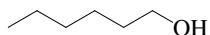


FIGURE 11.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1-pentanol.

11.1.1.10 1-Hexanol



Common Name: 1-Hexanol

Synonym: amylcarbinol, 1-hexanol, *n*-hexyl alcohol

Chemical Name: *n*-hexyl alcohol, 1-hexanol

CAS Registry No: 111-27-3

Molecular Formula: $C_6H_{14}O$, $CH_3CH_2CH_2CH_2CH_2CH_2OH$

Molecular Weight: 102.174

Melting Point ($^{\circ}C$):

−47.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

157.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8136 (Weast 1982–83)

0.81875, 0.81534 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

126.0 (calculated-density, Lande & Banerjee 1981)

148.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.40 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5000* ($20^{\circ}C$, shake flask-turbidity, measured range 0 – $110^{\circ}C$, Fühner 1924)

6240 (shake flask-interferometer, Butler et al. 1933)

5025 ($20^{\circ}C$, shake flask-turbidity, Laddha & Smith 1948)

6400* ($20^{\circ}C$, synthetic method, measured range 0 – $220^{\circ}C$, von Erichsen 1952)

6000 (shake flask-titration, Crittenden & Hixon 1954)

6300 (estimated, McGowan 1954)

6000 (surface tension, Kinoshita et al. 1958)

5838* (shake flask-refractive index, measured range 5.5 – $33.6^{\circ}C$, Hill & White 1974)

3590 (shake flask-GC, Korenman et al. 1974)

4230 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

6000* (recommended best value, IUPAC Solubility Series, temp range 0 – $220^{\circ}C$, Barton 1984)

6660* ($20^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.3^{\circ}C$, Stephenson et al. 1984)

5354 (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

95.86* ($24.98^{\circ}C$, extrapolated-modified isoteniscope data, measured range 60.11 – $152.77^{\circ}C$, Butler et al. 1935)

$\log(P/mmHg) = 51.0030 - 5068/(T/K) - 13.80 \cdot \log(T/K)$, temp range 60 – $152^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

151.1* (interpolated-regression of tabulated data, temp range 24.4 – $157^{\circ}C$, Stull 1947)

88.25 (extrapolated, ebulliometry, measured range 52 – $157^{\circ}C$, Kemme & Kreps 1969)

760* ($52.2^{\circ}C$, ebulliometry-differential thermal analysis, measured range 52.3 – $157.3^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 7.28781 - 1422.031/(t/^{\circ}C + 165.444)$; temp range 52 – $157^{\circ}C$ or pressure range 5.7 – $757.3\ mmHg$ (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

$\log(P/mmHg) = [-0.2185 \times 12708.5/(T/K)] + 9.367617$; temp range 24.4 – $157^{\circ}C$ (Antoine eq., Weast 1972–73)

- 130.6 (20°C, Verschueren 1983)
 79.65, 79.7 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.20107 - 1305.63/(153.901 + t/^\circ\text{C})$; temp range 52.2–157.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.26314 - 1334.63/(156.297 + t/^\circ\text{C})$; temp range 60.11–152.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 55.5 (extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
 52.9, 254, 888 (20, 40, 60°C, evaporation rate-gravimetric method, Gückel et al. 1982)
 109.5 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.86045 - 1707.26/(196.66 + t/^\circ\text{C})$; temp range 35–157°C (Antoine eq., Dean 1985, 1992)
 110 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.41271 - 1422.031/(t/^\circ\text{C} + 165.444)$; temp range not specified (Riddick et al. 1986)
 111 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.41271 - 1422.031/(-107.706 + T/\text{K})$; temp range 325–431 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 10.60355 - 3986.406/(46.713 + T/\text{K})$; temp range 298–343 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 53.9686 - 4.9501 \times 10^3/(T/\text{K}) - 15.199 \cdot \log(T/\text{K}) - 6.6922 \times 10^{-10} \cdot (T/\text{K}) + 2.3647 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 229–611 K (vapor pressure eq., Yaws 1994)
 113* (static method-manometry, measured range 278.15–323.15 K, Garriga et al. 1996)
 $\ln(P/\text{kPa}) = 8.472727 - 1275.055/(T/\text{K} - 178.568)$; temp range 278.15–323.15 K (Antoine eq., static method-manometry, Garriga et al. 1996)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 1.562 (measured partial pressure/mole fraction x at dilute aqueous solution, Butler et al. 1935)
 1.735 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
 1.562 (exptl., Hine & Mookerjee 1975)
 1.88, 2.367 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 1.46 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 1.60 (calculated-MCI χ , Nirmalakhandan & Speece 1988b)
 1.896 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 1.56 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 1.016 (wetted-wall column-GC, Altschuh et al. 1999)
 2.60 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{\text{AW}} = 11.705 - 5538.7/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.03 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1971; Hansch & Dunn III 1972)
 1.99 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
 2.03 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 1.86 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 2.03 (HPLC- k' correlation, Funasaki et al. 1986)
 2.04 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 2.03 (generator column-GC, Schantz & Martire 1987)
 2.05 (calculated from measured γ , Schantz & Martire 1987)
 1.50 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 2.03 (recommended, Sangster 1989, 1993)
 2.03 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 5.18 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.711 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC} :

1.01	(soil, quoted exptl., Meylan et al. 1992)
0.92	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.01	(calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate of 1.85×10^{-5} mol·cm⁻²·h⁻¹ was determined by gravimetric method with an air flow rate of (50 ± 1) L·h⁻¹ at $(20 \pm 0.1)^\circ\text{C}$ (Gückel et al. 1973).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH}(\text{exptl}) = (12.4 \pm 0.7) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹, $k_{OH}(\text{calc}) = 10.0 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH}(\text{exptl}) = 1.24 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at 298 K, and $k(\text{soln}) = 1.20 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ for the reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 12.4 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1989)

$k_{OH} = (12.2 \pm 2.4) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ by pulse radiolysis-UV spectroscopy; $k_{OH} = (12.9 \pm 1.2) \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 10.48 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water:

Groundwater:

Sediment:

Soil:

Biota

TABLE 11.1.1.10.1

Reported aqueous solubilities of 1-hexanol at various temperatures

1.

Fühner 1924		von Erichsen 1952		Hill & White 1974		Barton 1984	
synthetic method		synthetic method		shake flask-interferometry		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	7800	0	8100	5.51	7879	0	7900
10	6700	10	7000	6.85	7655	10	6900
20	5900	20	6400	8.15	7375	20	6200
30	5450	30	5900	11.0	7061	25	6000
40	5200	40	5400	12.94	6820	30	5700
50	5150	50	5000	14.68	6651	40	5300
60	5300	60	5200	17.04	6427	50	5100
70	5650	70	5600	20.71	6124	60	5200
80	6200	80	6100	22.99	5894	70	5600

(Continued)

TABLE 11.1.1.10.1 (Continued)

Fühner 1924		von Erichsen 1952		Hill & White 1974		Barton 1984	
synthetic method		synthetic method		shake flask-interferometry		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
90	6800	90	6900	25.01	5838	80	6200
100	7850	100	8000	26.99	5764	90	6900
110	8900	110	9100	28.94	5702	100	7900
		120	10400	30.92	5639	110	9000
		130	11900	33.59	5560	120	10000
		140	13700			130	12000
		150	16300			140	14000
		160	20500			150	16000
		170	27000			160	21000
		180	36100			170	27000
		190	48700			180	36000
		200	67500			190	49000
		210	97000			200	68000
		220	163000			210	97000
						220	163000

2.

Stephenson et al. 1984

shake flask-GC/TC	
t/°C	S/g·m ⁻³
0	9640
10.2	7590
20.0	6660
29.7	5580
39.8	5140
50.0	4970
60.0	5180
70.3	5770
80.3	6250
90.3	6380

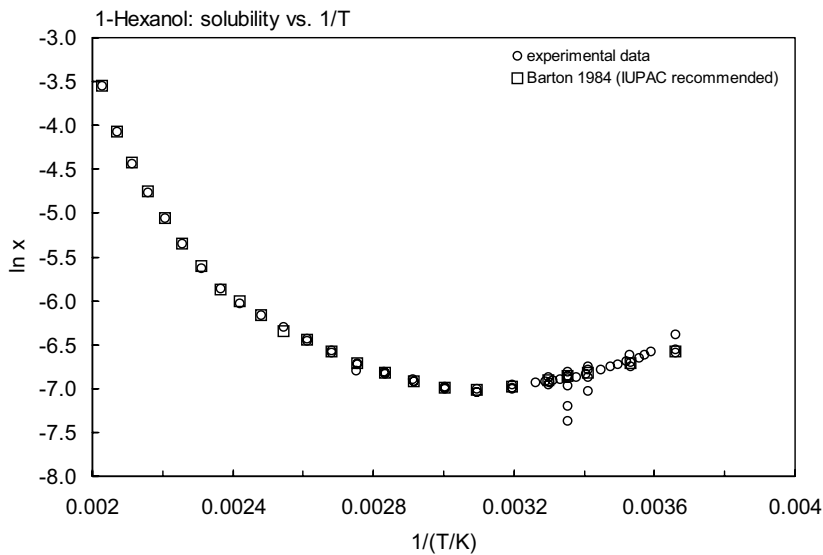


FIGURE 11.1.1.10.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-hexanol.

TABLE 11.1.1.10.2
Reported vapor pressures of 1-hexanol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)	ln P = A –B/(C + T/K)		(3a)		
log P = A – B/(T/K) – C·log (T/K)		(4)					
Butler et al. 1935		Stull 1947		Kemme & Kreps 1969		Garriga et al. 1996	
static method-isoteniscope		summary of literature data		differential thermal analysis		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	95.86	24.4	133.3	52.2	760.0	5	13
60.11	1300	47.2	666.6	60.4	1293	10	24
70.29	2365	58.2	1333	67.4	2040	15	45
80.58	4213	70.3	2666	72.6	2733	20	68
90.83	7275	83.7	5333	79.2	3973	25	113
101.16	12000	92.0	7999	85.0	5436	30	169
110.19	18012	102.8	13332	91.1	7373	35	251
120.55	27624	119.6	26664	98.7	10666	40	369
130.88	41303	138.0	53329	107.6	16105	45	517
141.67	60901	157.0	101325	119.7	26798	50	713
152.77	87966			130.1	40237		
		mp/°C	–51.6	144.5	66661	Antoine eq.	
bp/°C	155.7			157.3	100965	eq. 3a	P/kPa
D ²⁵	0.8183					A	8.472727
				Antoine eq.		B	1275.055
eq. 4	P/mmHg			eq. 2	P/mmHg	C	–178.875
A	51.003			A	7.28781		
B	5068			B	1422.031		
C	13.80			C	165.444		
ΔH _v /(kJ mol ^{–1}) = 62.84							
at 25°C							

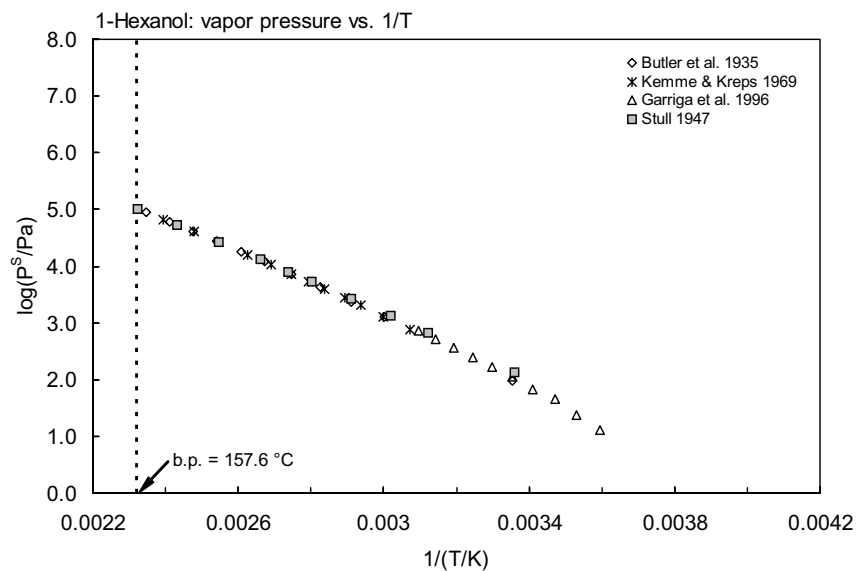
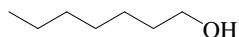


FIGURE 11.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-hexanol.

11.1.1.11 1-Heptanol



Common Name: 1-Heptanol

Synonym: 1-heptanol, *n*-heptyl alcohol

Chemical Name: *n*-heptyl alcohol, 1-heptanol

CAS Registry No: 111-70-6

Molecular Formula: $C_7H_{16}O$, $CH_3(CH_2)_6OH$

Molecular Weight: 116.201

Melting Point ($^{\circ}C$):

−33.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

176.45 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.82053 ($25^{\circ}C$, Butler et al. 1935)

0.8219 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

142.0 (calculated-density, Lande & Banerjee 1981)

170.2 (calculated- Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

930* ($18^{\circ}C$, shake flask-turbidity, measured range 70 – $130^{\circ}C$, Fühner 1924)

1804 (shake flask-interferometer, Butler et al. 1933)

1720 ($20^{\circ}C$, shake flask-titration, Addison 1943)

3288 (shake flask-centrifuge, Booth & Everson 1948)

1200 (shake flask-turbidimetric method, Harkins & Oppenheimer 1949)

2000* ($20^{\circ}C$, synthetic method, measured range 0 – $245^{\circ}C$, von Erichsen 1952)

1800 (estimated, McGowan 1954)

1700 (surface tension, Kinoshita et al. 1958)

1500* ($20^{\circ}C$, surface tension, 15 – $60^{\circ}C$, measured range Vochten & Petre 1973)

1676* (shake flask-interferometric method, measured range 6 – $34.9^{\circ}C$, Hill & White 1974)

1313 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

1740* (recommended best value, IUPAC Solubility Data Series, temp range 0 – $240^{\circ}C$, Barton 1984)

1840* ($20.2^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.5^{\circ}C$, Stephenson et al. 1984)

1510 (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

29.86* (extrapolated, modified isoteniscope method, measured range 60 – $110^{\circ}C$, Butler et al. 1935)

$\log (P/mmHg) = 55.1972 - 5580/(T/K) - 15.41 \cdot \log (T/K)$; temp range 60 – $152^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

44.04* (extrapolated-regression of tabulated data, temp range 42.4 – $175.8^{\circ}C$, Stull 1947)

22.2 (extrapolated-Antoine eq., ebulliometry, Kemme & Kreps 1969)

626.6* ($63.5^{\circ}C$, ebulliometry-differential thermal analysis, measured range 63.6 – $176.4^{\circ}C$, Kemme & Kreps 1969)

$\log (P/mmHg) = 6.85450 - 1266.783/(139.663 + t/^{\circ}C)$; temp range 63.6 – $176.4^{\circ}C$, or pressure range 5.3 – 760 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

31.30 (calculated-Antoine eq., Jordan 1970)

$\log (P/mmHg) = [-0.2185 \times 13920.9/(T/K)] + 9.720613$; temp range 42.4 – $175.8^{\circ}C$ (Antoine eq., Weast 1972–73)

- 12.8 (20°C, extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
 24.0 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.10824 - 1323.566/(146.241 + t/^\circ\text{C})$; temp range 63.6–176.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.01857 - 1278.78/(146.403 + t/^\circ\text{C})$; temp range 60.11–152.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 17.64 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 6.64767 - 1140.64/(126.56 + t/^\circ\text{C})$; temp range 60–176°C (Antoine eq., Dean 1985, 1992)
 $\log(P_L/\text{kPa}) = 5.9794 - 1256.783/(-133.487 + T/\text{K})$; temp range 336–450 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.10408 - 1322.62/(-126.87 + T/\text{K})$; temp range 335–450 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = -19.9205 - 4.3239 \times 10^3/(T/\text{K}) + 18.794 \cdot \log(T/\text{K}) - 5.0553 \times 10^{-2} \cdot (T/\text{K}) + 2.6161 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 239–632 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 1.909 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 1.880 (exptl., Hine & Mookerjee 1975)
 2.656, 3.583 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 2.015 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 1.176 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
 5.55 (calculated-molecular structure, Russell et al. 1992)
 5.62 (gas stripping-GC, Shiu & Mackay 1997)
 1.165 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.53 (Hansch & Dunn III 1972)
 2.41 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
 2.57 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 2.39 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 2.60 (HPLC- k' correlation, Funasaki et al. 1986)
 2.65 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 2.57 (shake flask, Log P Database, Hansch & Leo 1987)
 2.57 (generator column-GC, Schantz & Martire 1987)
 2.57 (calculated-activity coeff. γ , Schantz & Martire 1987)
 1.83 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 2.62 (recommended, Sangster 1989, 1993)
 2.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

- 1.09 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, $\log K_{oc}$:

- 1.48 (calculated-MCI χ , Gerstl & Helling 1987)
 1.14 (soil, quoted exptl., Meylan et al. 1992)
 1.19 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 1.14 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate of $6.804 \times 10^{-6} \text{ mol cm}^{-2} \text{ h}^{-1}$ was determined by gravimetric method with an air flow rate of $(50 \pm 1) \text{ L h}^{-1}$ at 20°C (Gückel et al. 1973).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical in air (Darnall et al. 1976)

$k_{\text{OH}}(\text{exptl}) = (13.6 \pm 1.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 10.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{\text{OH}}(\text{exptl}) = 1.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k(\text{soln}) = 1.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the s reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}} = (13.7 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (relative rate method, Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical in air (Darnall et al. 1976).

Surface water:

Sediment:

Soil:

Biota:

TABLE 11.1.1.11.1

Reported aqueous solubilities of 1-heptanol at various temperatures

1.

Fühner 1924		von Erichsen 1952		Vochten & Petre 1973		Hill & White 1974	
synthetic method		synthetic method		surface tension measurement		shake flask-interferometer	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
70	1250	0	3400	15	2000	6.0	2204
80	1700	10	2600	20	1500	10.2	2020
90	2250	20	2000	30	1500	10.54	1998
100	2800	30	1600	40	1300	15.08	1868
110	3350	40	1300	50	1400	17.94	1794
120	4300	50	1100	60	1500	20.03	1750
130	5150	60	1100			21.9	1685
		70	1500			24.99	1676
		80	1900			25.07	1665
		90	2300			26.04	1652
		100	2900			28.02	1639
		110	3500			30.14	1623
		120	4300			30.16	1625
		130	5300			32.9	1610
		140	6500			34.9	1605
		150	8000				
		160	9800				
		170	12300				
		180	16000				
		190	20800				
		200	25400				
		210	34800				

(Continued)

TABLE 11.1.1.11.1 (Continued)

Fühner 1924		von Erichsen 1952		Vochten & Petre 1973		Hill & White 1974	
synthetic method		synthetic method		surface tension measurement		shake flask-interferometer	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
		220	46800				
		230	67000				
		240	101000				
		245	139600				

2.

Barton 1984				Stephenson et al. 1984	
IUPAC recommended				shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	3400	120	4300	0	2360
10	2500	130	5200	10.5	2530
20	1700	140	6500	20.2	1840
25	1740	150	8000	30.6	1540
30	1600	160	10000	39.8	1660
40	1300	170	12000	50.1	1620
50	1200	180	16000	60.0	1780
60	1300	190	21000	70.1	2040
70	1400	200	26000	80.1	2170
80	1800	210	35000	90.5	2430
90	2300	220	47000		
100	2900	230	67000		
110	3400	240	101000		

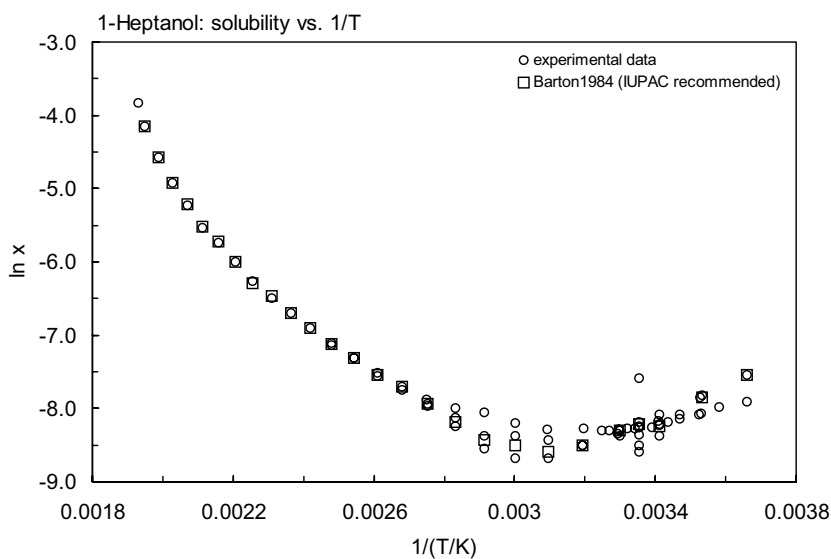
FIGURE 11.1.1.11.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-heptanol.

TABLE 11.1.1.11.2
Reported vapor pressures of 1-heptanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Butler et al. 1935		Stull 1947		Kemme & Kreps 1969	
isoteniscopes method		summary of literature data		differential thermal analysis	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	29.86	42.4	133.3	63.6	626.6
68.11	505	64.3	666.6	76.1	1453
70.29	997	74.7	1333	81.5	2000
80.58	1913	85.8	2666	87.6	2813
90.83	3430	99.8	5333	94.3	4026
101.16	5882	108.0	7999	99.9	5360
110.10	9061	119.5	13332	106.4	7399
120.55	14292	136.6	26664	114.5	10732
130.88	21811	155.6	53329	124.1	16319
141.67	32864	175.8	101325	136.5	26798
152.77	48596			147.8	40463
		mp/°C	34.6	162.8	66794
bp/°C	175.6			178.4	101432
D ²⁵	0.8205				
		Antoine eq.			
eq. 4	P/mmHg			eq. 2	P/mmHg
A	56.1972			A	6.85450
B	5580			B	1256.783
C	15.41			C	139.663
$\Delta H_v/(\text{kJ mol}^{-1}) = 68.66$					
at 25°C					

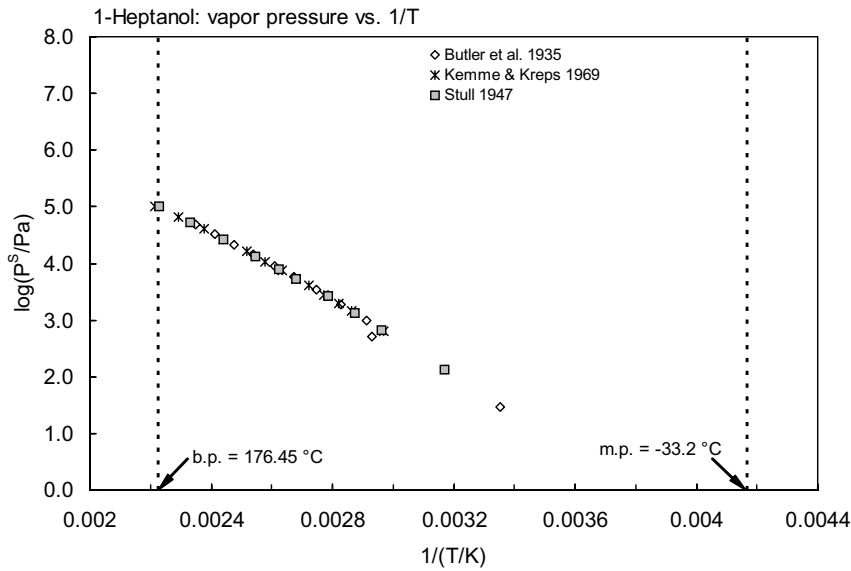
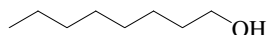


FIGURE 11.1.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for 1-heptanol.

11.1.1.12 1-Octanol (*n*-Octyl alcohol)

Common Name: 1-Octanol

Synonym: 1-octanol, *n*-octyl alcohol, capryl alcohol, heptylcarbinol

Chemical Name: *n*-octyl alcohol, 1-octanol

CAS Registry No: 111-87-5

Molecular Formula: $C_8H_{18}O$, $CH_3(CH_2)_7OH$

Molecular Weight: 130.228

Melting Point ($^{\circ}C$):

−14.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

195.15 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.827 (Weast 1982–83)

0.82499, 0.82157 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

158.0 (calculated-density, Rohrschneider 1973; Lande & Banerjee 1981)

192.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

42.3 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

586 (shake flask-interferometer, Butler et al. 1933)

760 ($30^{\circ}C$, shake flask-titration, Sobotka & Glick 1934.)

420 ($20^{\circ}C$, shake flask-surface tension, Addison 1945)

590 (shake flask-turbidimeter, McBain & Richard 1946)

500 (shake flask-titration, Crittenden & Hixon 1954)

582 (estimated, McGowan 1954)

490 (shake flask-surface tension, Kinoshita et al. 1958)

495 (shake flask-turbidity, Shinoda et al. 1959)

1000 ($30^{\circ}C$, shake flask-turbidimeter, Rao et al. 1961)

330 (calculated- K_{OW} , Hansch et al. 1968)

530 ($15^{\circ}C$, shake flask-surface tension, Vochten & Petre 1973)

600, 600 (40 , $60^{\circ}C$, shake flask-titration, Lavrova & Lesteva 1976)

10000, 5000 (95 , $115^{\circ}C$, shake flask-polythermic method, Zhuravleva et al. 1977)

540* (recommended best value, IUPAC Solubility Data Series, temp range 15 – $115^{\circ}C$, Barton 1984)

490* ($20.5^{\circ}C$, shake flask-GC/TC, measured range 20.5 – $90.3^{\circ}C$, Stephenson et al. 1984)

517 (shake flask-GC, Li et al. 1992)

417 (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11.06* ($25^{\circ}C$, extrapolated-modified isoteniscope data, measured range 60.12 – $110^{\circ}C$, Butler et al. 1935)

$\log (P/mmHg) = 40.2105 - 4100/(T/K) - 10.35 \cdot \log (T/K)$; temp range 20 – $110^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

18.8* (extrapolated-regression of tabulated data, temp range 54 – $195.2^{\circ}C$, Stull 1947)

$\log (P/mmHg) = 8.29442 - 2302.3/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

7604* ($121.99^{\circ}C$, ebulliometry, measured range 121.99 – $195.28^{\circ}C$, Dreisbach & Shrader 1949)

- 5.28 (extrapolated-Antoine eq., ebulliometry- DTA, Kemme & Kreps 1969)
- 706.6* (78.9°C, ebulliometry-differential thermal analysis, measured range 78.9–195.3°C, Kemme & Kreps 1969)
- $\log (P/\text{mmHg}) = 6.62354 - 1196.639/(124.107 + t/^\circ\text{C})$; temp range 78.9–195.3°C, or pressure range 5.3–760 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
- 10* (comparative ebulliometry, measured range 113.274–206.123 K, Ambrose & Sprake 1970)
- $\log (P/\text{Pa}) = 5.79413 - 1434.755/(T/\text{K} - 149.407)$; restricted temp range 113.274–151.974°C, (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- $\log (P/\text{Pa}) = 5.88511 - 1264.322/(T/\text{K} - 142.420)$; temp range 113.274–206.123°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- 142* (54.88°C, comparative ebulliometry, measured range 328.03–386.96 K, data fitted to Chebyshev polynomial, Ambrose et al. 1974)
- 2.78 (20°C, extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
- 4.07, 32.3, 177 (20, 40, 60°C, evaporation rate-gravimetric method, Gückel et al. 1982)
- $\log (P/\text{mmHg}) = [-0.2185 \times 14262.4/(T/\text{K})] + 9.601156$; temp range: 54–195°C, (Antoine eq., Weast 1972–73)
- 10.06, 6.89, 5.74, 9.95 (extrapolated-Antoine eq., Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.80512 - 1752.302/(174.07 + t/^\circ\text{C})$; temp range 54.88–113.9°C (Antoine eq. from reported exptl. data of Ambrose et al. 1974, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 5.98227 - 1322.952/(137.413 + t/^\circ\text{C})$; temp range 79.9–195.4°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 5.87970 - 1260.554/(130.23 + t/^\circ\text{C})$; temp range 113.3–206.1°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.00162 - 1356.232/(144.452 + t/^\circ\text{C})$; temp range 229.05–250.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 13.43 (calculated-Antoine eq., Dean 1985)
- $\log (P/\text{mmHg}) = 12.0701 - 4506.8/(319.9 + t/^\circ\text{C})$; temp range 0–80°C (Antoine eq., Dean 1985, 1992)
- $\log (P/\text{mmHg}) = 6.83790 - 1310.62/(136.05 + t/^\circ\text{C})$; temp range 70–195°C (Antoine eq., Dean 1985, 1992)
- 14.5 (static measurement, Berti et al. 1986)
- 10.0 (Riddick et al. 1986)
- $\log (P/\text{kPa}) = 5.88511 - 1264.322/(t/^\circ\text{C} + 130.73)$; temp range not specified (Riddick et al. 1986)
- 13.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.90052 - 1273.291/(-141.417 + T/\text{K})$; temp range 386–480 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.342 - 3343/(T/\text{K})$; temp range 267–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 18.014 - 5507/(T/\text{K})$; temp range 238–251 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.7934 - 1208.201/(-149.366 + T/\text{K})$; temp range 430–474 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.39406 - 1540.599/(-114.618 + T/\text{K})$; temp range 328–400 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.90632 - 1276.86/(-140.996 + T/\text{K})$; temp range 397–479 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
- 10.58 (Daubert & Danner 1989; quoted, Howard 1993)
- $\log (P/\text{mmHg}) = -26.3876 - 4.2263 \times 10^3/(T/\text{K}) + 21.093 \cdot \log(T/\text{K}) - 5.0048 \times 10^{-2} \cdot (T/\text{K}) + 2.4611 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 258–653 K (vapor pressure eq., Yaws 1994)
- 8.0* (static method-manometry, measured range 278.15–323.15 K, Garriga et al. 1996)
- $\ln (P/\text{kPa}) = 13.058110 - 2443.493/(T/\text{K} - 162.071)$; temp range 278.15–323.15 K (Antoine eq., static method-manometry, Garriga et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C):

- 2.454 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
- 2.479 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
- 2.422 (exptl., Hine & Mookerjee 1975)
- 3.344, 6.085 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 2.537 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

- 1.609 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 1.537 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW} :

- 3.15 (shake flask-CR, Collander 1951)
 2.84 (calculated- π constant, Hansch et al. 1968)
 3.03 (Hansch & Dunn III 1972)
 2.95, 2.97; 2.84 (calculated-f const.; calculated- π constant, Rekker 1977)
 2.97 (HPLC- k' correlation, Könemann et al. 1979)
 2.80 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
 2.92 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 3.16 (shake flask-GC, Platford 1983)
 2.97 (Hansch & Leo 1985)
 3.27 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 2.14 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 3.07 (recommended, Sangster 1989, 1993)
 3.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

- 6.03 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 0.307 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)
 0.097 (calculated-S, Lyman et al. 1982; quoted, Howard 1993)
 1.651 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC} :

- 2.99 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)
 2.14 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1993)
 1.56, 1.76 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
 1.56 (soil, quoted exptl., Meylan et al. 1992)
 1.45 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 1.56 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate $k = 1.752 \times 10^{-6} \text{ mol}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$ was determined by gravimetric method with an air flow rate $k = (50 \pm 1) \text{ L h}^{-1}$ at $20 \pm 0.1^\circ\text{C}$ (Gückel et al. 1973);

$t_{1/2} \sim 1.8 \text{ d}$ from a model river of 1-m deep flowing at 1 m/s with a wind speed of 3 m/s, based on calculated Henry's law constant (Lyman et al. 1982; quoted, Howard 1993);

$t_{1/2} \sim 8.2 \text{ d}$ from a model pond with the consideration of adsorption (USEPA 1987; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation half-life of 0.24–2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k \leq 0.8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = (13.6 \pm 1.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Wallington et al. 1988a; Atkinson 1989)

$k_{OH} = (14.4 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Nelson et al. 1990)

$k_{OH}(\text{calc}) = 11.67 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 1.3$ d in air, based on measured rate constant $k = 1.195 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ cm}^{-3}$ at 25°C in air (Atkinson 1987; quoted, Howard 1993).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.12.1

Reported aqueous solubilities of 1-octanol at various temperatures

Barton 1984		Stephenson et al. 1984	
tentative or recommended		shake flask-GC/TC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
15	530	20.5	490
20	420	30.6	640
25	540	40.1	650
30	760	50.0	1050
40	600	60.3	880
60	600	70.3	770
95	1000	80.1	870
115	500	90.3	860
25	540*		
30	900*		

*"best" values

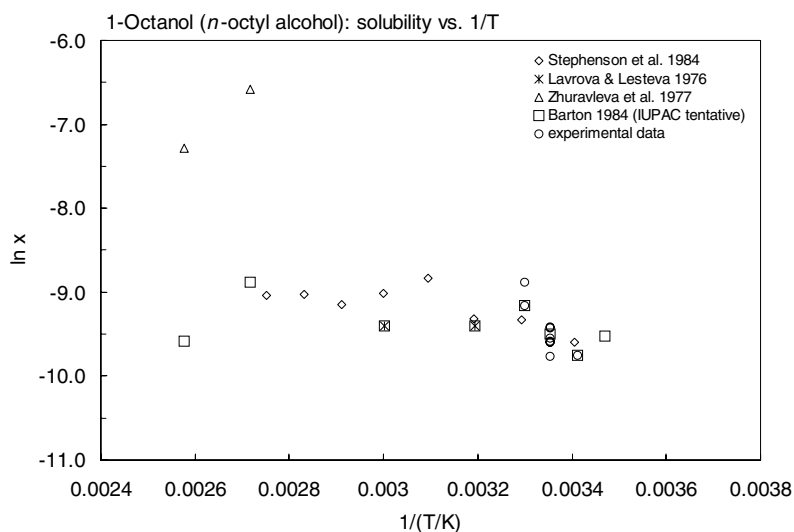
FIGURE 11.1.1.12.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-octanol.

TABLE 11.1.1.12.2

Reported vapor pressures of 1-octanol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & \ln P = A - B/(C + T/K) & (3a) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Butler et al. 1935		Stull 1947		Dreisbach & Shrader 1949		Kemme & Kreps 1969	
isoteniscope method		summary of literature data		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	11.066	54.0	133.3	121.99	7604	78.9	706.6
60.12	220.0	76.5	666.6	125.42	8851	88.8	1360
70.3	441.3	88.3	1333	140.37	16500	95.4	2000
80.59	890.6	101.0	2666	166.09	42066	101.5	2800
90.84	1589	115.2	5333	181.17	67661	108.4	4000
101.17	2868	123.8	7999	195.28	101325	114.0	5266
110.2	4456	135.2	13332			120.9	7253
120.56	7202	152.0	26664			131.2	11386
130.89	11390	173.8	53329			140.2	16505
141.68	17683	195.2	101325			166.1	42063
152.78	26858					181.2	67674
		mp/°C	-15.4			195.3	101325
bp/°C	194.5						
D ²⁵	0.8232					Antoine eq.	
						eq. 2	P/mmHg
eq. 4	P/mmHg					A	6.62354
A	65.2106					B	1196.639
B	6190					C	124.107
C	18.40						
$\Delta H_v(\text{kJ mol}^{-1}) = 72.93$							
at 25°C							

2.

Ambrose & Sprake 1970		Ambrose et al. 1974		Garriga et al. 1996	
comparative ebulliometry		comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
113.274	5065	54.88	142	5	< 2
117.718	6261	64.11	281	10	< 2
122.526	7810	70.44	431	15	< 2
127.503	9742	73.91	544	20	3
133.164	12400	77.69	700	25	8
139.162	15845	79.86	803	30	15
147.224	21679	82.36	938	35	25
151.974	25859	84.65	1078	40	45
157.372	31373	87.26	1259	45	77
161.868	36654	89.24	1415	50	116
167.897	44832	91.26	1591		
173.981	54475	95.52	2022	Antoine eq.	

TABLE 11.1.1.12.2 (Continued)

Ambrose & Sprake 1970		Ambrose et al. 1974		Garriga et al. 1996	
comparative ebulliometry		comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
179.523	64637	101.66	2817	eq. 3a	P/Pa
184.300	74519	105.12	5376	A	13.058110
190.026	87866	109.57	4226	B	2443.493
195.114	101222	113.81	5236	C	−162.071
195.504	102265	data fitted to Chebyshev polynomial, see ref.			
201.198	119164				
206.123	135431				
Antoine eq. for full range					
eq. 3	P/Pa				
A	5.88511				
B	1264.322				
C	−142.420				
Data also fitted to Cragoe equation, see ref.					

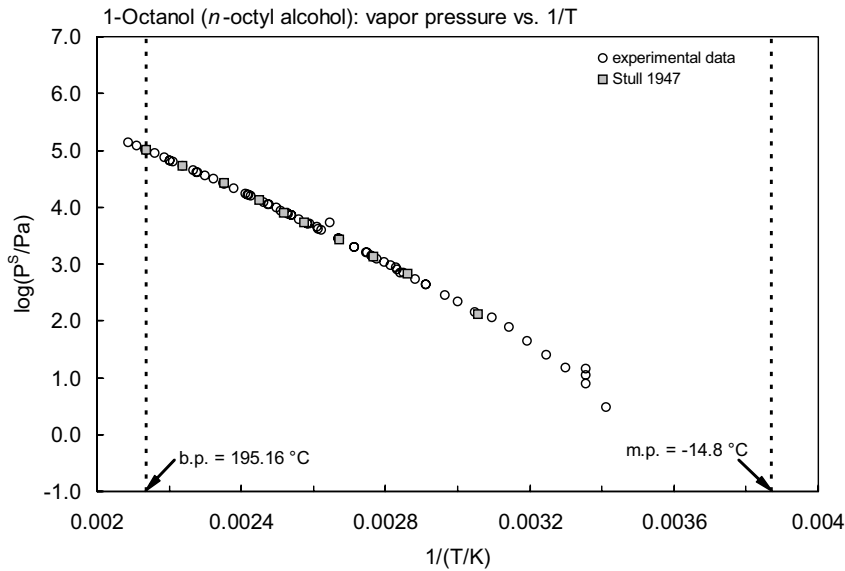
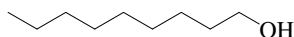


FIGURE 11.1.1.12.2 Logarithm of vapor pressure versus reciprocal temperature for 1-octanol.

11.1.1.13 1-Nonanol



Common Name: 1-Nonanol

Synonym: *n*-nonyl alcohol

Chemical Name: 1-nonanol

CAS Registry No: 143-08-8

Molecular Formula: $C_9H_{20}O$, $CH_3(CH_2)_8OH$

Molecular Weight: 144.254

Melting Point ($^{\circ}C$):

−5 (Lide 2003)

Boiling Point ($^{\circ}C$):

213.37 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8273 (Weast 1982–83)

Molar Volume (cm^3/mol):

174.4 ($20^{\circ}C$, Stephenson and Malanowski 1987)

214.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

140 (shake flask-surface tension, Kinoshita et al. 1958)

140 ($15^{\circ}C$, shake flask-surface tension, Vochten and Petre 1973)

130 (recommended-IUPAC Solubility Data Series, Barton 1984)

280* ($20^{\circ}C$, shake flask-GC/TC, measured range 9.8 – $90.5^{\circ}C$, Stephenson & Stuart 1986)

128 ($20^{\circ}C$, shake flask/slow stirring-GC, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($59.5^{\circ}C$, summary of literature data, temp range 59.5 – $213.5^{\circ}C$, Stull 1947)

746.6* ($91.7^{\circ}C$, ebulliometry-differential thermal analysis, measured range 91.7 – $213.6^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 6.83667 - 1373.417/(133.968 + t/^{\circ}C)$; temp range 91.7 – $213.6^{\circ}C$, or pressure range 5.6 – 757.5 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

$\log(P/mmHg) = [-0.2185 \times 14065.1/(T/K)] + 8.99150$; temp range 69.5 – $231^{\circ}C$ (Antoine eq., Weast 1972–73)

7.466 ($20^{\circ}C$, extrapolated from data of Stull 1947, Gückel et al. 1973)

1.87 ($20^{\circ}C$, evaporation rate-gravimetric method, Gückel et al. 1973)

12680* ($152.15^{\circ}C$, ebulliometry, measured range 152 – $221.35^{\circ}C$, Hon et al. 1976)

0.106 ($20^{\circ}C$, evaporation rate-gravimetric method, Gückel et al. 1982)

$\log(P_L/kPa) = 5.9049 - 1341.28/(-142.64 + T/K)$; temp range 381 – 495 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.9454 - 1366.566/(-139.73 + T/K)$; temp range 368 – 500 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 103.0308 - 8.1526 \times 10^3/(T/K) - 31.641 \cdot \log(T/K) - 7.230 \times 10^{-10} \cdot (T/K) + 6.0332 \times 10^{-6} \cdot (T/K)^2$; temp range 280 – 690 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1.675 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.77	(generator column-GC, Tewari et al. 1982)
4.26	(shake flask, Log P Database, Hansch & Leo 1987)
4.26	(recommended, Sangster 1993)
4.26	(shake flask, recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 11.1.1.13.1

Reported aqueous solubilities of 1-nonanol at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
9.8	350
20.0	280
29.6	310
39.6	340
49.8	320
60.1	340
70.5	330
80.2	280
90.5	300

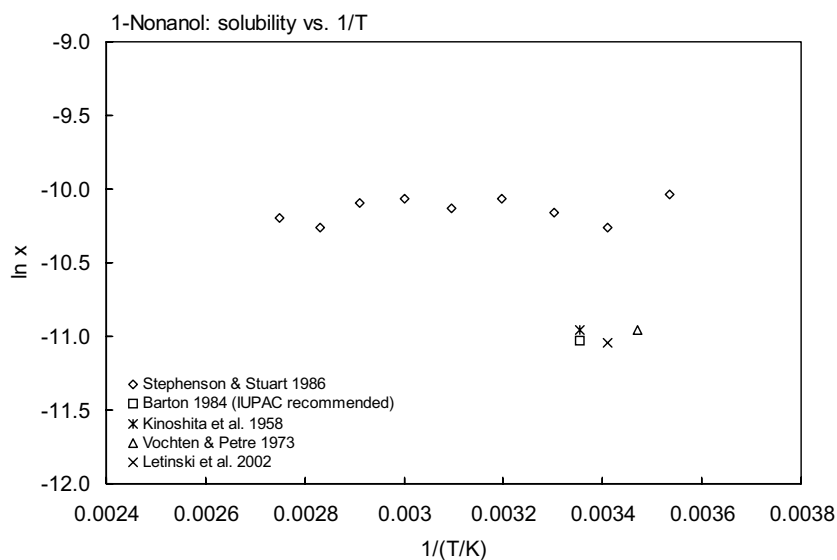


FIGURE 11.1.1.13.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-nonanol.

TABLE 11.1.1.13.2

Reported vapor pressures of 1-nonanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)			
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Kemme & Kreps 1969		Hon et al. 1976	
summary of literature data		differential thermal analysis		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
ebulliometry					
59.5	133.1	91.7	746.6	152.15	12680
86.1	666.6	102.1	1400	170.20	25385
99.7	1333	108.9	2040	181.03	37146
113.8	2666	114.4	2706	187.49	46110
129.0	5333	122.4	4026	194.80	58337
139.0	7999	128.8	5413	203.95	77352
151.3	13332	135.8	7399	207.76	86645
170.5	26664	144.7	10719	213.44	101948
192.1	53329	155.0	16092	213.97	103527
213.5	101325	169.0	26851	217.73	115289
		181.0	40317	221.35	127515
mp/°C	-5	198.0	66994		
		213.6	101845	bp/°C	213.17
		Antoine eq.		eq. 2	P/mmHg
		eq. 2	P/mmHg	A	7.60022
		A	6.83667	B	1793.77
		B	1373.417	C	166.91
		C	133.968		

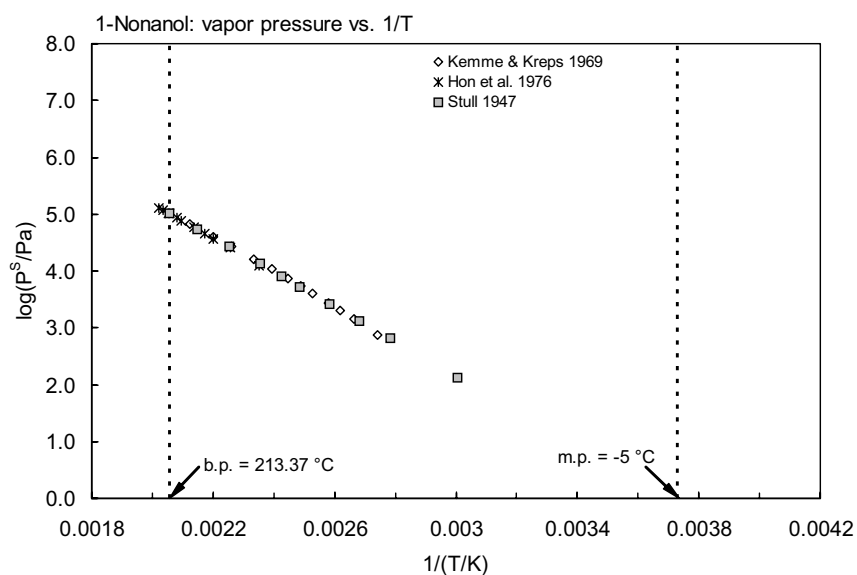
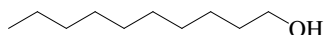


FIGURE 11.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for 1-nonanol.

11.1.1.14 1-Decanol



Common Name: 1-Decanol

Synonym: decyl alcohol

Chemical Name: 1-decanol

CAS Registry No: 112-30-1

Molecular Formula: $C_{10}H_{22}O$, $CH_3(CH_2)_8CH_2OH$

Molecular Weight: 158.281

Melting Point ($^{\circ}C$):

6.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

231.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8297 (Weast 1982–83)

Molar Volume (cm^3/mol):

190.8 ($20^{\circ}C$, calculated-density, Stephenson and Malanowski 1987)

236.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

- 50 (shake flask-turbidimetric method, Stearns et al. 1947)
- 36 ($20^{\circ}C$, shake flask-surface tension, Addison and Hutchinson 1949)
- 50 (shake flask-turbidimetric method-photometer, Harkins and Oppenheimer 1949)
- 37 (shake flask-surface tension, Kinoshita et al. 1958)
- 32 ($15^{\circ}C$, shake flask-surface tension, Vochten and Petre 1973)
- 10000, 8000 ($102.5, 120.5^{\circ}C$, polythermic method, Zhuravleva et al. 1977)
- 37* (recommended-IUPAC Solubility Data Series, temp range 15 – $120^{\circ}C$, Barton 1984)
- 210* ($29.6^{\circ}C$, shake flask-GC/TC, measured range 29.6 – $90.4^{\circ}C$, Stephenson 1992)
- 35.9 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 133.3* ($69.5^{\circ}C$, summary of literature data, temp range 69.5 – $231.0^{\circ}C$, Stull 1947)
- 747* ($105.0^{\circ}C$, ebulliometry-differential thermal analysis, measured range 105 – $231^{\circ}C$, Kemme & Kreps 1969)
- $\log (P/mmHg) = 6.39379 - 1180.306/(104.321 + t/^{\circ}C)$; temp range 105 – $231^{\circ}C$, or pressure range 5.6 – 757.5 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
- 1.0* (comparative ebulliometry, measured range 127.261 – $255.2^{\circ}C$, Ambrose & Sprake 1970)
- $\log (P/Pa) = 5.94387 - 1434.755/(T/K - 139.888)$; restricted temp range 127.261 – $194.484^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- $\log (P/Pa) = 5.86571 - 1373.916/(T/K - 147.202)$; temp range 127.16 – $255.2^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- 124* ($76.23^{\circ}C$, comparative ebulliometry, measured range 349.38 – $406.19\ K$, data fitted to Chebyshev polynomial, Ambrose et al. 1974)
- $\log (P/mmHg) = [-0.2185 \times 13849.2/(T/K)] + 9.115470$; temp range 59.5 – $213.5^{\circ}C$ (Antoine eq., Weast 1972–73)
- 0.5866 ($20^{\circ}C$, evaporation rate-gravimetric method, Gückel et al. 1973)
- 1.10 ($20^{\circ}C$, evaporation rate-gravimetric method, Gückel 1982)

$\log (P/\text{kPa}) = 5.76028 - 1315.079/(119.128 + t/^{\circ}\text{C})$, temp range 105–231°C (Antoine eq. derived from exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.84611 - 1365.892/(124.619 + t/^{\circ}\text{C})$, temp range 127.2–255.2°C (Antoine eq. derived from data of Ambrose & Sprake 1970, Boublik et al. 1984)

$\log (P_{\text{S}}/\text{kPa}) = 17.615 - 6028/(T/\text{K})$; temp range 264–279 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 6.57397 - 1761.308/(-113.992 + T/\text{K})$; temp range 349–410 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 5.8587 - 1374.347/(-147.547 + T/\text{K})$; temp range 405–528 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 111.7949 - 8.3502 \times 10^3/(T/\text{K}) - 34.786 \cdot \log(T/\text{K}) + 3.3682 \times 10^{-10} \cdot (T/\text{K}) + 7.2697 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 268–673 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

2.689 (computer value, Yaws et al. 1991)

3.222 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.98 (HPLC-RT correlation, D'Amboise & Hani 1982)

4.57 (shake flask, Log P Database, Hansch & Leo 1987)

4.57 (recommended, Sangster 1993)

4.57 (shake flask, recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constant, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 11.1.1.14.1

Reported aqueous solubilities of 1-decanol at various temperatures

Barton 1984		Stephenson & Stuart 1986	
IUPAC recommended		shake flask-GC/TC	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
15	32	29.6	210
20	36	40.3	260
25	37	50.0	260
102	10000#	60.3	280
120	8000#	70.2	220
	# tentative	80.2	240
		90.4	230
		mp/ $^{\circ}\text{C}$	5

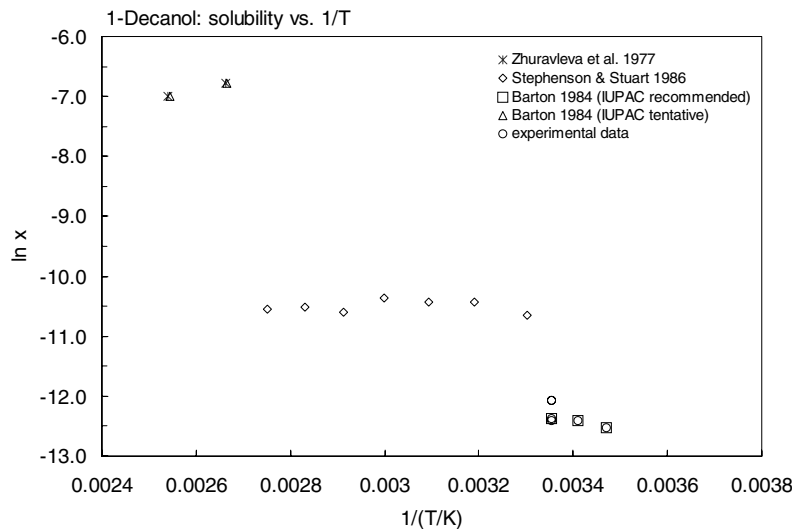


FIGURE 11.1.14.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-decanol.

TABLE 11.1.14.2
Reported vapor pressures of 1-decanol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Kemme & Kreps 1969		Ambrose & Sprake 1970		Ambrose & Sprake 1974	
summary of literature data		differential thermal analysis		comparative ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
69.5	133.3	105.0	747	127.261	2656	349.38	124
97.3	666.6	114.5	1360	129.526	2968	358.67	235
111.3	1333	121.7	2000	133.573	3600	364.21	339
125.8	2666	127.3	2680	138.245	4468	364.26	352
142.1	5333	135.6	3986	141.817	5242	371.15	528
152.9	7999	142.2	5346	147.863	6250	371.30	534
165.8	13332	149.9	7466	149.414	7266	375.86	701
186.2	26664	159.2	10812	154.602	8995	379.24	854
208.6	53329	169.9	16172	159.206	10799	380.38	917
231.0	101325	183.9	25398	163.693	12835	383.04	1061
mp/°C	7.0	197.4	40397	168.653	15439	385.72	1236
		215.3	67301	174.653	19146	388.16	1408
		231.0	101005	177.568	21193	392.43	1769
				182.748	25250	395.02	2025
		Antoine eq		189.377	31359	397.42	2283
		eq. 2	P/mmHg	194.484	36807	401.34	2774
		A	6.39397	201.039	44875	403.08	3017

(Continued)

TABLE 11.1.1.14.2 (Continued)

Stull 1947		Kempe & Kreps 1969		Ambrose & Sprake 1970		Ambrose & Sprake 1974	
summary of literature data		differential thermal analysis		comparative ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		B	1180.306	207.352	55899	404.70	3263
		C	104.321	213.119	63364	406.19	3504
				218.923	74244		
				225.489	87994		
				230.471	99886		
				237.598	118863		

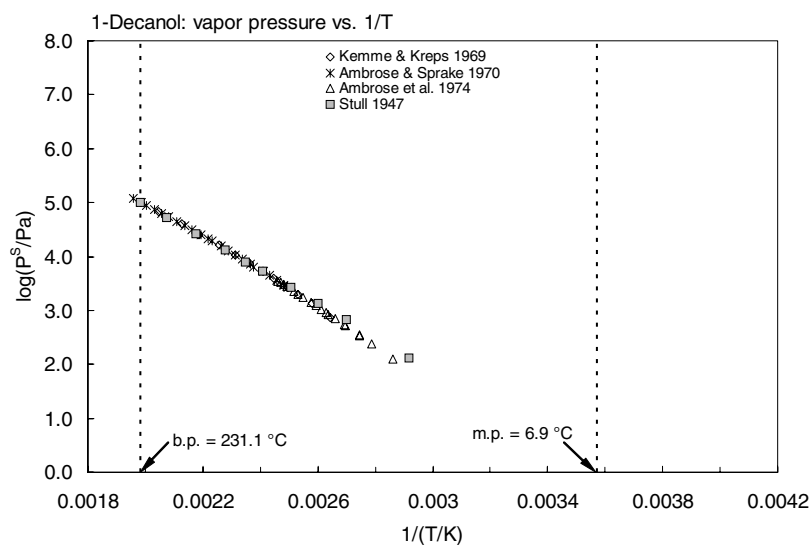
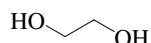


FIGURE 11.1.1.14.2 Logarithm of vapor pressure versus reciprocal temperature for 1-decanol.

11.1.1.15 Ethylene glycol



Common Name: Ethylene glycol

Synonym: 1,2-ethanediol, 1,2-dihydroxyethane, MEG

Chemical Name: 1,2-ethanediol, ethylene glycol

CAS Registry No: 107-21-1

Molecular Formula: $C_2H_6O_2$, $HOCH_2CH_2OH$

Molecular Weight: 62.068

Melting Point ($^{\circ}C$):

−12.69 (Lide 2003)

Boiling Point ($^{\circ}C$):

197.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1088 (Weast 1982–83)

Molar Volume (cm^3/mol):

55.8 (Rohrschneider 1973)

66.6 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

14.22 (Dean 1985)

14.24 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.958 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985; Howard 1990; Yaws et al. 1990)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

22.39 (extrapolated-Antoine eq., differential manometer, Gallagher & Hibbert 1937)

$\log (P/mmHg) = 9.2087 - 2976.6/(T/K)$; temp range 40 – $120^{\circ}C$ (Antoine eq. from differential Hg manometry measurements, Gallagher & Hibbert 1937)

133.3* ($53.0^{\circ}C$, summary of literature data, temp range 53.0 – $197.3^{\circ}C$, Stull 1947)

$\log (P/mmHg) = [-0.2185 \times 14032.4/(T/K)] + 9.394685$; temp range: 53 – $197.3^{\circ}C$ (Antoine eq., Weast 1972–73)

11.70* (ebulliometry, extrapolated-Antoine eq., measured range 270 – $310 K$, Ambrose & Hall 1981)

$\log (P/kPa) = 11.1828 - 2611.2/[(T/K) - 40.0]$; temp range 270 – $310 K$ (ebulliometry, Antoine eq., Ambrose & Hall 1981)

$\log (P/kPa) = 6.83995 - 1818.591/[(T/K) - 94.499]$; temp range 374.01 – $495.4 K$ (Antoine eq., ebulliometry, Ambrose & Hall 1981)

7.40* ($20^{\circ}C$, average, gas saturation-GC/FID, Hales et al. 1981)

$\log (P/mmHg) = 23.7259 - 4648.55/(T/K) - 503391/(T/K)^2$; temp range 283 – $373 K$ (empirical vapor pressure eq., gas saturation, Hales et al. 1981)

14.90 ($20^{\circ}C$, evaporation method, Gückel et al. 1982)

6.67, 26.66 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

0.73, 9.30 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.69339 - 1093.154/(98.821 + t/^{\circ}C)$; temp range 122.5 – $186.5^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 7.13856 - 2035.185/(1936.936 + t/^{\circ}C)$; temp range 50 – $200^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

11.86 (extrapolated-Antoine eq., Dean 1985)

11.7 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.83995 - 1818.591/(178.651 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 8.3726 - 2994.4/(T/\text{K})$, temp range 130–190°C, (Antoine eq., Riddick et al. 1986)
 $\log (P/\text{mmHg}) = 8.0908 - 2088.9/(203.5 + t/^{\circ}\text{C})$; temp range 50–200°C (Antoine eq., Dean 1985, 1992)
 10.1 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.98465 - 1928.08/(-83.45 + T/\text{K})$; temp range 323–473 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.86912 - 1817.439/(-95.859 + T/\text{K})$, temp range 363–418 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 12.26 (Howard et al. 1986; quoted, Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 82.4062 - 6.3472 \times 10^3/(T/\text{K}) - 25.433 \cdot \log(T/\text{K}) - 2.3732 \times 10^{-9} \cdot (T/\text{K}) + 8.7467 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 160–645 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.006 (calculated- C_W/C_A , Hine & Mookerjee 1975)
 5.81×10^{-6} , 2.37×10^{-5} (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

-1.93 (shake flask, Hansch & Leo 1979)
 -1.34 (shake flask-RC, Cornford 1982)
 -1.36 (shake flask, Log P Database, Hansch & Leo 1987)
 -1.36 (recommended, Sangster 1993)
 -1.36 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.00 (golden ide, after 3 d, Freitag et al. 1985)
 2.28 (algae, after 1 d, Freitag et al. 1985)
 2.30 (activated sludge, after 5 d, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate $k = 2.915 \times 10^{-6} \text{ mol cm}^{-2} \text{ h}^{-1}$ was determined by gravimetric method with an air flow rate $k = (50 \pm 1) \text{ L h}^{-1}$ at $20 \pm 0.1^{\circ}\text{C}$ (Gückel et al. 1973);
 evaporation rate $k = 2.97 \times 10^{-8} \text{ mol cm}^{-2} \text{ h}^{-1}$ was determined at 20°C (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 photooxidation $t_{1/2} = 267 \text{ d}$ –64.6 yr in water, based on measured rate constant for the reaction with OH radical (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)
 photooxidation $t_{1/2} = 0.24$ –2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
 $k_{OH} = (7.7 \pm 1.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K in air (Wiedermann & Zetzsch 1982; quoted, Atkinson 1985)
 photooxidation $t_{1/2} = 8.3$ –83 h in air, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

Hydrolysis:

Biodegradation:

$k = 41.7 \text{ mg COD g}^{-1} \text{ h}^{-1}$, average rate based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
 $k = 0.026$ –0.035 h^{-1} in 30 mg/L activated sludge after a time lag of 10–15 h (Urano & Kato 1986b)
 $t_{1/2}(\text{aq. aerobic}) = 48$ –288 h, based on grab sample from river die-away studies (Evans & David 1974; selected, Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 192–1152 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2}$ = 8.3–83 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2}$ = 267 d–64.6 yr, based on measured rate constant for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; Dorfman & Adams 1973; quoted, Howard et al. 1991); $t_{1/2}$ = 48–288 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2}$ = 96–576 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 48–288 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota

TABLE 11.1.1.15.1

Reported vapor pressures of ethylene glycol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C/(T/K)^2$	(5)	$\ln P = A - B/(T/K) - C/(T/K)^2$	(5a)

1.

Stull 1947		Ambrose & Hall 1981		Hales et al. 1981			
summary of literature data		comparative ebulliometry		transpiration-GC analysis			
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
				“continuous” measurements		“collection” measurements	
53.0	133.3	100.86	2208	10.0	2.698	9.0	2.711
79.7	666.6	103.869	2584	9.68	2.834	9.8	2.706
92.1	1333	107.59	3121	8.97	2.656	9.79	2.938
105.8	2666	111.997	3885	10.01	7.285	10.02	2.873
120.2	5333	115.971	4705	19.91	7.565	9.73	2.825
129.5	7999	120.647	5857	20.05	7.174	9.94	2.805
141.8	13332	124.645	7032	39.85	14.94	10.09	2.795
158.5	26664	129.735	8800	39.97	43.54	19.9	7.254
178.5	53329	133.244	10244	39.77	42.48	19.05	7.084
197.3	101325	182.095	62918	59.72	44.12	19.93	7.577
		187.372	74338	59.94	184.9	20.51	7.911
mp/ $^{\circ}\text{C}$	–15.6	192.976	88398	60.04	187.8	19.93	7.495
		197.704	101829	59.72	197.8	20.0	7.210
		203.13	119270	74.55	466.2	20.0	7.710
		207.615	135464	74.57	476.9	39.97	41.84
		212.932	156959	73.74	472.6		
		217.989	179863	100.17	2166.0		
		222.287	201399	100.15	2098.0	overall best fit equation	
		25.0	11.70			eq. 5a	
						P/Pa	

(Continued)

TABLE 11.1.1.15.1 (Continued)

Stull 1947		Ambrose & Hall 1981		Hales et al. 1981			
summary of literature data		comparative ebulliometry		transpiration-GC analysis			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		(extrapolated value)				A	23.7259
						B	4648.55
		bp/°C	297.54			C	503391
		eq. 3	P/kPa				
		A	6.83995				
		B	1818.591				
		C	-94.499				

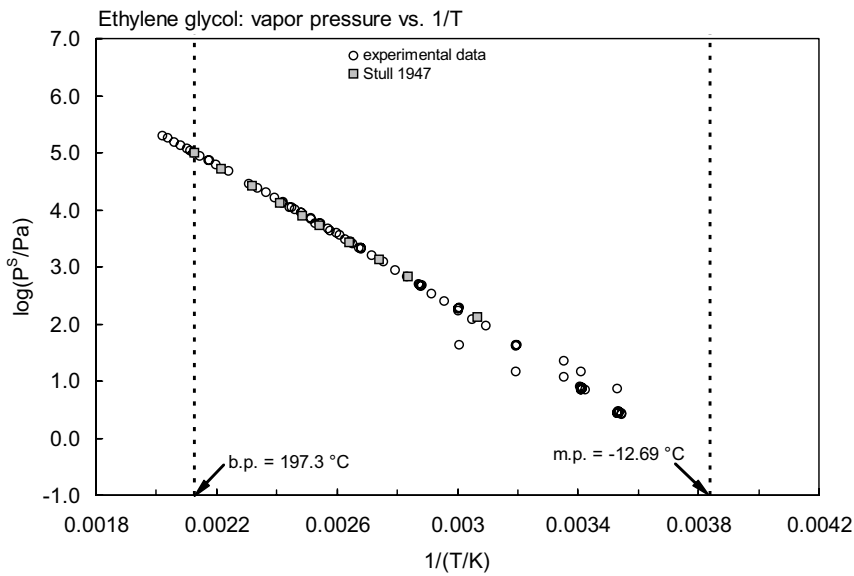
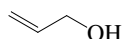


FIGURE 11.1.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for ethylene glycol.

11.1.1.16 Allyl alcohol



Common Name: Allyl alcohol

Synonym: propenylalcohol, 2-propen-1-ol, 1-propene-3-ol, vinylcarbinol

Chemical Name: allyl alcohol, 1-propene-3-ol, 2-propen-1-ol

CAS Registry No: 107-18-6

Molecular Formula: C_3H_6O , $CH_2=CHCH_2OH$

Molecular Weight: 58.079

Melting Point ($^{\circ}C$):

-129 (Stull 1947; Weast 1982–83; Verschueren 1983; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

97.1 (Weast 1982–83; Dean 1985; Riddick et al. 1986)

97 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.854 (Weast 1982–83; Dean 1985)

0.85511 ($15^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

64.8 (Kamlet et al. 1986; Leahy 1986)

74.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

15.5 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2666* ($21.7^{\circ}C$, temp range -20 to $96.6^{\circ}C$, Stull 1947)

3140 (Hoy 1970)

$\log(P/mmHg) = [-0.2185 \times 10577.7/(T/K)] + 9.143231$; temp range -20 to $96.6^{\circ}C$ (Antoine eq., Weast 1972–73)

2666, 4266 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

3750 (Riddick et al. 1986)

$\log(P/kPa) = 31.75070 - 3451.8/(T/K) - 7.94975 \log(T/K)$; temp not specified (Riddick et al. 1986)

3298 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.40725 - 1790.13/(-38.295 + T/K)$; temp range 253 – 370 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 21.3978 - 2.9525 \times 10^3/(T/K) - 3.8137 \cdot \log(T/K) - 2.7145 \times 10^{-3} \cdot (T/K) + 1.8811 \times 10^{-6} \cdot (T/K)^2$; temp range 144 – 545 K (vapor pressure eq., Yaws 1994)

6954* ($38.28^{\circ}C$, ebulliometry, measured range 311.42 – 355.70 K, Lubomska & Malanowski 2004)

$\log(P/kPa) = 6.936209 - 1513.129/[(T/K) - 63.131]$; temp range 311.42 – 355.70 K (Antoine eq., ebulliometric method, Lubomska & Malanowski 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.506 (calculated- C_W/C_A , Hine & Mookerjee 1975)

0.510 (calculated-bond contribution, Hine & Mookerjee 1975)

0.564 (computed, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.17	(shake flask, Hansch & Leo 1979)
0.17	(recommended, Sangster 1989)
0.17	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 334 \text{ d}$ – 37 yr , based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; quoted, Howard et al. 1991)

photooxidation $t_{1/2} = 2.2$ – 22 h , based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{OH} = 25.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 440 K (Atkinson 1989)

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 24$ – 168 h , based on estimated unacclimated aqueous aerobic biodegradation screening test data (Sasaki 1978; quoted, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 96$ – 672 h , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.2$ – 22 h , based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 334 \text{ d}$ – 37 yr , based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 48$ – 336 h , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 24$ – 168 h , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 11.1.1.16.1

Reported vapor pressures of allyl alcohol at various temperatures

Stull 1947		Lubomska & Malanowski 2004	
summary of literature data		ebulliometry	
$t/^\circ\text{C}$	P/Pa	T/K	P/Pa
–20.0	133.3	311.42	6954
0.20	666.6	315.81	8869
10.5	1333	319.97	11079
21.7	2666	326.70	15672
33.4	5333	331.84	20194
40.3	7999	334.20	22603
50.0	13332	337.96	26943
64.5	26664	341.54	31723

TABLE 11.1.1.16.1 (Continued)

Stull 1947		Lubomska & Malanowski 2004	
summary of literature data		ebulliometry	
t/°C	P/Pa	T/K	P/Pa
80.2	53329	344.27	35822
96.6	101325	346.97	40304
		351.37	48613
mp/°C	−129	353.15	52334
		353.59	53299
		355.70	58108

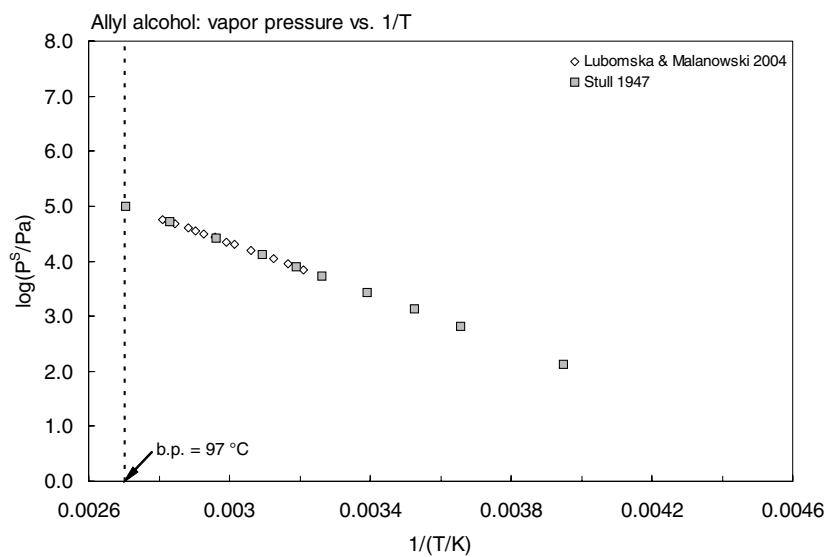
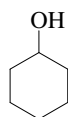


FIGURE 11.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for allyl alcohol.

11.1.1.17 Cyclohexanol



Common Name: Cyclohexanol

Synonym: adronol, anol, cyclohexylalcohol, hexahydrophenol, hexalin, hydralin, hydrophenol

Chemical Name: cyclohexanol

CAS Registry No: 108-93-0

Molecular Formula: $C_6H_{11}OH$

Molecular Weight: 100.158

Melting Point ($^{\circ}C$):

25.93 (Lide 2003)

Boiling Point ($^{\circ}C$):

160.84 (Lide 2003)

Density (g/cm^3):

0.9624 (Lide 2003)

Molar Volume (cm^3/mol):

104.0 (calculated-density, Lande & Banerjee 1981)

125.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

1.70 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

37000* (shake flask-synthetic method, temp range 7.2 – $184.72^{\circ}C$, Sidgwick & Sutton 1930)

39200 (shake flask-interferometry, Hansen et al. 1949)

32920 (residue volume, Booth & Everson 1942)

40000* ($20^{\circ}C$, synthetic method, measured range 0 – $184^{\circ}C$, Zil'berman 1951)

48960 (shake flask-interferometry, Donahue & Bartell 1952)

36000 ($26.7^{\circ}C$, shake flask-turbidity, Skrzec & Murphy 1954)

38000* (recommended "best" value, IUPAC Solubility Data Series, temp range 0 – $180^{\circ}C$, Baron 1984)

37500 (selected, Riddick et al. 1986)

44400* ($19.7^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.3^{\circ}C$, Stephenson & Stuart 1986)

38200 (selected, Yaws et al. 1990)

37500 (dialysis tubing equilibration-GC. Etzweiler et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

467* ($34.0^{\circ}C$, Ramsay-Young method, measured range 34.0 – $149.0^{\circ}C$, Gardner & Brewer 1937)

133.1*, 194 ($21^{\circ}C$, interpolated-regression of tabulated data, temp range 21 – $161^{\circ}C$, Stull 1947)

7177* ($93.73^{\circ}C$, temp range 93.73 – $160.70^{\circ}C$, Novak et al. 1960; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 11935.8/(T/K)] + 8.909086$; temp range 21 – $161^{\circ}C$ (Antoine eq., Weast 1972–73)

174.8 (calculated-Cox eq., Chao et al. 1983)

$\log(P/mmHg) = [1 - 434.658/(T/K)] \times 10^{\{0.951396 - 8.46102 \times 10^{-4} \cdot (T/K) + 8.87926 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 294.15 – $434.15\ K$ (Cox eq., Chao et al. 1983)

37.53 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.2553 - 912.87/(109.13 + t/^{\circ}C)$; temp range 94 – $161^{\circ}C$ (Antoine eq., Dean 1985, 1992)

1300 ($56^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 5.92859 - 1199.10/(t/^{\circ}C + 145.0)$; temp range 107 – $160^{\circ}C$ (Riddick et al. 1986)

97.36 (interpolated, solid, Antoine eq.-I, Stephenson & Malanowski 1987)

80.0, 84.85 (extrapolated, liquid, Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log(P_S/\text{kPa}) = 9.631 - 3173.1/(T/\text{K})$; temp range 272–298 K (Antoine eq.-I, for solid, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.1634 - 1318.5/(-116.55 + T/\text{K})$; temp range 318–434 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.27792 - 1381.8/(-110.132 + T/\text{K})$; temp range 300–434 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

106.6 (Daubert & Danner 1989)

14.66, 196.0 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 49.9123 - 4.8446 \times 10^3/(T/\text{K}) - 13.711 \cdot \log(T/\text{K}) + 3.5451 \times 10^{-9} \cdot (T/\text{K}) + 1.5932 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 297–625 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

0.581 (calculated- C_W/C_A , Hine & Mookerjee 1975)

2.48, 2.37 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

0.281 (calculated-P/C, Howard 1993)

0.278 (correlated-molecular structure, Russell et al. 1992)

0.446 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.23 (shake flask-AS, Hansch & Anderson 1967, Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)

1.36 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

1.23 (recommended, Sangster 1989, 1993)

1.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

5.18 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

0.708 (estimated- K_{OW} , Lyman et al. 1990)

0.176 (estimated-S, Lyman et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

2.045 (soil, estimated- K_{OW} , Lyman et al. 1990; quoted, Howard 1993)

1.114 (soil, estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 145$ d estimated from a model environmental pond with the consideration of the effect of adsorption (USEPA 1987; quoted, Howard 1993);

based on the Henry's law constant, $t_{1/2} \sim 13.3$ d from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s at 25°C (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 17.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radical concentration of 5×10^5 per cm^3 in air at 25°C corresponds to an atmosphere $t_{1/2} = 22$ h (Atkinson 1987; quoted, Howard 1993)

Hydrolysis:

Biodegradation: average rate of biodegradation $k = 28.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 22$ h, based on estimated reaction rate constant of 17.4×10^{-12} cm³ molecule⁻¹ s⁻¹ for the vapor phase reaction with 5×10^5 hydroxyl radical per cm³ in air at 25°C (Howard 1993).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 11.1.1.17.1

Reported aqueous solubilities of cyclohexanol at various temperatures

Sidgwick & Sutton 1930		Zil'berman 1951		Barton 1984		Stephenson & Stuart 1986	
synthetic method		synthetic method		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
7.2	50000	0	53400	0	53000	0	67700
9.4	47800	10	45700	10	46200	9.5	54000
9.7	45800	20	40000	20	39700	19.7	44400
11.2	44100	30	36000	25	38000	30.6	37400
12.0	45500	40	33300	30	35500	40.0	36300
14.2	42300	50	31400	40	33000	50.0	34900
15.2	42900	54	31000	50	31000	60.3	33700
16.3	40900	62	31000	60	31000	70.1	34400
20.6	39500	70	31900	70	32000	80.2	36000
20.8	38200	80	34100	80	34000	90.3	37500
24.6	37500	90	36500	90	37000		
27.55	35200	100	39300	100	39000		
28.7	35700	110	42800	110	43000		
31.85	33700	120	47000	120	49000		
33.6	34100	130	53000	130	56000		
40.4	32600	140	61000	140	64000		
40.45	31800	150	72000	150	77000		
45.8	31900	160	88000	160	93000		
121.95	51400	170	115000	170	120000		
156.9	92200	180	178000	180	190000		
174.3	150000	184	339000				
179.4	192000						
184.72	324000						

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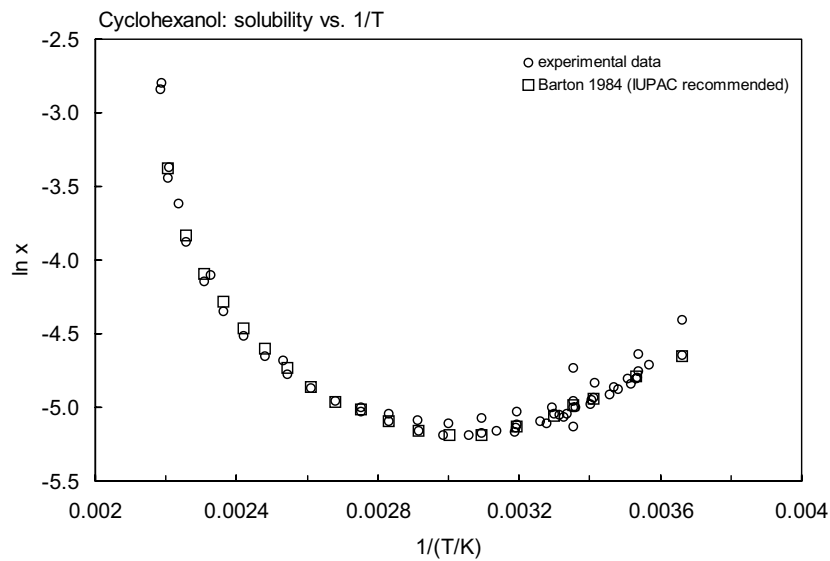


FIGURE 11.1.1.17.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for cyclohexanol.

TABLE 11.1.1.17.2
Reported vapor pressures of cyclohexanol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K)$$
$$\log P = A - B/(C + t/^{\circ}\text{C})$$
$$\log P = A - B/(C + T/K)$$
$$\log P = A - B/(T/K) - C \cdot \log(T/K)$$

(1)

(2)

(3)

(4)

$$\ln P = A - B/(T/K)$$
$$\ln P = A - B/(C + t/^{\circ}\text{C})$$

(1a)

(2a)

Gardner & Brewer 1937		Stull 1947		Novak et al. 1960	
Ramsay-Young method		summary of literature data		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
34.0	467	21.0	133.3	93.73	7177
37.5	560	44.0	666.6	97.02	9210
46.4	587	56.0	1333	99.71	10426
47.8	693	68.8	2666	102.52	11876
53.6	907	83.0	5333	104.83	13159
59.4	1133	91.8	7999	108.82	15372
73.0	2773	103.7	13332	112.70	18252
80.5	4146	121.7	26664	116.86	21891
97.8	9826	141.4	53329	120.35	25264
119.1	13771	161.0	101325	125.54	30864
136.9	47036			130.95	37543
149.0	71994	mp/°C	23	136.22	45356
				142.41	56448
bp/°C	162.3			148.72	69487
				155.71	86046
				160.70	99192
				in Boublik et al. 1984	
				eq. 2	P/kPa
				A	5.34182
				B	894.818
				C	106.797
				bp/°C	161.425

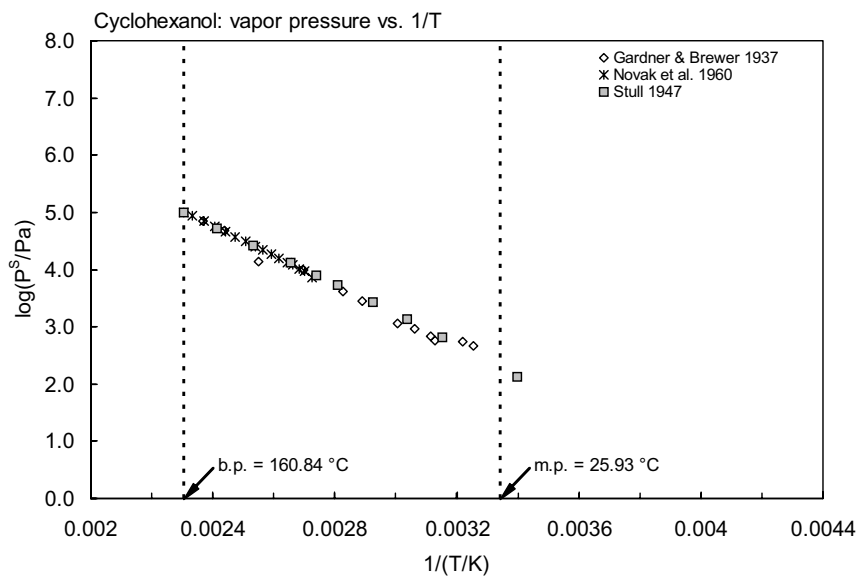
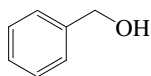


FIGURE 11.1.17.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexanol.

11.1.1.18 Benzyl alcohol



Common Name: Benzyl alcohol

Synonym: benzenemethanol, (hydroxymethyl)benzene, *o*-hydroxy toluene, phenylcarbinol, phenylmethanol

Chemical Name: benzyl alcohol

CAS Registry No: 100-51-6

Molecular Formula: C_7H_8O , $C_6H_5CH_2OH$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

−15.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

205.31 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.04535, 1.04156 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.04127 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

103.5 (calculated-density, Rohrschneider 1973)

125.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

48.13, 61.42 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.406 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

38020 (Seidell 1941)

34200 (estimated, McGowan 1954)

38000 (20 – $25^{\circ}C$, shake flask-GC, Urano et al. 1982)

35000 ($20^{\circ}C$, Verschueren 1983)

42900 (shake flask-LSC, Banerjee 1985)

43000* ($20.1^{\circ}C$, shake flask-GC/TC, measured range 0 – $50^{\circ}C$, Stephenson & Stuart 1986)

46070 (shake flask-GC, Li et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($60.9^{\circ}C$, static method, measured range 60.9 – $152.1^{\circ}C$, Kahlbaum 1898)

26.7* ($38.8^{\circ}C$, ebulliometry, measured range 38.8 – $151.6^{\circ}C$, Gardner & Brewer 1937)

15.40* (extrapolated-regression of tabulated data, temp range 58 – $205.7^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.90550 - 2187.8/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

6287* ($122.52^{\circ}C$, ebulliometry, measured range 122.52 – $205.41^{\circ}C$, Dreisbach & Shrader 1949)

19.59 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.58200 - 1904.3/(200.0 + t/^{\circ}C)$; temp range 112 – $330^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

12.0 (Hoy 1970)

$\log(P/mmHg) = [-0.2185 \times 14093.2/(T/K)] + 9.391874$; temp range 58 – $204.7^{\circ}C$ (Antoine eq., Weast 1972–73)

8.35*, 10.06 ($20^{\circ}C$, $25^{\circ}C$, extrapolated-Antoine eq., gas-saturation method, Grayson & Fosbraey 1982)

$\log(P/Pa) = 29.0 - 7958/(T/K)$; temp range 29.5 – $60.1^{\circ}C$ (Antoine eq., gas saturation, Grayson & Fosbraey 1982)

4.750 (extrapolated-Cox eq., Chao et al. 1983)

- $\log (P/\text{mmHg}) = [1 - 479.624/(T/K)] \times 10^4 \{ 1.02742 - 6.26739 \times 10^{-4} \cdot (T/K) + 1.28791 \times 10^{-7} \cdot (T/K)^2 \}$; temp range 340.95–463.65 K (Cox eq., Chao et al. 1983)
 12.07, 9.69 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.34897 - 1650.313/(174.623 + t/^{\circ}\text{C})$; temp range 122.5–205.4°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.39383 - 1655.003/(171.85 + t/^{\circ}\text{C})$; temp range 38.8–151.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 11.72 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.19817 - 1632.593/(172.79 + t/^{\circ}\text{C})$; temp range 122–205°C (Antoine eq., Dean 1985, 1992)
 15.0 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 8.963 - 3214/(T/K)$; temp range not specified (Antoine eq., Riddick et al. 1986)
 15.25 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.7069 - 1904.3/(-73.15 + T/K)$; temp range 385–573 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.963 - 3214/(T/K)$; temp range 293–315 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 7.395 (ebulliometry, fitted to Antoine eq., Ambrose & Ghassee 1990)
 12.0 (calculated-Wagner eq., Ambrose & Ghassee 1990)
 $\log (P/\text{mmHg}) = -36.2189 - 3.3475 \times 10^3/(T/K) + 23.337 \cdot \log(T/K) - 4.46 \times 10^{-2} \cdot (T/K) + 2.1443 \times 10^{-5} \cdot (T/K)^2$; temp range 258–677 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 0.0231 (quoted estimated value of Hine & Mookerjee 1975, Howard 1993)
 0.0396 (calculated-P/C, Howard 1993)
 < 0.0273 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 1.10 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968)
 1.10 ± 0.02 (shake flask-UV, Iwasa et al. 1965)
 1.10 (shake flask-UV, Hansch et al. 1968)
 1.10 (shake flask-RC, Cornford 1982)
 1.00 (shake flask-UV, Mayer et al. 1982)
 1.16 ± 0.02 (exptl.-ALPM, Garst & Wilson 1984)
 1.06 (HPLC-k' correlation, Eadsforth 1986)
 1.58 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 1.05 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
 1.05 (recommended, Sangster 1989, 1993)
 1.22 (centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)
 0.96 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)
 1.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 0.602 (calculated- K_{ow} , Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{oc}$:

- 1.193 (red-brown Australian soil with 1.09% organic carbon, Briggs 1981; quoted, Howard 1993)
 0.790 (calculated- K_{ow} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 97$ d for a model river of 1 m deep, flowing at 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 7.99 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, estimated from Atmospheric Oxidation Program; $k_{\text{OH}}(\text{exptl}) = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{\text{OH}}(\text{calc}) = 7.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, estimated from Fate of Atmospheric Pollutants Program, (Meylan & Howard 1993)

$k_{\text{OH}}(\text{calc}) = 0.85 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{exptl}) = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation: biodegradation rate constant $k = 0.042\text{--}0.062 \text{ h}^{-1}$ in 30 mg L^{-1} activated sludge after a lag time of 5–15 h (Urano & Kato 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the estimated $t_{1/2} \sim 2 \text{ d}$ for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Atkinson 1985; quoted, Howard 1993).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.18.1

Reported aqueous solubilities of benzyl alcohol at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	48000
9.8	47000
20.1	43000
29.6	43000
40.2	45000
50.0	52000

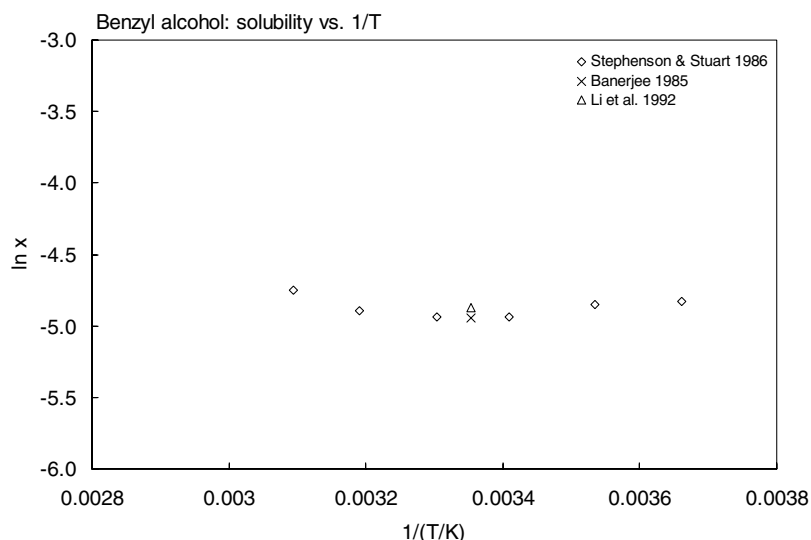


FIGURE 11.1.1.18.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for benzyl alcohol.

TABLE 11.1.1.18.2

Reported vapor pressures of benzyl alcohol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Kahlbaum 1898		Gardner & Brewer 1937		Stull 1947		Grayson & Fosbraey 1982	
static method		ebulliometry		summary of literature data		gas saturation-GC/LC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
60.9	133.3	38.8	26.7	58.0	133.3	29.5	18.29
67.8	266.6	42.5	80.0	80.8	666.6	30.2	22.77
72.9	400.0	46.8	106.7	92.6	1333	39.8	44.22
77.2	533.3	50.5	120.0	105.8	2666	40.1	46.11
80.8	666.6	85.2	906.6	119.8	5333	49.7	101.41
92.8	1333.2	97.2	1747	129.3	7999	60.1	221.10
99.9	1999.8	113.5	3880	141.7	13332	20	8.35
105.3	2666.4	128.8	7786	160.0	26664		
109.7	3333.06	151.6	18918	183.0	53329	eq. 1a	P/Pa
113.4	3999.7			204.7	101325	A	29.0
116.7	4666.3	bp/°C	206.9			B	7958
119.6	5332.9			mp/°C	−15.3		
122.2	5999.5						
124.4	6666.1						
133.9	9999.2						
141.3	13332						
152.1	19998						
				Dreisbach & Shrader 1949			
				ebulliometry			
				t/°C	P/Pa		
				122.52	6287		
				127.12	7605		
				130.90	8851		
				134.28	10114		
				147.09	16500		
				190.50	67661		
				205.41	101325		

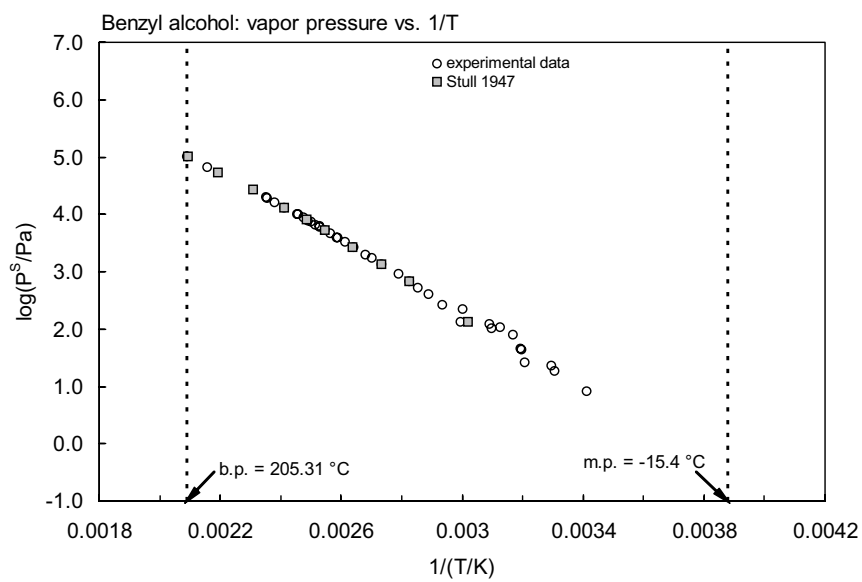


FIGURE 11.1.18.2 Logarithm of vapor pressure versus reciprocal temperature for benzyl alcohol.

11.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 11.2.1
Summary of physical properties of alcohols

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C	Molar volume, V_M cm ³ /mol	
							MW/ ρ at 20°C	Le Bas
Methanol	67-56-1	CH ₃ OH	32.042	-97.53	64.6	1	40.49	37.0
Ethanol	64-17-5	C ₂ H ₅ OH	46.068	-114.14	78.29	1	58.36	59.2
Propanol (<i>n</i> -Propyl alcohol)	71-23-8	C ₃ H ₇ OH	60.095	-124.39	97.2	1	74.79	81.4
Isopropanol (<i>i</i> -Propyl alcohol)	67-63-0	<i>i</i> C ₃ H ₇ OH	60.095	-87.9	82.3	1	76.51	81.4
1-Butanol (<i>n</i> -Butyl alcohol)	71-36-3	C ₄ H ₉ OH	74.121	-88.6	117.73	1	91.56	103.6
Isobutanol (<i>i</i> -Butyl alcohol)	78-83-1	<i>i</i> C ₄ H ₉ OH	74.121	-101.9	107.89	1	92.47	103.6
<i>sec</i> -Butyl alcohol	78-92-2	<i>s</i> C ₄ H ₉ OH	74.121	-88.5	99.51	1	91.90	103.6
<i>tert</i> -Butyl alcohol	75-65-0	<i>t</i> C ₄ H ₉ OH	74.121	25.69	82.4	1	94.88	103.6
1-Pentanol (<i>n</i> -Amyl alcohol)	71-41-0	C ₅ H ₁₁ OH	88.148	-77.6	137.98	1	108.23	125.8
2-Pentanol	6032-29-7	C ₅ H ₁₁ OH	88.148	-73	119.3	1	108.91	125.8
1-Hexanol	111-27-3	C ₆ H ₁₃ OH	102.174	-47.4	157.6	1	124.79	148.0
1-Heptanol	111-70-6	C ₇ H ₁₅ OH	116.201	-33.2	176.45	1	141.38	170.2
1-Octanol (<i>n</i> -Octyl alcohol)	111-87-5	C ₈ H ₁₇ OH	130.228	-14.8	195.16	1	157.85	192.4
1-Nonanol	143-08-8	C ₉ H ₁₉ OH	144.254	-5	213.37	1	174.37	214.6
1-Decanol	112-30-1	C ₁₀ H ₂₁ OH	158.281	6.9	231.1	1	190.77	236.8
Ethylene glycol	107-21-1	(CH ₂ OH) ₂	62.068	-12.69	197.3	1	55.98	66.6
Allyl alcohol	107-18-6	C ₃ H ₅ OH	58.079	-129	97	1	67.92	74.0
Cyclopentanol	96-41-3	C ₅ H ₉ OH	86.132	-17.5	140.42	1	90.78	106.9
Cyclohexanol	108-93-0	C ₆ H ₁₁ OH	100.158	25.93	160.84	1	104.07	125.6
Benzyl alcohol	100-51-6	C ₇ H ₇ OH	108.138	-15.4	205.31	1	103.85	125.6

TABLE 11.2.2
Summary of selected physical-chemical properties of alcohols at 25°C

Compound	Selected properties				log K _{OW} calcd P/C	Henry's law constant H/(Pa·m ³ /mol)		
	Solubility		Vapor pressure			exptl (a)	exptl (b)	exptl (c)
	S/(g/m ³)	C _L /(mol/m ³)	P _L /Pa					
Methanol	miscible	miscible	16210	−0.77		0.45		0.45
Ethanol	miscible	miscible	7800	−0.31		0.53		0.527
Propanol	miscible	miscible	2780	0.25				0.751
Isopropanol	miscible	miscible	5700	0.05				0.80
1-Butanol	74000	998.4	900	0.82	0.9014	0.80	0.892	0.80
Isobutanol	81000	1093	1500	0.76	1.3726	0.99		0.99
<i>sec</i> -Butyl alcohol	181000	2442	2300	0.61	0.9419	0.80		0.918
<i>tert</i> -Butyl alcohol	miscible	miscible	5500	0.35		1.46		1.46
1-Pentanol	22000	249.6	300	1.50	1.202	1.314		
2-Pentanol	45000	510.5	777	1.14	1.522			
1-Hexanol	6000	58.72	110	2.03	1.873	1.562	1.735	
1-Heptanol	1740	14.97	24	2.62	1.603	1.909		
1-Octanol	540	4.146	11	3.07	2.653	2.454	2.48	
1-Nonanol	130	0.9012		4.26				
1-Decanol	37	0.2338		4.57				
Ethylene glycol	miscible	miscible	12	−1.36		0.006		
Allyl alcohol	miscible	miscible	3750	0.17				
Cyclopentanol			292					
Cyclohexanol	38000	379.4	85	1.23	0.224			
Benzyl alcohol	80	0.7398	12	1.10	16.22			

(a) Butler et al. 1935

(b) Buttery et al. 1969

(c) Snider & Dawson 1985

TABLE 11.2.3
Suggested half-life classes of alcohols in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Methanol	4	3	3	4
Ethanol	3	3	3	4
Propanol (<i>n</i> -Propyl alcohol)	3	3	3	4
Isopropanol (<i>i</i> -Propyl alcohol)	3	3	3	4
1-Butanol (<i>n</i> -Butyl alcohol)	3	3	3	4
Isobutanol (<i>i</i> -Butyl alcohol)	3	3	3	4
<i>tert</i> -Butyl alcohol	4	4	4	5
1-Pentanol (<i>n</i> -Amyl alcohol)	3	3	3	4
1-Hexanol	3	3	3	4
1-Octanol (<i>n</i> -Octyl alcohol)	3	3	3	4
Ethylene glycol	3	3	3	4
Allyl alcohol	3	3	3	4
Cyclohexanol	3	3	3	4
Benzyl alcohol	3	3	3	4

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

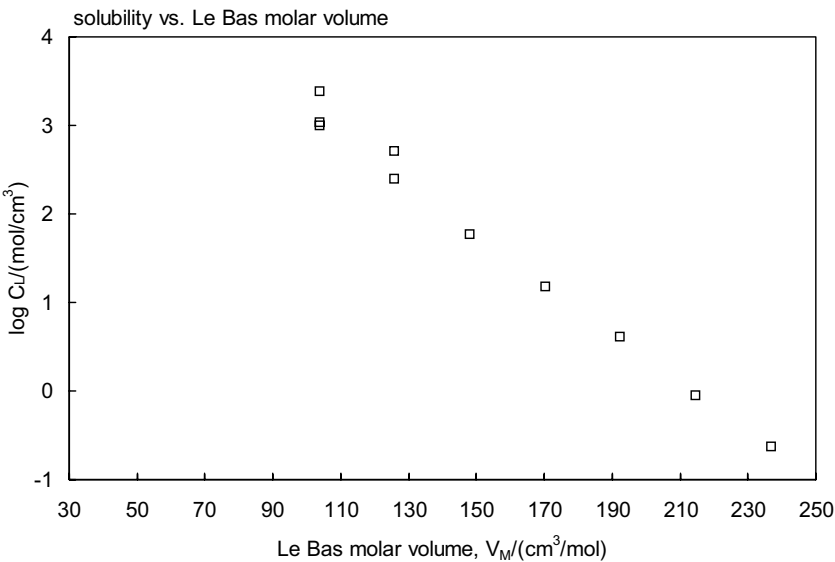


FIGURE 11.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alcohols.

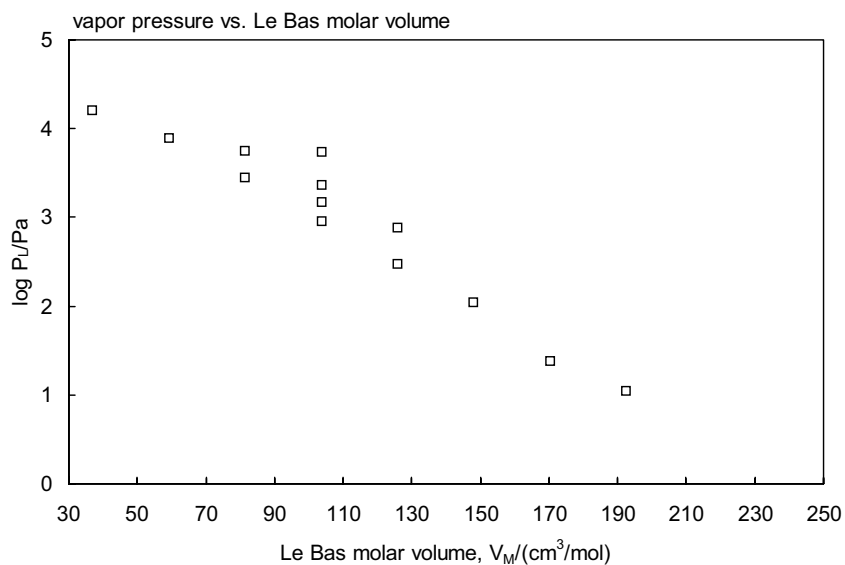


FIGURE 11.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alcohols.

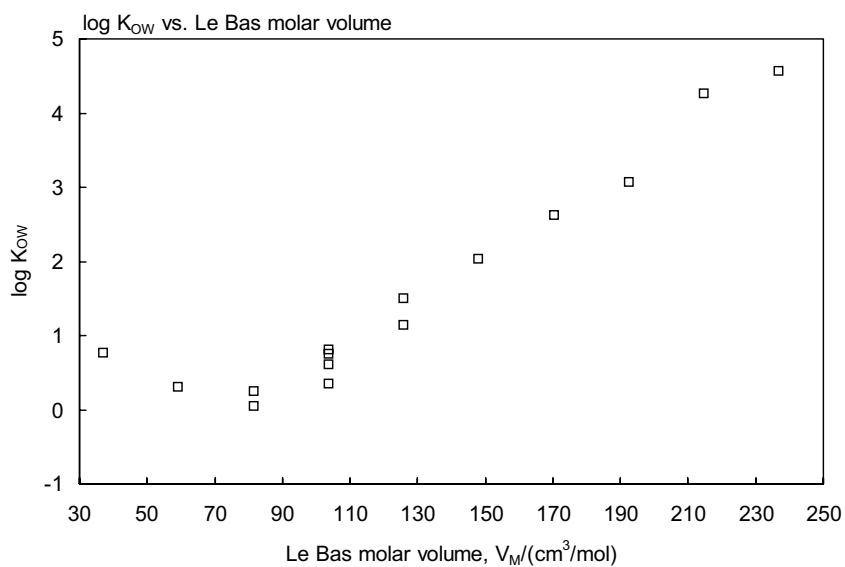


FIGURE 11.2.3 Octanol-water partition coefficient versus Le Bas molar volume for alcohols.

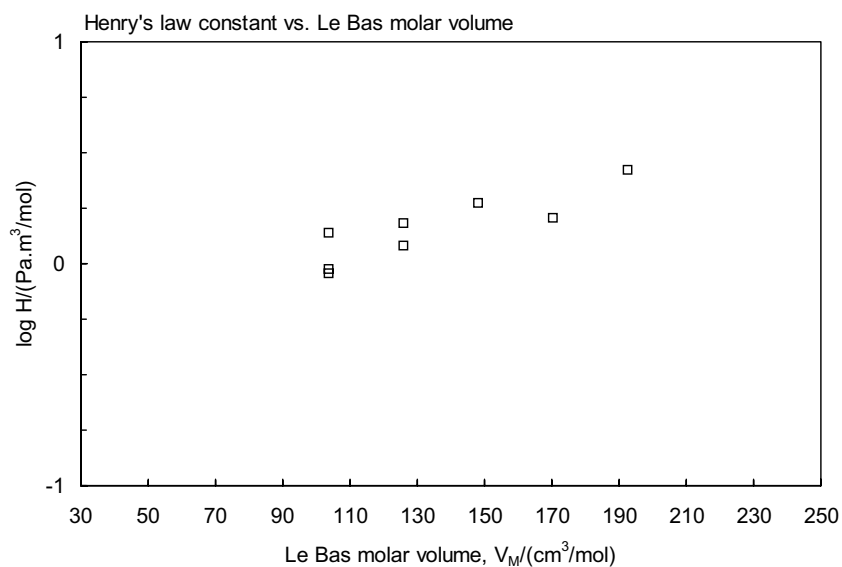


FIGURE 11.2.4 Henry's law constant versus Le Bas molar volume for alcohols.

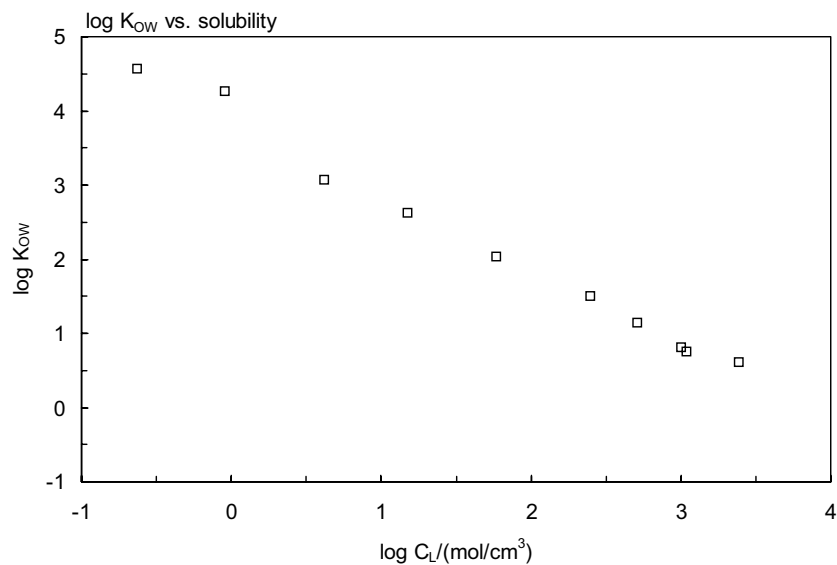


FIGURE 11.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alcohols.

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12 Aldehydes and Ketones

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12.1 LIST OF CHEMICALS AND DATA COMPILATIONS

12.1.1 ALDEHYDES

12.1.1.1 Methanal (Formaldehyde)



Common Name: Formaldehyde

Synonym: formalin, methanal, oxomethane

Chemical Name: formaldehyde

CAS Registry No: 50-00-0

Molecular Formula: CH₂O, HCHO

Molecular Weight: 30.026

Melting Point (°C):

-92.0 (Weast 1982–83; Dean 1985; Lide 2003)

Boiling Point (°C):

-19.1 (Lide 2003)

Density (g/cm³):

0.815 (-20°C, Weast 1982–83)

0.815 (-20°C, Verschueren 1983; Dean 1985)

Molar Volume (cm³/mol):

36.8 (-20°C, Stephenson & Malanowski 1987)

29.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K.), F: 1.0Water Solubility (g/m³ or mg/L at 25°C):

1220000 (Dean 1985)

very soluble, up to 55% (Budavari 1989, Howard 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

88566* (-22.29°C, static method-differential manometer, measured range -109.39 to -22.29°C, Spencer & Wild 1935)

101325* (-19.5°C, summary of literature data, temp range -88 to -19.5°C, Stull 1947)

log (P/mmHg) = [-0.2185 × 5917.9/(T/K)] + 7.985746; temp range -88 to -19.5°C (Antoine eq., Weast 1972–73)

1333 (-88°C, Verschueren 1983)

log (P/kPa) = 6.32524 - 972.5/(244.329 + t/°C), temp range (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 7.1958 - 970.65/(244.1 + t/°C); temp range -109 to -22°C (Antoine eq., Dean 1985, 1992)

log (P_L/kPa) = 6.5475 - 1062.4/(-19.92 + T/K), temp range 184–251 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.4306 - 1013.206/(-24.883 + T/K); temp range 163–251 K (Antoine eq.-II, Stephenson & Malanowski 1987)

517690 (1 atm, Howard 1989)

log (P/mmHg) = 41.9603 - 2.1355 × 10³/(T/K) - 13.765·log (T/K) + 9.568 × 10⁻³·(T/K) - 5.1101 × 10⁻¹²·(T/K)²; temp range 181–408 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0331 (20°C, porous membrane gas-liquid equilibration system, Dong & Dasgupta 1986)

0.0169 (review, Gaffney et al. 1987)

0.0341* (gas stripping-headspace GC, measured range 15–45°C, Betterton & Hoffmann 1988)

0.0298* (gas-stripping-HPLC-UV, freshwater, measured range 10–45°C, Zhou & Mopper 1990)
 $\ln [K_H'/(M/atm)] = -6.0 + 2844/(T/K)$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
 $\ln [K_H'/(M/atm)] = -6.7 + 3069/(T/K)$, temp range 25–45°C (gas stripping-HPLC measurements, seawater (salinity $35 \pm 1\%$), Zhou & Mopper 1990)
 0.021 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 4.621 - 2840/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.35 (shake flask, Johnson & Piret 1948)
 -1.54 (Kenaga & Goring 1980)
 0.00 (Verschuereen 1983)
 0.35 (recommended, Sangster 1989)
 0.35 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

no bioconcentration. in fish and shrimp observed (Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: sunlight photolysis $t_{1/2} = 1.25$ – 6.0 h, based on measured gas-phase photolysis by simulated sunlight (Calvert et al. 1972; Su et al. 1979; quoted, Howard et al. 1991);
 rate constant $k = 8.0 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carrier et al. 1986);
 calculated lifetime of 4 h (Atkinson 2000).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius equation see reference:

$k_{OH} = 1.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

aqueous photooxidation $t_{1/2} = 4813$ – 190000 h, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; quoted, Howard et al. 1991)

$k_{OH} = 1.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (long-path Fourier transform IR, Niki et al. 1978)

$k_{NO_3} = 3.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 1 K (review, Atkinson & Lloyd 1984)

$k = (0.1 \pm 0.03) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{HO_2} = 4.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with HO_2 radical at 298 K (review, Baulch et al. 1984; quoted, Carrier et al. 1986)

$k_{OH} = 1.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Baulch et al. 1984; quoted, Carrier et al. 1986)

$k_{OH}(\text{calc}) = 7.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 9.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

atmospheric photooxidation half-life of 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k_{OH}^* = 9.77 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{NO_3} = 5.8 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{OH}(\text{calc}) = 17.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: degradation complete in 20 h under aerobic conditions and 48 h under anaerobic conditions in a die-away test using water from a stagnant lake (Howard 1989)

aqueous aerobic half-life of 24–168 h, based on unacclimated aqueous aerobic biodegradation screening test data; aqueous anaerobic half-life of 96–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: half-life is a few hours in the sunlit troposphere; $t_{1/2} = 19$ and 50 h by dry deposition and wet removal, respectively; $t_{1/2} = 12$ d when reacts with NO_3 radical by H-atom abstraction. (Howard 1989)

photooxidation $t_{1/2} = 7.13\text{--}71.3$ h, based on measured rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);

$t_{1/2} = 1.26\text{--}6.0$ h, based on photolysis half-life in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994);

calculated lifetimes of 1.2 d, 80 d and > 4.5 yr for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.1.1.1

Reported vapor pressures of methanal (formaldehyde) at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Spencer & Wild 1935		Stull 1947	
differential manometer		summary of literature data	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-109.39	127	-88.0	1333
-104.39	237	-79.6	2666
-98.29	480	-70.6	5333
-95.19	647	-65.0	7999
-89.09	1157	-57.3	13332
-85.59	1633	-46.0	26664
-78.89	2802	-33.0	53329
-78.29	2946	-19.5	101325
-71.29	4720		
-68.55	6190	mp/ $^{\circ}\text{C}$	-92
-65.29	7859		
-64.59	8219		
-63.69	8693		
-55.79	14799		
-53.99	16625		
-49.29	21745		
-40.59	35544		
-39.09	38743		
-34.29	49182		
-28.39	66208		
-22.29	88566		

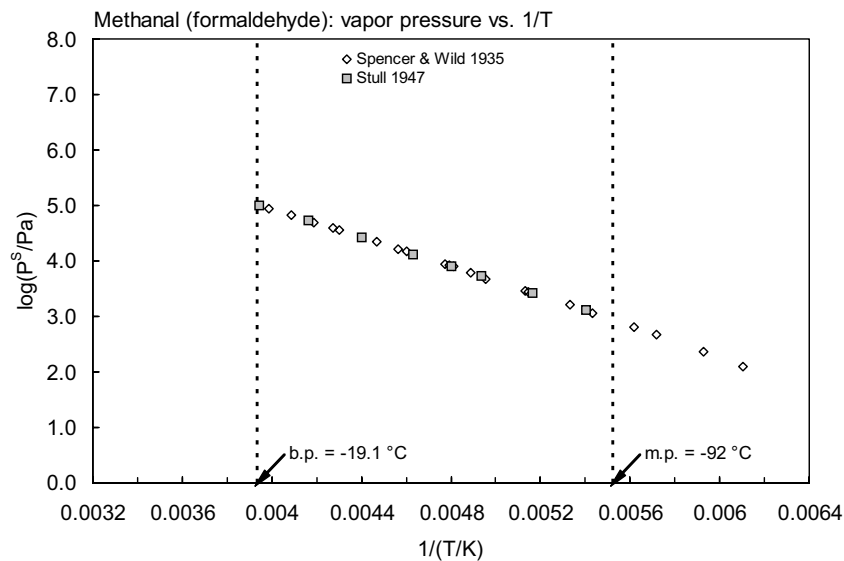


FIGURE 12.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methanal.

TABLE 12.1.1.1.2
Reported Henry's law constants of methanal (formaldehyde) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		
Betterton & Hoffmann 1988		Zhou & Mopper 1990	
gas stripping-fluorescence		gas stripping-HPLC/UV	
gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
		t/°C	H/(Pa m³/mol)
		fresh water	
15	0.01386	10	0.01023
15	0.01031*	17	-
25	0.0341	25	0.0298
35	0.0675	30	0.0507
45	0.1506	35	0.0675
		40	0.0921
		45	0.125
$\Delta H/(\text{kJ mol}^{-1}) = -59.8$			
* in 0.5 M HSO ₄ solution		eq. 1a	$K_H'/(M/\text{atm})$
		A	-6.00
		B	-2844
		eq. 1a	$K_H'/(M/\text{atm})$
		A	-6.70
		B	-3069

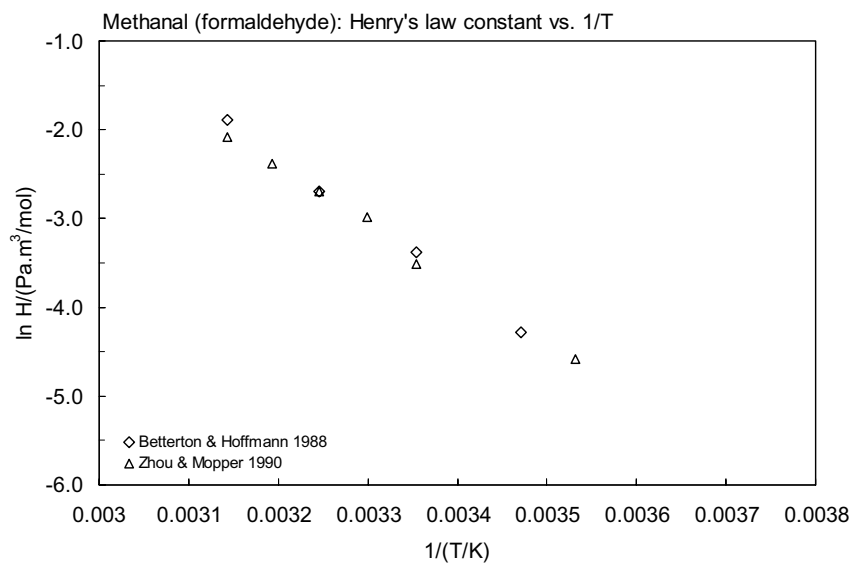


FIGURE 12.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for methanal.

12.1.1.2 Ethanal (Acetaldehyde)



Common Name: Acetaldehyde

Synonym: acetic aldehyde, aldehyde, ethanal, ethylaldehyde

Chemical Name: acetaldehyde, ethanal

CAS Registry No: 75-07-0

Molecular Formula: C_2H_4O , CH_3CHO

Molecular Weight: 44.052

Melting Point ($^{\circ}C$):

−123.37 (Lide 2003)

Boiling Point ($^{\circ}C$):

20.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7834 ($18^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

56.23 ($18^{\circ}C$, calculated-density)

51.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

−10.2 (pK_b , Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

3.243 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Palit 1947; Riddick et al. 1986)

miscible (Verschueren 1983; Dean 1985)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

101300* ($20.2^{\circ}C$, summary of literature data, temp range -81.5 to $5.9^{\circ}C$, Stull 1947)

102125* ($20.7^{\circ}C$, measured range -0.20 to $34.4^{\circ}C$, Coles & Popper 1950)

120060 (Hoy 1970)

$\log(P/\text{mmHg}) = [-0.2185 \times 7267.8/(T/K)] + 8.327803$; temp range -81.5 to $20.2^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 6622.1/(T/K)] + 7.82060$; temp range -24.3 to $27.5^{\circ}C$ (Antoine eq., Weast 1972–73)

98640 ($20^{\circ}C$, Verschueren 1983)

102125, 120220 ($20.7^{\circ}C$, quoted exptl., interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 7.14122 - 1606.85/(292.482 + t/^{\circ}C)$, temp range: -0.2 to $34.3^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

120230 (calculated-Antoine eq., Dean 1985, 1992)

$\log(P/\text{mmHg}) = 8.00552 - 1600.017/(291.809 + t/^{\circ}C)$, temp range: liquid (Antoine eq., Dean 1985, 1992)

121300 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.1814 - 1070.6/(236.0 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

120700 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.1410 - 1034.5/(-43.15 + T/K)$; temp range 272 – 294 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.03292 - 1012.828/(-41.823 + T/K)$; temp range 293 – 377 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 87.3702 - 3.6822 \times 10^3/(T/K) - 31.548 \cdot \log(T/K) + 2.0114 \times 10^{-2} \cdot (T/K) + 5.5341 \times 10^{-13} \cdot (T/K)^2$; temp range 150 – 461 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 6.692 (shake flask-concentration ratio-GC, Buttery et al. 1969)
- 8.924 (calculated K_{AW} s, Buttery et al. 1969)
- 6.672 (exptl., Hine & Mookerjee 1975)
- 5.946, 5.423 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 1.336, 8.0 (0, 25°C, gas stripping-GC, Snider & Dawson 1985)
- 6.75 (review, Gaffney et al. 1987)
- 2.578* (gas stripping-headspace GC, measured range 15–35°C, Betterton & Hoffmann 1988)
- 6.80* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)
- $\ln [K_{\text{H}}'/(M/\text{atm})] = -6.03 + 276/(T/K)$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
- $\ln [K_{\text{H}}'/(M/\text{atm})] = -5.21 + 1984/(T/K)$, temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity $35 \pm 1\text{‰}$), Zhou & Mopper 1990)
- 10.18 (calculated-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
- 5.47* (20°C, headspace-GC, measured range 10–40°C, Benkelberg et al. 1995)
- 8.72* (headspace-GC, artificial seawater, measured range 16–40°C, Benkelberg et al. 1995)
- $\ln (k_{\text{H}}/\text{atm}) = (20.4 \pm 0.1) - (5671 \pm 22)/(T/K)$; temp range 10–40°C (headspace-GC measurements, Benkelberg et al. 1995)
- 5.14 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
- 6.33 (solid-phase microextraction SPME-GC, Bartelt 1997)
- 6.69 (equilibrium headspace-GC, Marin et al. 1999)
- 5.39 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
- $\log K_{\text{AW}} = 5.324 - 2340/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.52 (generator column-HPLC, Wasik et al. 1981)
- 0.36 (generator column-GC, Tewari et al. 1982)
- 0.43 (calculated, Verschueren 1983)
- 0.45 (recommended, Sangster 1989, 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 2.3.0 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986);
calculated lifetime of 6 d (Atkinson 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and or Arrhenius equation see reference:

$k_{\text{OH}} = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{\text{OH}} = 1.6.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (long-path Fourier transform IR, Niki et al. 1978)

$k = 0.1 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with half-life of $8 \times 10^4 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with half-life $> 00 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{OH}} = (12.8 \pm 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Kerr & Sheppard 1981; quoted, Atkinson 1985)

$k = (1.5 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}} = (12.2 \pm 2.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Semmes et al. 1985; quoted, Atkinson 1985)

$k_{\text{O}_3} = (3.4 \pm 0.5) \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (Stedman & Niki 1973; quoted, Atkinson & Carter 1984)

$k_{\text{OH}} = 9.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k_{\text{O}_3} \leq 6 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ $296 \pm 2 \text{ K}$ (Atkinson et al. 1981, 1982; quoted, Atkinson & Carter 1984; Atkinson 1985)

$k_{\text{HO}_2} = 1.0 \times 10^{-17} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with HO_2 radical at 293 K in the atmosphere (Barnes et al. 1982; quoted, Carlier et al. 1986)

$k_{\text{OH}} = 1.62 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$; and $k_{\text{NO}_3} = 3.02 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K in air (Atkinson et al. 1984)

$k_{\text{NO}_3} = 1.40 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ $298 \pm 1 \text{ K}$ (review, Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{OH}} = 1.60 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)

$k_{\text{OH}} = (14.7 \pm 2.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Michael et al. 1985; quoted, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 1.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}} = 1.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.7 d^{-1} , $k_{\text{O}_3} \leq 6.0 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $\leq 0.0004 \text{ d}^{-1}$, $k_{\text{NO}_3} = 2.5 \times 10^{-15} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.05 d^{-1} (review, Atkinson 1985)

$k_{\text{OH}}^* = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 16.22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 3.02 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{\text{NO}_3} = 2.78 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{\text{OH}} = 10.64 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} < 0.24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994);

calculated lifetimes of 8.8 h, 17 d and $> 4.5 \text{ yr}$ for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.2.1

Reported vapor pressures of ethanal (acetaldehyde) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
Stull 1947	Coles & Popper 1950		
summary of literature data	isoteniscope method		
t/°C	P/Pa	t/°C	P/Pa
-81.5	133.3	-0.20	44263
-65.1	666.6	2.70	49996
-56.8	1333	6.70	59062
-47.8	2666	9.30	65861
-37.8	5333	11.6	70794
-31.4	7999	15.3	76927
-22.6	13332	17.6	90926
-10.0	26664	20.7	102125
4.90	53329	30.8	149321
20.2	101325	34.4	167852
mp/°C	-123.5	bp/°C	20.4
		eq. 1	P/mmHg
		A	7.694
		B	1413

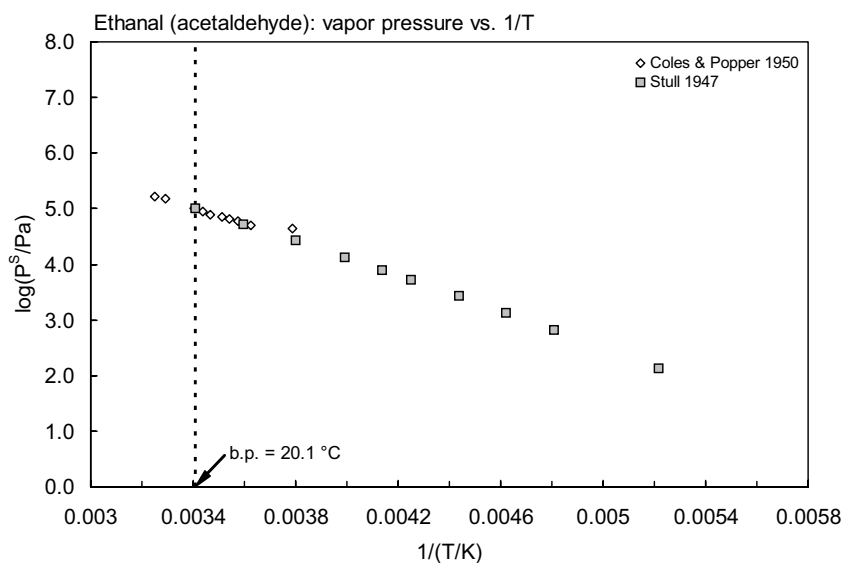


FIGURE 12.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethanal.

TABLE 12.1.1.2.2

Reported Henry's law constants of ethanal (acetaldehyde) at various temperatures and temperature dependence equations

$$\begin{aligned}\ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) & (4) & \ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K) & (4a) \\ K_{AW} &= A - B\cdot(T/K) + C\cdot(T/K)^2 & (5) & & \end{aligned}$$

1.

Snider & Dawson 1985		Betterton & Hoffmann 1988		Zhou & Mopper 1990			
gas stripping-GC		gas stripping-GC, spec.		gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
				fresh water		sea water	
0	1.336	5	1.829	10	2.277	10	3.147
25	8.00	10	2.578	17	-	17	5.170
		25	8.888	25	6.80	25	7.735
enthalpy of transfer:		35	15.446	30	8.238	30	9.296
$\Delta H/(\text{kJ mol}^{-1}) = -46.024$		$\Delta H/(\text{kJ mol}^{-1}) = -52.1$		35	10.55	35	11.78
		at 25°C		40	-	40	14.90
				45	15.59	45	17.78
				eq. 1a	$K_H'/(M/\text{atm})$	eq. 1a	$K_H'/(M/\text{atm})$
				A	-6.03	A	-5.21
				B	-2164	B	-1894

2.

Benkelberg et al. 1995			
equilibrium vapor phase concentration-headspace GC			
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
deionized water		artificial sea water	
10	2.754	16	5.070
15	3.940	25	8.718
20	5.472	30	11.69
30	10.268	40	19.716
40	18.968		
for deionized and rain water:			
eq. 3	k_H/atm		
A	20.4 ± 0.1		
B	5671 ± 22		
$\Delta H/(\text{kJ mol}^{-1}) = -47.15$			

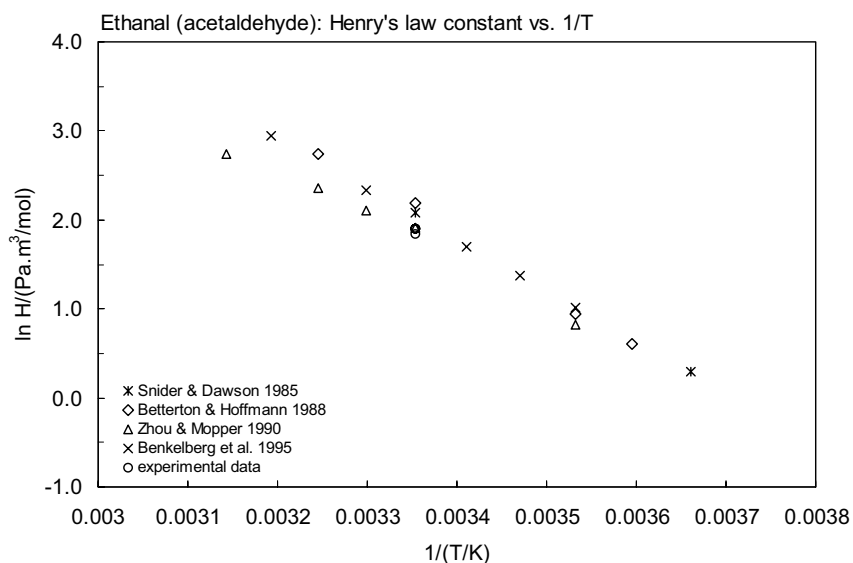
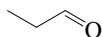


FIGURE 12.1.1.2.2 Logarithm of Henry's law constant versus reciprocal temperature for ethanal.

12.1.1.3 Propanal (Propionaldehyde)



Common Name: Propionaldehyde

Synonym: propanal

Chemical Name: propionaldehyde, propanal

CAS Registry No: 123-38-6

Molecular Formula: C_3H_6O , CH_3CH_2CHO

Molecular Weight: 58.079

Melting Point ($^{\circ}C$):

−80 (Lide 2003)

Boiling Point ($^{\circ}C$):

48 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8058 (Weast 1982–83)

0.7970 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

72.9 (calculated-density, Stephenson & Malanowski 1987)

74.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

160000 ($20^{\circ}C$, Seidell 1941)

200000 ($20^{\circ}C$, Verschueren 1983)

306000 (Dean 1985; Riddick et al. 1986)

405000 (selected, Yaws et al. 1990)

310000*, 269000 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 12.3 – $50^{\circ}C$, Stephenson 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

67661* ($39.07^{\circ}C$, ebulliometry, measured range 39.07 – $50.29^{\circ}C$, Dreisbach & Shrader 1949)

$\log(P/mmHg) = 7.08683 - 1178.9/(230 + t/^{\circ}C)$; temp range not specified (Antoine eq., Dreisbach & Martin 1949)

42300* ($23^{\circ}C$, measured range 13.1 – $48.06^{\circ}C$, Ambrose & Sprake 1974)

42340 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.2902 - 1210.87/(234.65 + t/^{\circ}C)$, temp range 13.1 – $48.06^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose & Sprake 1974, Boublik et al. 1984)

42490, 42360 (interpolated-Antoine eq. I and II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.2047 - 1166.99/(-43.15 + T/K)$; temp range 290–322 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.2336 - 1180/(-42.0 + T/K)$; temp range 250–330 K (Antoine eq.-II, Stephenson & Malanowski 1987)

23190 (calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/mmHg) = 26.1637 - 2.3059 \times 10^3/(T/K) - 6.5289 \cdot \log(T/K) - 2.3065 \times 10^{-10} \cdot (T/K) + 2.5454 \times 10^{-6} \cdot (T/K)^2$; temp range 193–496 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7.436 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)

7.486 (exptl., Hine & Mookerjee 1975)

- 8.40, 8.21 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 8.305* (gas stripping-HPLC/UV, measured range 10–45°C, Zhou & Mopper 1990)
 $\ln [K_H'/(M/atm)] = -7.15 + 2467/(T/K)$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
 $\ln [K_H'/(M/atm)] = -6.60 + 2273/(T/K)$, temp range 25–35°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 11), Zhou & Mopper 1990)
 7.486, 13.62 (quoted, correlated-molecular structure, Russell et al. 1992)
 5.48 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 5.324 - 2237/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.83 (calculated, Verschueren 1983)
 0.59 (shake flask, Log P Database, Hansch & Leo 1987)
 0.59 (recommended, Sangster 1989)
 0.59 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 3.02 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 3.2 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 3.06 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

photooxidation $t_{1/2} < 0.24 \text{ h}$ for the gas-phase reaction with OH radicals in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH} = 2.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (long-path Fourier transform IR, Niki et al. 1978)

$k_{OH} = (18.5 \pm 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Audley et al. 1981; quoted, Atkinson 1985),

$k_{OH} = (19.5 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Kerr & Sheppard 1981; quoted, Atkinson 1985)

$k = (2.5 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 1.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{OH} = (17.1 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Semmes et al. 1985; quoted, Atkinson 1985)

$k_{OH}(\text{calc}) = 2.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 3.3\text{--}33 \text{ h}$ in air, based on measured reaction rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991)

$k_{OH} = 1.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}(\text{calc}) = 16.55 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: biodegradation rate constants $k = 0.046\text{--}0.063 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b); aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on aerobic biological screening test data (Gerhold & Malaney 1966; Dore et al. 1975; Urano & Kato 1986; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} < 0.24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2}$ = 3.3–33 h in air, based on measured reaction rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).
Surface water: $t_{1/2}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Ground water: $t_{1/2}$ = 48–336 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Sediment:
Soil: $t_{1/2}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Biota:

TABLE 12.1.1.3.1
Reported aqueous solubilities and vapor pressures of propanal (propionaldehyde) at various temperatures

Aqueous solubility		Vapor pressure					
Stephenson 1993		Dreisbach & Shrader 1949		Dreisbach & Martin 1949		Ambrose & Sprake 1974	
shake flask-GC/TC		ebulliometry		ebulliometry		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.3	477000	39.07	67661	data presented in		13.1	25300
15.6	368000	50.29	101325	log P = A – B/(C + t/°C)		23.0	42300
20.0	310000			eq. 2	P/mmHg	29.5	51000
30.0	269000			A	7.08683	47.95	101300
40.0	235000			B	1178.9	48.06	101700
50.0	197000			C	230		
				bp/°C	50.29		

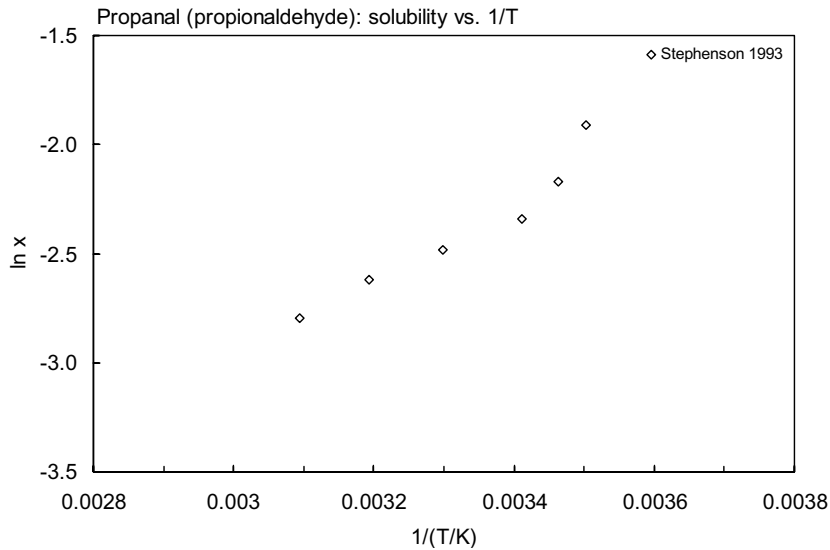


FIGURE 12.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for propanal.

TABLE 12.1.1.3.2

Reported Henry's law constants of propanal (propionaldehyde) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Zhou & Mopper 1990

gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
fresh water		sea water	
10	2.605	10	3.389
17	-	17	6.495
25	8.305	25	10.13
30	10.67	30	12.67
35	14.07	35	16.34
40	-	40	22.03
45	23.56	45	28.15
eq. 1a	K _H '/(M/atm)	eq. 1a	K _H '/(M/atm)
A	-7.15	A	-6.60
B	-2467	B	-2273

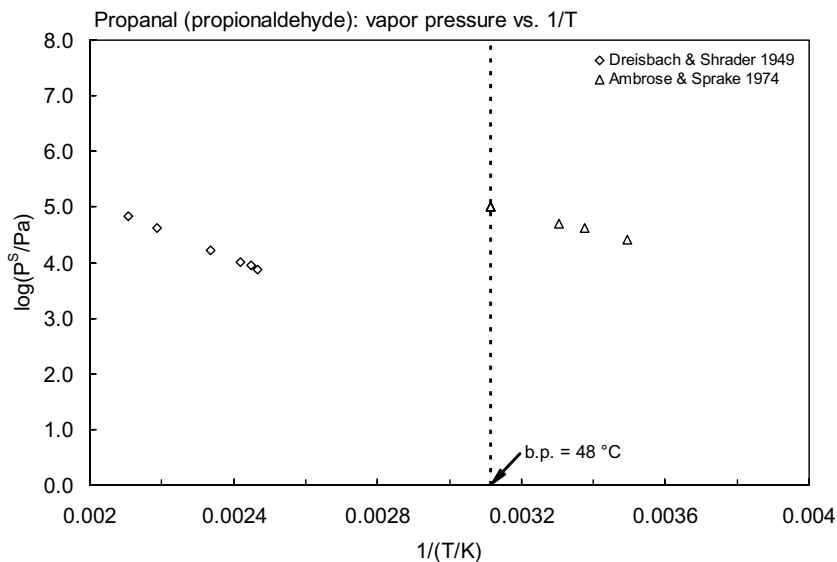


FIGURE 12.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for propanal.

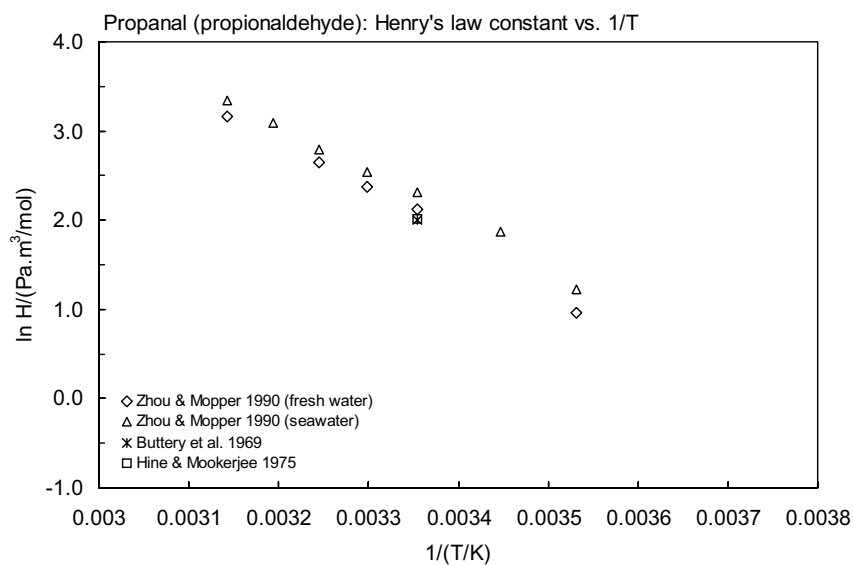
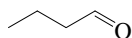


FIGURE 12.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for propanal.

12.1.1.4 Butanal (*n*-Butyraldehyde)

Common Name: *n*-Butyraldehyde

Synonym: 1-butanal, butylaldehyde, butyric aldehyde

Chemical Name: butyraldehyde, butanal

CAS Registry No: 123-72-8

Molecular Formula: C_4H_8O , $CH_3CH_2CH_2CHO$

Molecular Weight: 72.106

Melting Point ($^{\circ}C$):

−96.86 (Lide 2003)

Boiling Point ($^{\circ}C$):

74.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8170 (Weast 1982–83; Verschueren 1983)

0.8016 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

90.0 ($20^{\circ}C$, calculated-density)

96.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

11.088 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

36000 ($20^{\circ}C$, quoted, Palit 1947)

37840 (Deno & Berkheimer 1960)

37000, 71000 (lit. values, Verschueren 1983)

71000 (Dean 1985; Riddick et al. 1986)

83700 (selected, Yaws et al. 1990)

74400*, 54800 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $70^{\circ}C$, Stephenson 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19372* ($30.71^{\circ}C$, measured range 30.71 – $74.03^{\circ}C$, Seprakova et al. 1959; quoted, Boublik et al. 1984)

9464 ($20^{\circ}C$, Verschueren 1983)

14798 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.52728 - 921.802/(186.564 + t/^{\circ}C)$; temp range 30.71 – $74.03^{\circ}C$ (Antoine eq. from reported exptl. data of Seprakova et al. 1959, Boublik et al. 1984)

14785 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.91048 - 946.35/(246.68 + t/^{\circ}C)$; temp range -87 to $7^{\circ}C$ (Antoine eq., Dean 1985, 1992)

15700 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.1461 - 1233.0/(223.0 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

14780 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.68618 - 994.1/(-78.05 + T/K)$; temp range 293 – 349 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.40874 - 1182.472/(T/K)$; temp range 348 – 423 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 66.8411 - 3.6784 \times 10^3/(T/K) - 22.609 \cdot \log(T/K) + 1.1697 \times 10^{-2} \cdot (T/K) + 2.9647 \times 10^{-13} \cdot (T/K)^2$; temp range 177 – 525 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11.65 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)

11.59, 11.594, 12.14 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

11.65 (gas stripping-HPLC, Zhou & Mopper 1990)

3.237, 11.65, 15.59, 20.68, 36.19 (10, 25, 30, 35, 45°C, gas-stripping-HPLC-UV, Zhou & Mopper 1990)

$\ln [K_H'/(M/\text{atm})] = -8.07 + 2701/(T/K)$; temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

$\ln [K_H'/(M/\text{atm})] = -8.20 + 2698/(T/K)$; temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 11), Zhou & Mopper 1990)

11.59, 11.59 (quoted, correlated-molecular structure, Russell et al. 1992)

7.26 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.244 - 2571/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.20 (Hansch & Leo 1979)

0.88 (shake flask, Log P Database, Hansch & Leo 1987)

0.88 (recommended, Sangster 1989)

0.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.39 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 2.7 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:

photooxidation $t_{1/2} = 114 \text{ d}$ to 19 yr in water, based on measured rate constant for the reaction with OH radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

$k_{OH} = (26.2 \pm 3.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Audley et al. 1981; quoted, Atkinson 1985)

$k_{OH} = (25.3 \pm 0.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Kerr & Sheppard 1981; quoted, Atkinson 1985)

$k_{OH} = 25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k = (2.5 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = (30.8 \pm 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence technique. Semmes et al. 1985; quoted, Atkinson 1985)

$k_{OH}(\text{calc}) = 2.55 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 2.8\text{--}28 \text{ h}$ in air, based on measured rate constant for the gas-phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991)

$k_{OH}^* = 2.35 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation: rate constants $k = 0.044\text{--}0.069 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b);

aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on aerobic biological screening test data (Lamb & Jenkins 1952; Heukelekian & Rand 1955; Dore et al. 1975; Urano & Kato 1986b; selected, Howard et al. 1991);
 aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.8\text{--}28$ h, based on measured rate constant for the gas-phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);
 calculated lifetimes of 5.9 d for reaction with OH radical (Atkinson 2000).

Surface water: photooxidation $t_{1/2} = 114$ d to 19 yr, based on measured rate constant for the reaction with OH radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991);
 $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.1.4.1

Reported aqueous solubilities and vapor pressures of butanal (*n*-butyraldehyde) at various temperatures

Aqueous solubility		Vapor pressure	
Stephenson 1993		Seprakova et al. 1959	
shake flask-GC/TC		in Boublik et al. 1984	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
0	118200	30.71	19372
10.0	91200	38.36	26771
20.0	74400	43.93	33584
30.0	54800	48.33	39997
40.0	47100	52.36	46663
50.0	42500	55.90	53329
60.0	41700	62.29	66661
70.0	38900	67.73	79993
		74.03	97512
bp/ $^{\circ}\text{C}$	75		
eq in Boublik et al. 1984			
$\log P = A - B/(C + t/^{\circ}\text{C})$			
eq. 2			
		P/kPa	
		A	5.52728
		B	921.802
		C	186.564
		bp/ $^{\circ}\text{C}$	75.195

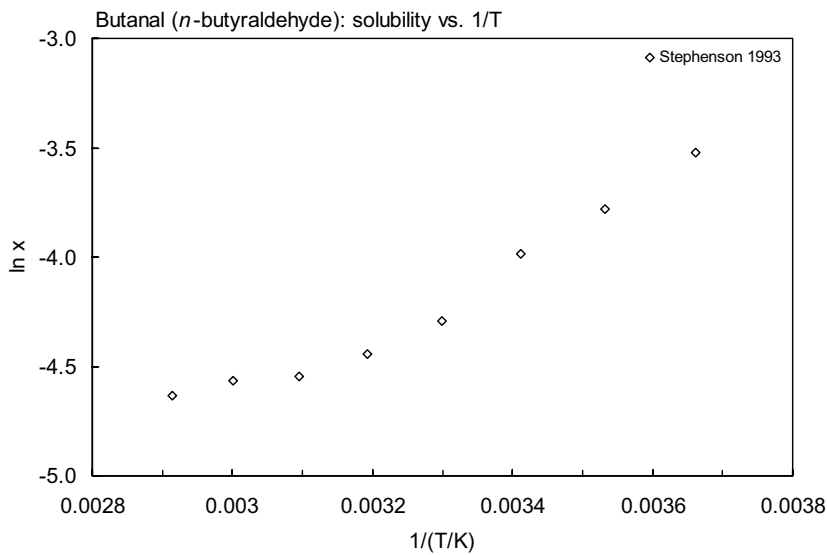


FIGURE 12.1.1.4.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for butanal.

TABLE 12.1.1.4.2
Reported Henry’s law constants of butanal (*n*-butyraldehyde) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Zhou & Mopper 1990

gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
fresh water		sea water	
10	3.237	10	4.312
17	-	17	8.660
25	11.65	25	16.08
30	15.83	30	20.68
35	20.68	35	28.15
40	-	40	38.97
45	36.18	45	50.66
eq. 1a	$K_H'/(M/\text{atm})$	eq. 1a	$K_H'/(M/\text{atm})$
A	-8.07	A	-8.20
B	-2704	B	-2698

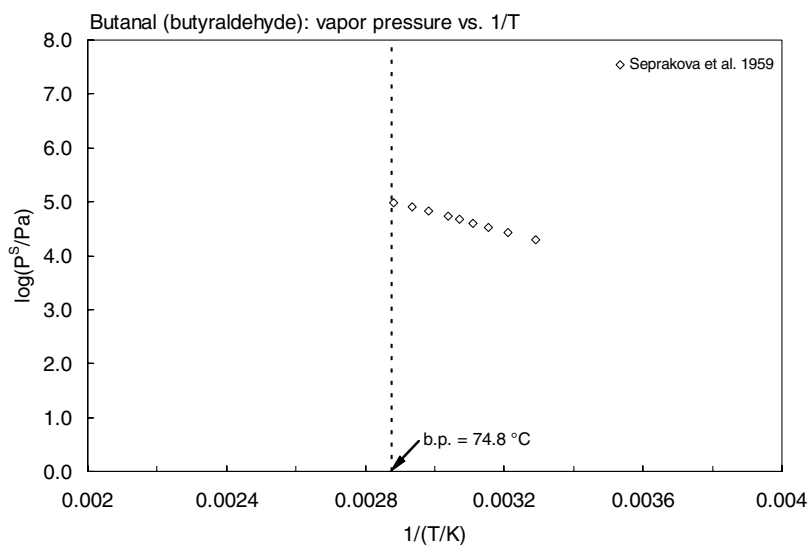


FIGURE 12.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for butanal.

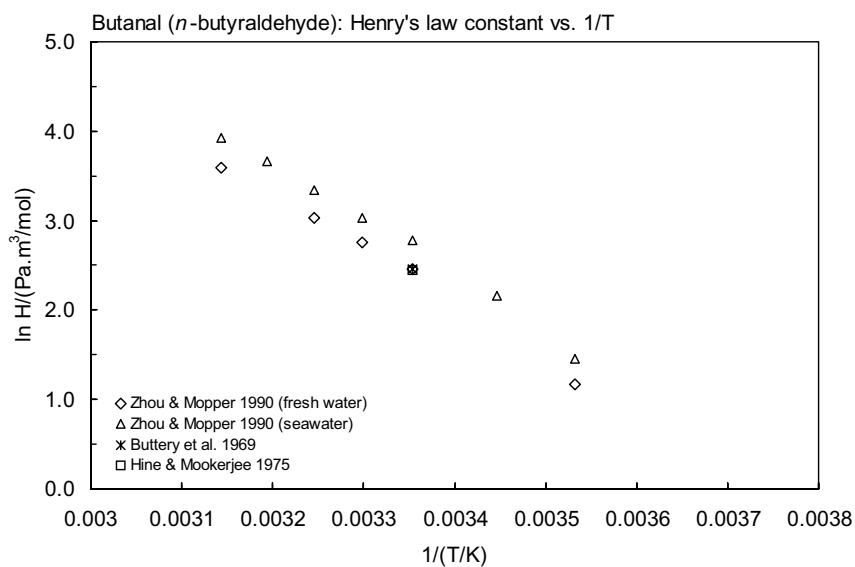
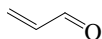


FIGURE 12.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for butanal.

12.1.1.5 2-Propenal (Acrolein)



Common Name: Acrolein

Synonym: 2-propenal, acraldehyde, acrylic aldehyde, allylaldehyde, acrylaldehyde, aqualin

Chemical Name: 2-propenal

CAS Registry No: 107-02-8

Molecular Formula: C_3H_4O , $CH_2=CHCHO$

Molecular Weight: 56.063

Melting Point ($^{\circ}C$):

−87.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

52.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8389 (Riddick et al. 1986)

Dissociation Constant:

Molar Volume (cm^3/mol):

66.8 ($20^{\circ}C$, calculated-density)

66.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

208000 ($20^{\circ}C$, Günther et al. 1968; Callahan et al. 1979; Verschueren 1977, 1983)

102020 (shake flask-radioactive analysis, Veith et al. 1980)

208000 (selected, Riddick et al. 1986)

229000*, 230000 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range $0-53^{\circ}C$, Stephenson 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

26664* ($17.5^{\circ}C$, summary of literature data, temp range -64.5 to $52.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 7628.8/(T/K)] + 8.033866$; temp range: -64.5 to $52.5^{\circ}C$, (Antoine eq., Weast 1972–73)

29330, 44000 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1977, 1983)

35300 (Riddick et al. 1986, Howard 1989)

36610, 35360 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.19181 - 1204.95/(-37.8 + T/K)$; temp range 208–326 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.2878 - 1231.003/(-38.405 + T/K)$; temp range 250–306 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 57.9815 - 3.0933 \times 10^3/(T/K) - 19.638 \cdot \log(T/K) + 1.1486 \times 10^{-2} \cdot (T/K) - 2.3854 \times 10^{-14} \cdot (T/K)^2$; temp range 185–506 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.84, 13.77 (0 , $25^{\circ}C$, headspace-GC, Snider & Dawson 1985)

12.36 (review, Gaffney et al. 1987)

0.446 (Howard 1989)

5.48 ($20^{\circ}C$, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 4.823 - 2110/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

−0.09 (quoted, Callahan et al. 1979)

0.90 (measured value, Veith et al. 1980)

- −0.10 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Sangster 1993)
 −0.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 2.54 (bluegill sunfish, Barrows et al. 1980)
 2.54 (bluegill sunfish, Veith et al. 1980)
 −0.22 (estimated- K_{OW} , Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.38 (estimated- K_{OW} , Howard et al. 1989)
 −0.219 (calculated- K_{OW} , Kolliig 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 10$ d from a model river (Howard 1989);

Photolysis: $t_{1/2} = 3.5$ d, based on measured quantum yields (Howard 1989).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = 6.4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson & Carter 1984)

$k_{OH} = (1.90 - 2.53) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in air (Atkinson 1985)

$k_{OH} = 20.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 23.5°C using propylene as reference compound, with a atmospheric lifetime of 0.56 d (Edney et al. 1986)

$k_{NO_3} = 5.9 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime of 16 d, $k_{OH} = 2.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 1.2 d; and $k_{O_3} = 2.8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 59 d at room temp. (Atkinson et al. 1987)

$k_{OH}(\text{calc}) = 2.29 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = 1.99 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

atmospheric $t_{1/2} = 3.4\text{--}33.7$ h, based on rate constant for reaction with OH radical (Howard et al. 1991)

$k_{OH} = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 1.15 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ((Sabljić & Güsten 1990; Müller & Klein 1991)

$k_{OH}(\text{calc}) = 17.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable groups (Callahan et al. 1979).

Biodegradation: $t_{1/2} = 29$ h (natural unsterilized water) and $t_{1/2} = 43$ h in sterilized (thymol-treated) water (Bowmer & Higgins 1976, quoted, Howard 1989);

aqueous aerobic $t_{1/2} = 168\text{--}672$ h, based on acclimated aqueous screening test data; and aqueous anaerobic $t_{1/2} = 672\text{--}2880$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $t_{1/2} < 4$ d (Callahan et al. 1979)

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: atmospheric lifetime of 0.56 d due to reaction with OH radical (Edney et al. 1986);

calculated atmospheric lifetimes: 16 d for reaction with NO_3 radical, 1.2 d with OH radical and 59 d with O_3 (Atkinson et al. 1987);

$t_{1/2} = 10\text{--}13$ h for reaction with photochemically generated hydroxyl radical, $t_{1/2} = 18$ d for reaction with ozone and $t_{1/2} = 3.5$ d for photodissociation in the atmosphere (Howard 1989);

$t_{1/2} = 3.4\text{--}33.7$ h, based on photooxidation half-life in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: removal $t_{1/2} = 2.0$ to 2.5 d from water (Howard 1989);

First order $k = 0.163 \text{ h}^{-1}$ in 8 agricultural canals and varies between 0.104 and 0.211 h^{-1} at pH 7.1 to 7.5 and water temperature of 16–24°C, the mean value corresponds to $t_{1/2} = 4.25$ h at 21°C (Bowmer & Sainty 1977)

$t_{1/2} \sim 8$ and 23 d for reacting with singlet oxygen and alkylperoxy radicals in natural sunlit water (estimated, Howard 1989),

aqueous aerobic $t_{1/2}$ = 168–672 h, based on acclimated aqueous screening test data; and aqueous anaerobic $t_{1/2}$ = 672–2880 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)
k = 0.015 h⁻¹ at 21°C and pH 7.0, corresponding to $t_{1/2}$ = 46 h in dilute buffered solutions of acrolein in distilled water. (Nordone et al. 1996)
Dissipation k = 0.068 h⁻¹ with $t_{1/2}$ = 10.2 h and k = 0.028 h⁻¹ with $t_{1/2}$ = 7.3 h in weedy (Pump Canal, 12–20°C) and non-weedy agricultural canals (Lateral 1, 12–18°C), respectively, dissipation is the result of numerous processes including degradation, volatilization, adsorption and dilution (Nordone et al. 1996)
Ground water: $t_{1/2}$ = 336–1344 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $t_{1/2}$ = 168–672 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biota:

TABLE 12.1.1.5.1
Reported aqueous solubilities and vapor pressures of 2-propenal(acrolein) at various temperatures

Aqueous solubility		Vapor pressure	
Stephenson 1993		Stull 1947	
shake flask-GC/TC		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	P/Pa
0	197000	−64.5	133.3
10.0	209000	−46.0	666.6
20.0	229000	−36.7	1333
30.0	230000	−26.3	2666
40.0	242000	−15.0	5333
53.0	245000	−7.5	7999
		2.5	13332
		17.5	26664
		34.5	53329
		52.5	101325
		mp/°C	−87.7

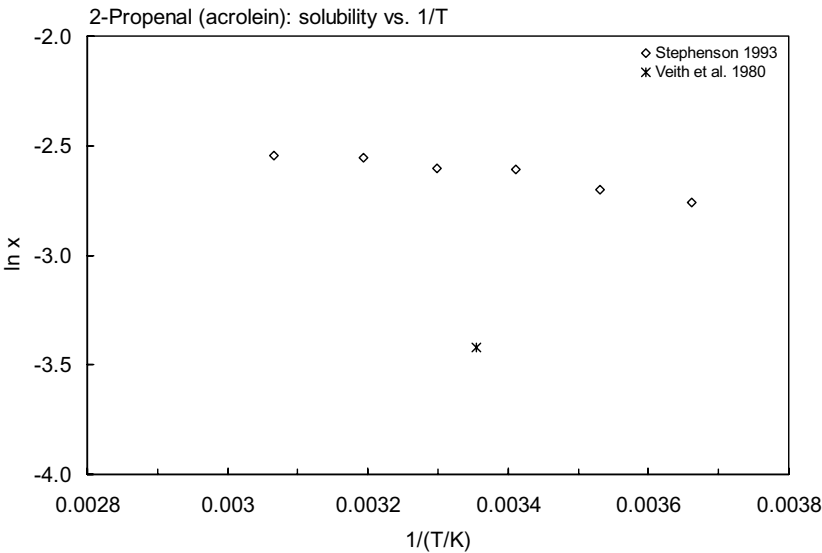


FIGURE 12.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-propenal.

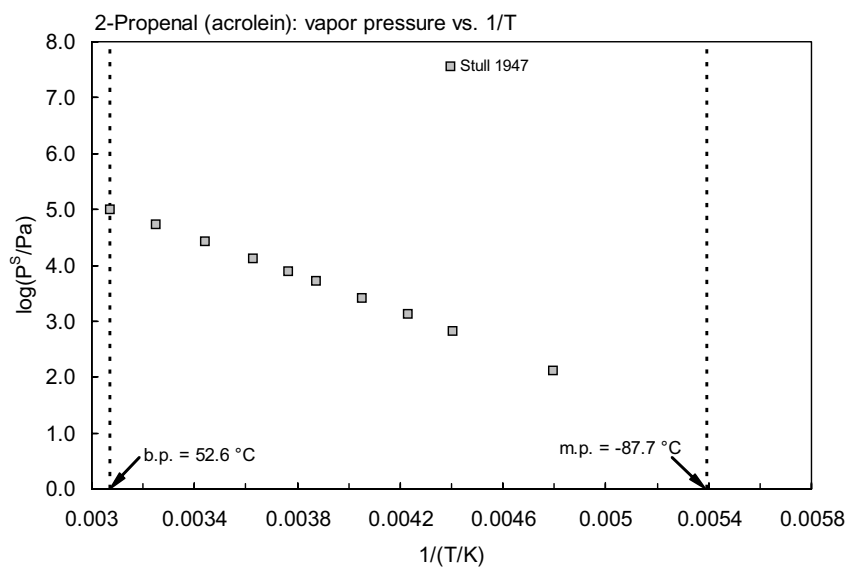
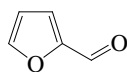


FIGURE 12.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 2-propenal.

12.1.1.6 Furfural (2-Furaldehyde)



Common Name: Furfural

Synonym: 2-furaldehyde, 2-furancarboxaldehyde; furfurole, 2-furancarboxal, fural, furfuraldehyde, furole

Chemical Name: furfural

CAS Registry No: 98-01-1

Molecular Formula: $C_5H_4O_2$

Molecular Weight: 96.085

Melting Point ($^{\circ}C$):

−38.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

161.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.16 (Verschuereen 1983)

Dissociation Constant:

Molar Volume (cm^3/mol):

82.9 (calculated-density, Stephenson & Malanowski 1987)

92.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

82000 ($40^{\circ}C$, synthetic method, Jones 1929)

91593 (shake flask-volumetric method, Booth & Everson 1948)

92900 ($26.7^{\circ}C$, shake flask-turbidity, Skrzec & Murphy 1954)

77830 (generator column-HPLC/UV, Tewari et al. 1982)

79400*, 84000 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $90^{\circ}C$, Stephenson 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1066.6* ($39.9^{\circ}C$, ebulliometry, measured range 40 – $170.6^{\circ}C$, Evans & Aylesworth 1926)

220.4* (interpolated-regression of tabulated data, temp range 18.5 – $161.8^{\circ}C$, Stull 1947)

1767* ($55.67^{\circ}C$, Ramsay-Young method, measured range 55.6 – $170^{\circ}C$, Matthews et al. 1950)

$\log(P/mmHg) = A - B/(T/K) - C \log(T/K)$; temp range 55.6 – $170^{\circ}C$ (Kirchhoff eq., Matthews et al. 1950)

$\log(P/mmHg) = [-0.2185 \times 11614.6/(T/K)] + 8.729884$; temp range 18.5 – $161.8^{\circ}C$ (Antoine eq., Weast 1972–73)

133.3, 400 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

$\log(P/kPa) = 5.62941 - 1124.583/(148.829 + t/^{\circ}C)$, temp range 92.3 – $170.6^{\circ}C$ (Antoine eq. derived from Evans & Aylesworth 1926 data, Boublik et al. 1984)

$\log(P/kPa) = 5.76606 - 1236.745/(167.368 + t/^{\circ}C)$, temp range 55.87 – $160.8^{\circ}C$ (Antoine eq. derived from Matthews et al. 1950 data, Boublik et al. 1984)

208.0 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.91048 - 946.35/(246.68 + t/^{\circ}C)$, temp range -87 to $7^{\circ}C$ (Antoine eq., Dean 1985, 1992)

333.3 (Riddick et al. 1986)

313.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_1/kPa) = 6.41784 - 1663.16/(-57.88 + T/K)$, temp range 357 – $435 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 32.0337 - 3.3161 \times 10^3/(T/K) + 10.171 \cdot \log(T/K) - 2.1115 \times 10^{-2} \cdot (T/K) + 9.2045 \times 10^{-6} \cdot (T/K)^2$; temp range 237 – $657 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.375 (calculated-P/C, Howard 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.34	(20°C, shake flask, Korenman 1972)
0.52	(generator column-HPLC/UV, Tewari et al. 1982)
0.41, 0.52	(shake flask, Log P Database, Hansch & Leo 1987)
0.46	(recommended, Sangster 1993)
0.41	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

0.079	(estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)
-2.097	(estimated-S, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

1.602	(soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)
0.00	(soil, estimated-S, Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: based on calculated Henry's law constant, the estimated $t_{1/2} \sim 9.9$ d from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: average rate of biodegradation 41.0 mg COD $g^{-1} h^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: estimated photooxidation $t_{1/2} \sim 0.44$ d for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard 1993).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.6.1

Reported aqueous solubilities of furfural (2-furaldehyde) at various temperatures

Stephenson 1993

shake flask-GC/TC	
t/°C	S/g·m⁻³
0	82200
10.0	78600
20.0	79400
30.0	84000
40.0	89400
50.0	95000
60.0	102800
70.0	109700
80.0	125600
90.0	147400

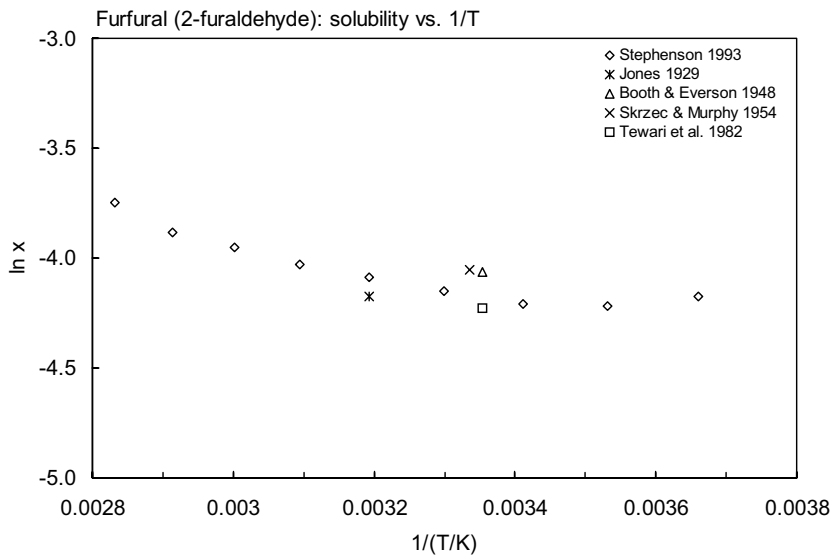


FIGURE 12.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for furfural.

TABLE 12.1.1.6.2
Reported vapor pressures of furfural (2-furaldehyde) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Evans & Aylesworth 1926		Stull 1947		Matthews et al. 1950			
ebulliometry		summary of literature data		Ramsay-Young method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
92.30	9199	18.5	133.3	55.67	1767	continued	
120.3	28531	42.6	666.6	56.07	1793	139.95	56368
131.6	41330	54.8	1333	64.50	2786	143.8	61635
140.2	54795	67.8	2666	67.70	3321	146.85	69034
154.4	83326	82.1	5333	75.05	4600	149.65	71727
159.0	94259	91.5	7999	76.47	5034	151.70	77247
160.9	99192	103.4	13332	84.95	7254	153.95	82473
163.8	108257	121.8	26664	87.38	8239	155.10	85459
170.6	128789	141.8	53329	92.15	9959	160.75	101885
		161.8	101325	93.05	10308	bp/K	433.8
				96.77	12060	$\Delta H_v/(\text{kJ mol}^{-1}) = 38.59$ at bp	
		mp/°C	−35.6	102.13	15079	Kirchhoff, Rakine, Dupre eq.	
				103.31	15705	eq. 4	P/mmHg
				103.09	17012	A	29.3205
				107.27	18292	B	3530.52
				111.65	21651	C	6.9418
				116.25	24731		
				118.40	27184		
				120.85	29744		
				124.75	34144		

(Continued)

TABLE 12.1.1.6.2 (Continued)

Evans & Aylesworth 1926		Stull 1947		Matthews et al. 1950			
ebulliometry		summary of literature data		Ramsay-Young method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				126.05	35064		
				126.35	35130		
				132.15	43583		
				133.80	45303		
				135.95	48942		
				138.35	53262		

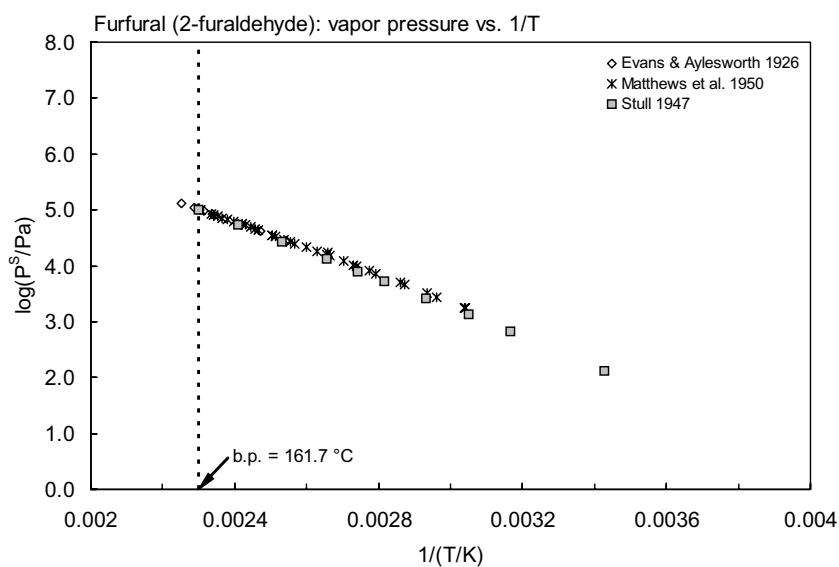
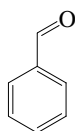


FIGURE 12.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for furfural.

12.1.1.7 Benzaldehyde



Common Name: Benzaldehyde

Synonym: benzenecarbonal, oil of bitter almonds

Chemical Name: benzaldehyde

CAS Registry No: 100-52-7

Molecular Formula: C_7H_6O , C_6H_5CHO

Molecular Weight: 106.122

Melting Point ($^{\circ}C$):

-57.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

178.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0401 (24.94 $^{\circ}C$, measured, Ambrose et al. 1975)

1.0447 (Dean 1985)

1.0446 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

102.0 (calculated-density, Chiou 1985)

118.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

9.322 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} J/mol K:

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2991 (quoted, Deno & Berkheimer 1960)

2857 (1 in 350 parts, Merck Index 1960)

3490, 3500 (quoted Ph. D. theses from University of London, Mitchell et al. 1964)

6550, 6580 (shake flask-gravimetric method, shake flask-GC/FID, Mitchell et al. 1964)

6900–7000 (shake flask-refractive index method, Carless & Swarbrick 1964)

7200 ($20^{\circ}C$, shake flask-GC, Tewari et al. 1982)

3000 (20 – $25^{\circ}C$, shake flask-GC, Urano et al. 1982)

3300 (Verschuereen 1983)

3279 (shake flask-GC, Chiou 1985)

3000 ($20^{\circ}C$, Riddick et al. 1986)

7200*, 7400 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $90^{\circ}C$, Stephenson 1993)

3514 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3*, 145.2 ($26.2^{\circ}C$, extrapolated-regression of tabulated data, temp range 26.2 – $179^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11657.8/(T/K)] + 8.580362$; temp range 26.2 – $179^{\circ}C$ (Antoine eq., Weast 1972–73)

137.0* (ebulliometry-extrapolated from Antoine eq., measured range 38.5 – $89.3^{\circ}C$, Ambrose et al. 1975b)

$\log(P/kPa) = 6.20251 - 1611.217/(T/K - 67.984)$; temp range 38.5 – $89.3^{\circ}C$, mercury as reference, Ambrose et al. 1975b)

$\log(P/kPa) = 6.22556 - 1628.007/(T/K - 66.119)$; temp range 74.9 – $190.8^{\circ}C$, water as reference, Ambrose et al. 1975b)

169.0 (calculated from different vapor eq., Ambrose et al. 1975)

160.5 (extrapolated-Antoine eq., Ambrose et al. 1979)

133.3 ($26.0^{\circ}C$, Verschuereen 1983)

160.5 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.21282 - 1618.669/(205.994 + t/^{\circ}\text{C})$; temp range 38.5–208°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

169.0 (Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 5.56823 - 1197.54/(-115.829 + T/\text{K})$; temp range 348–452 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.4764 - 2455.4/(T/\text{K})$; temp range 273–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.20256 - 1611.255/(-67.979 + T/\text{K})$; temp range 409–481 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.48764 - 1782.204/(-52.863 + T/\text{K})$; temp range 311–376 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.22745 - 1629.229/(-65.993 + T/\text{K})$; temp range 370–475 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 28.4711 - 3.4489 \times 10^3/(T/\text{K}) - 6.8363 \cdot \log (T/\text{K}) - 2.8173 \times 10^{-10} \cdot (T/\text{K}) + 9.5236 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 247–695 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.781, 1.494 (quoted exptl., calculated-bond contribution, Hine & Mookerjee 1975)

2.815 (Gaffney et al. 1987)

2.71* (gas stripping-GC, measured range 15–45°C, Betterton & Hoffmann 1988)

2.282* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)

$\ln [K_H'/(M/\text{atm})] = -5.00 + 1977/(T/\text{K})$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

$\ln [K_H'/(M/\text{atm})] = -5.90 + 2207/(T/\text{K})$, temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 11), Zhou & Mopper 1990)

3.08* (EPICS-UV spectroscopy, measured range 5–25°C, Allen et al. 1998)

$\ln K_{AW} = -6759/(T/\text{K}) + 15.93$ (EPICS-UV, temp range 5–25°C, Allen et al. 1998)

1.94 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.665 - 2276/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.48 (Leo et al. 1971; Hansch et al. 1972)

1.45 (shake flask-UV at pH 5.62, Umeyama et al. 1971)

1.43 (shake flask-UV, Holmes & Lough 1976)

1.45 ± 0.03 (shake flask at pH 7, Unger et al. 1978)

2.33 (HPLC-RT correlation, Veith et al. 1979)

1.56 (HPLC- k' correlation, Eadsforth 1986)

1.49 (shake flask, Eadsforth 1986)

1.44 (HPLC-RT correlation average, Ge et al. 1987)

1.54 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)

1.48 (recommended, Sangster 1989, 1993)

1.72 (shake flask-UV, Kramer & Henze 1990)

1.48 (shake flask-UV spec., Alcron et al. 1993)

1.48 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: loss rate $k = 3.4 \times 10^{-4} \text{ min}^{-1}$ in outdoor Teflon chambers in dark (Grosjean 1985).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:

$k < 2.0 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen in the aquatic systems at 25°C with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{OH}} = 1.3 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ determined by the long-path Fourier transform IR spectroscopic method with reference to that for C_2H_4 or C_2D_4 (Niki et al. 1978)

$k_{\text{OH}} = 7.6 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 0.74 \text{ d}$ (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{\text{OH}} = 7.8 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k = (2.5 \pm 0.5) \text{ M}^{-1} \text{ s}^{-1}$ for 2–10 mM to react with ozone in water at pH 1.7 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{\text{NO}_3} = < 9.6 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ (using relative rate technique to propene Carter et al. 1981; quoted, Atkinson 1991)

$k_{\text{NO}_3} = (2.55 \pm 0.08) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{NO}_3} = (1.13 \pm 0.25) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, compared to a previous measured value $k_{\text{NO}_3} < 5.2 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate technique, Atkinson et al. 1984)

$k_{\text{OH}} = .2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = 2.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (reevaluated value, Atkinson et al. 1987)

$k_{\text{OH}}(\text{exptl}) = 1.30 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 1.698 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (SAR, Atkinson 1987, 1990; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{\text{NO}_3} = 2.54 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 1.29 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 11.40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation $119.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976),

biodegradation rate constant $k = 0.065\text{--}0.074 \text{ h}^{-1}$ in 30 mg/L activated sludge after a lag time of 5–10 h (Urano & Kato 1986b).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9 \text{ d}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 0.74 \text{ d}$ based on rate constants for oxidation by OH radical in the atmosphere at 25°C (Mill 1982);

loss rate $k = (3.4 \pm 1.7) \times 10^{-4} \text{ min}^{-1}$ in outdoor Teflon chambers in the dark (Grosjean 1985);

calculated lifetimes of 11 h and 18 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.7.1
Reported aqueous solubilities of benzaldehyde at various temperatures

Stephenson 1993

shake flask-GC/TC

$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	8400
20.0	7200
30.0	7400
40.0	7900
50.0	8200
60.0	9300
70.0	10200
80.0	12400
90.0	14000

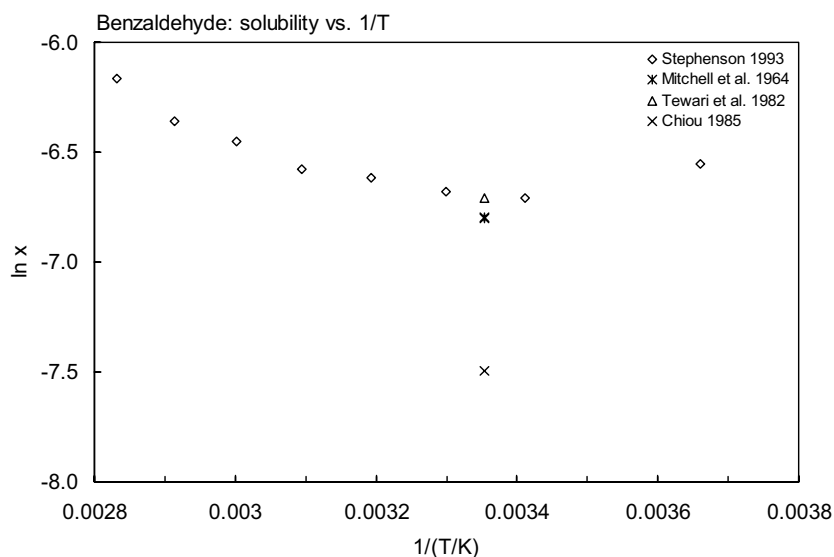


FIGURE 12.1.1.7.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for benzaldehyde.

TABLE 12.1.1.7.2

Reported vapor pressures of benzaldehyde at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		Ambrose et al. 1975b					
summary of literature data		comparative ebulliometry					
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
		mercury as reference		water as reference			
26.2	133.3	38.489	399	74.961	2837	25.0	169
50.1	666.6	41.273	473	77.570	3203	31.69	2000
62.0	1333	43.525	539	80.848	3723	76.85	3098
75.0	2666	45.584	608	85.231	4524	178.75	101325
90.1	5333	47.296	672	89.154	5352	213.35	225300
99.6	7999	48.838	722	93.610	6460	254.65	500000
112.5	13332	50.707	814	97.721	7644	421.65	4650000
131.7	26664	51.955	873	102.170	9124		
154.1	53329	56.352	1235	106.662	10854	bp/ $^{\circ}\text{C}$	178.75
179.0	101325	63.266	1592	111.251	12894		
		68.412	2057	115.947	15306	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
mp/ $^{\circ}\text{C}$	-26	75.098	2808	120.430	17945	at 25 $^{\circ}\text{C}$	50.3
		77.665	3150	126.350	21995	at bp	42.6
		80.998	3724	131.273	25910		
		83.392	4528	137.178	31339	density	
		89.251	5353	142.836	37379	T/K	$\rho/\text{kg m}^{-3}$
				148.806	44737	292.94	1044.85
				155.366	54140	298.09	1040.13
		Antoine eq.		161.067	63540	298.03	1040.22
		eq. 3	P/kPa	167.121	74923		

TABLE 12.1.1.7.2 (Continued)

Stull 1947		Ambrose et al. 1975					
summary of literature data		comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		A	6.20251	173.661	88998		
		B	1611.217	178.672	101131		
		C	-67.984	179.710	103800		
				185.556	119891		
				190.829	136055		
				Antoine eq.			
				eq. 3		P/kPa	
				A		6.22556	
				B		1628.007	
				C		-66.119	

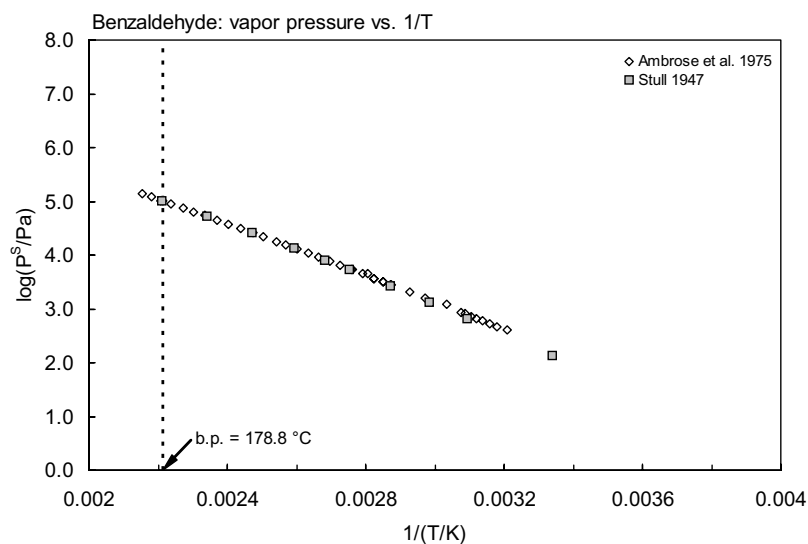


FIGURE 12.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for benzaldehyde.

TABLE 12.1.1.7.3

Reported Henry's law constants of benzaldehyde at various temperatures and temperature dependence equations

$$\begin{aligned} \ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) & (4) & \ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K) & (4a) \\ K_{AW} &= A - B\cdot(T/K) + C\cdot(T/K)^2 & (5) & & \end{aligned}$$

Zhou & Mopper 1990		Zhou & Mopper 1990		Betterton & Hoffmann 1988		Allen et al. 1998	
gas stripping-HPLC/UV		gas stripping-HPLC/UV		gas stripping-GC, spec.		EPICS-UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
	fresh water		sea water				
10	1.095	10	1.339	15	1.506	5	0.555
17	-	17	1.987	25	2.709	10	0.824
25	2.282	25	3.025	35	4.648	15	1.197
30	3.016	30	4.187	45	7.916	20	1.803
35	3.943	35	5.790			25	3.10
40	-	40	7.342				
45	6.413	45	9.296		$\Delta H/(\text{kJ mol}^{-1}) = -42.2$ at 25°C	eq. 1	K_{AW}
eq. 1a	$K_H'/(M/\text{atm})$	eq. 1a	$K_H'/(M/\text{atm})$			A	-6759
A	-5.00	A	-5.90			B	15.93
B	-1977	B	-2207				$\Delta H/(\text{kJ mol}^{-1}) = -56.2$ $\Delta S/(\text{J K}^{-1} \text{mol}^{-1}) = 132.4$

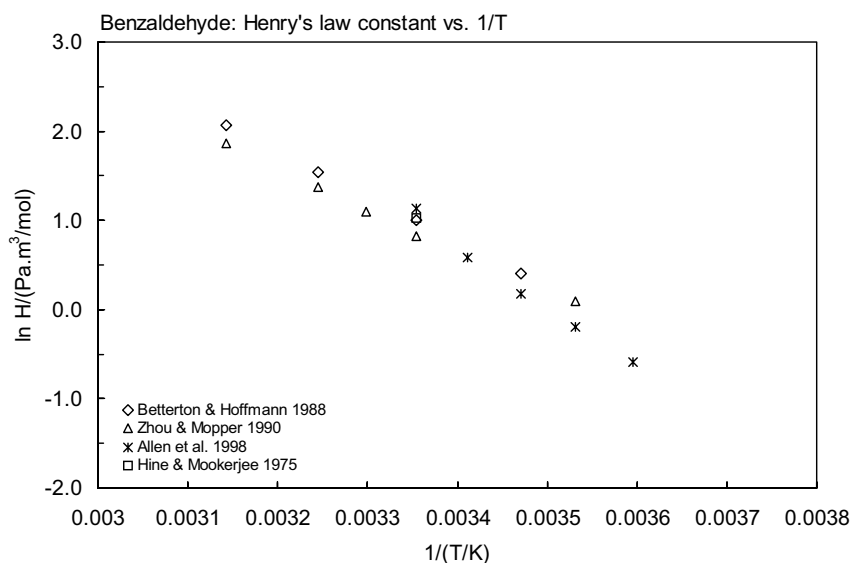


FIGURE 12.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for benzaldehyde.

12.1.2 KETONES

12.1.2.1 Acetone



Common Name: Acetone

Synonym: 2-propanone, dimethylketone, DMK

Chemical Name: acetone, 2-propanone

CAS Registry No: 67-64-1

Molecular Formula: C_3H_6O , CH_3COCH_3

Molecular Weight: 58.079

Melting Point ($^{\circ}C$):

−94.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

56.05 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7899 (Weast 1982–83)

0.7908 (Dean 1985)

Molar Volume (cm^3/mol):

73.5 ($20^{\circ}C$, calculated-density)

74.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

5.690 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

miscible ($20^{\circ}C$, Palit 1947)

miscible (Dean 1985; Yaws et al. 1990)

miscible (Riddick et al. 1986; Howard 1990)

217700, 453000 (pseudo-solubilities, Staples 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

29610* (interpolated-regression of tabulated data, temp range -59.4 to $56.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.19038 - 1233.4/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

30490 (Perry 1950)

51854* ($37.68^{\circ}C$, temp range 37.68 – $56.02^{\circ}C$, Brown & Smith 1957)

30800 (Buttery et al. 1969)

30810 (Hoy 1970)

29923* ($24.330^{\circ}C$, temp range -12.949 to $55.285^{\circ}C$, Boublik & Aim 1972; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 10577.7/(T/K)] + 9.143231$; temp range -20 to $96^{\circ}C$ (Antoine eq., Weast 1972–73)

30780, 30800 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/mmHg) = 7.15853 - 1231.232/(231.766 + t/^{\circ}C)$; temp range 37.6 – $56.02^{\circ}C$ (Antoine eq. from reported exptl. data of Brown & Smith 1957, Boublik et al. 1973)

$\log(P/mmHg) = 7.11714 - 1210.595/(229.664 + t/^{\circ}C)$; temp range -12.95 to $55.3^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

30810* (ebulliometry, fitted to Antoine eq., measured range 259 – $350.9 K$, Ambrose et al. 1974)

$\log(P/kPa) = 6.25632 - 1217.904/(T/K - 42.692)$; temp range 311.7 – $350.9 K$, or for pressure range 53 – $202 kPa$ (Antoine eq., ebulliometry, Ambrose et al. 1975a)

$\log(P/kPa) = 6.25478 - 1216.689/(T/K - 42.875)$; temp range 259.17 – $350.9 K$, or for pressure below $225 kPa$ (Antoine eq., ebulliometry, Ambrose et al. 1974)

30870, 31520 (quoted exptl., calculated-Antoine eq., Boublik et al. 1984)

- $\log (P/\text{kPa}) = 6.24039 - 1209.746/(229.574 + t/^{\circ}\text{C})$; temp range -12.95 to 55.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.26017 - 1214.208/(230.002 + t/^{\circ}\text{C})$; temp range -13.98 to 77.72°C (Antoine eq. from reported exptl. data of Ambrose et al. 1974, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.28185 - 1230.342/(231.665 + t/^{\circ}\text{C})$; temp range 37.6 – 56.02°C (Antoine eq. from reported exptl. data of Brown & Smith 1957, Boublik et al. 1984)
 30780 (calculated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.11714 - 1210.595/(229.664 + t/^{\circ}\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
 24227, 30806 (20, 25°C , Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.25478 - 1216.589/(230.275 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 30730 (interpolated-Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.24204 - 1210.6/(-43.49 + T/\text{K})$; temp range 261–329 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.75622 - 1566.69/(0.269 + T/\text{K})$; temp range 329–488 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 3.6452 - 469.5/(-108.21 + T/\text{K})$; temp range 178–243 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19735 - 1190.382/(-45.373 + T/\text{K})$; temp range 203–269 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.26483 - 1221.852/(-42.388 + T/\text{K})$; temp range 257–334 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.24554 - 1211.515/(-43.471 + T/\text{K})$; temp range 323–379 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.69966 - 1542.465/(0.447 + T/\text{K})$; temp range 374–464 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 28.5884 - 2.469 \times 10^3/(T/\text{K}) - 7.351 \cdot \log (T/\text{K}) + 2.8025 \times 10^{-10} \cdot (T/\text{K}) + 2.7361 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 178–508 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 3.34 (partial pressure, Butler & Ramchandani 1935)
 3.96 (shake flask, partial vapor pressure-GC, Burnett 1963)
 3.25 (28°C , concn. ratio-GC, Nelson & Hoff 1968)
 3.97 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
 4.02, 3.93, 2.91 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 4.05 (headspace-GC, Vitenberg et al. 1975)
 4.10 (calculated-activity coeff and vapor pressure, γ -P, Rathbun & Tai 1982)
 0.908, 3.93 (0, 25°C , headspace-GC, Snider & Dawson 1985)
 3.38 (review, Gaffney et al. 1987)
 2.928* (gas-stripping-HPLC-UV, measured range 10 – 45°C , Zhou & Mopper 1990)
 $\ln [K_H'/(M/\text{atm})] = -5.00 + 1977/(T/\text{K})$; temp range 10 – 45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
 $\ln [K_H'/(M/\text{atm})] = -3.60 + 1518/(T/\text{K})$; temp range 25 – 45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 11), Zhou & Mopper 1990)
 3.07* (gas stripping-GC, measured range -14.9 to 44.9°C , Betterton 1991)
 4.33 (computed, Yaws et al. 1991)
 0.722, 1.26, 2.045, 5.31, 7.514 (0.51, 9.0, 16.11, 31, 38.51°C , headspace-GC, de-ionized water, Benkelberg et al. 1995)
 3.735* (headspace-GC, rain water, measured range -30 to 39.51°C , Benkelberg et al. 1995)
 0.762, 2.19, 6.64, 10.30 (0, 14.51, 30, 39.51°C , headspace-GC, artificial seawater, Benkelberg et al. 1995)
 $\ln (k_H/\text{atm}) = (18.4 \pm 0.3) - (5386 \pm 100)/(T/\text{K})$, temp range 10 – 40°C (headspace-GC measurements, Benkelberg et al. 1995)
 2.56 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)
 9.92 (EPICS-GC, Ayuttaya et al. 2001)
 2.58 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 3.742 - 1965/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} :

-0.24	(shake flask-CR, Collander 1951)
-0.24	(shake flask at pH 7, Unger et al. 1978)
-0.48	(shake flask-GC, Tani et al. 1986)
-0.24	(recommended, Sangster 1989, 1993)
-0.31	(CPC centrifugal partition chromatography, Gluck & Martin 1990)
-0.37	(calculated-UNIFAC activity coeff., Dallos et al. 1993)
-0.24	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

2.31	(head-space GC, Abraham et al. 2001)
------	--------------------------------------

Bioconcentration Factor, log BCF:

-0.187	(calculated, Staples 2000)
--------	----------------------------

Sorption Partition Coefficient, log K_{OC} :

-0.586	(calculated- K_{OW} , Kollig 1993)
-0.523	(quoted calculated value, Staples 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 20$ h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: rate constant $k = 1.4 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986); calculated lifetime $\tau \sim 60$ d in air (Atkinson 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:

photooxidation $t_{1/2} = 11.3\text{--}453$ yr, based on measured data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH} = (0.23 \pm 0.03) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (flash photolysis-resonance fluorescence, Zetzsch 1982; quoted, Atkinson 1985)

$k_{OH} = (0.62 \pm 0.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate technique to *n*-hexane, Chiorboli et al. 1983; quoted, Atkinson 1985)

$k = 0.032 \pm 0.006 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 279\text{--}2790$ h, based on measured data for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991)

$k_{OH} = 2.16 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K and $k = 1.80 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the aqueous-phase reaction with hydroxyl radical in solution (Wallington & Kurylo 1987)

$k_{OH} = 2.16 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH}^* = 2.26 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}(\text{calc}) = 0.18 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: biodegradation rate constants, $k = 0.016\text{--}0.020 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 20–25 h (Urano & Kato 1986b);

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168$ h, based on unacclimated aqueous screening test data (Bridie et al. 1979; Dore et al. 1975; selected, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 96\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$k(\text{exptl}) = 0.0440 \text{ h}^{-1}$ compared to predicted rate constants by group contribution method: $k = 0.0433 \text{ h}^{-1}$ (nonlinear) and $k = 0.043 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9 \text{ d}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 279\text{--}2790 \text{ h}$, based on measured data for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

calculated lifetimes $\tau = 53 \text{ d}$ and $\tau > 11 \text{ yr}$ for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000);

photooxidation and photolysis $t_{1/2} = 36 \text{ h}$ (Staples 2000).

Surface water: photooxidation $t_{1/2} = 11.3\text{--}453 \text{ yr}$, based on measured data for the reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991);

$t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

aerobic biodegradation $t_{1/2} = 96\text{--}168 \text{ h}$ (Staples 2000).

Ground water: $t_{1/2} = 48\text{--}336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: anaerobic biodegradation $t_{1/2} = 384 \text{ h}$ or 16 d (Staples 2000).

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

aerobic biodegradation $t_{1/2} = 96\text{--}168 \text{ h}$ (Staples 2000).

Biota:

TABLE 12.1.2.1.1

Reported vapor pressures of acetone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Stull 1947		Brown & Smith 1957		Boublik & Aim 1972			
summary of literature data		Austr. J. Chem. 10, 423-		ref. in Boublik et al. 1984*			
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
-59.4	133.3	37.68	51854	-12.949	4524	36.649	49704
-40.5	666.6	41.58	60127	-5.424	6967	42.094	61295
-31.1	1333	44.96	68271	-0.103	9306	48.344	77125
-20.8	2666	45.0	68367	4.882	12046	55.285	98572
-9.40	5333	47.01	73603	8.666	14549	bp/ $^\circ\text{C}$	56.102
-2.0	7999	49.31	79969	13.019	17921	Antoine eq. eq. 2	
7.7	13332	51.91	87727	16.831	21314		P/kPa
22.7	26664	56.02	101199	20.939	25780		6.24039
39.5	53329			24.330	29923		1209.746
56.5	101325			28.351	35493		229.574
				32.138	41470	C	
mp/ $^\circ\text{C}$	-94.6						

*ref. Collection Czech. Chem. Commun 37, 3513 (1972)

TABLE 12.1.2.1.1 (Continued)

2.

Ambrose et al. 1974

comparative ebulliometry

t/°C	P/Pa	t/°C	P/Pa
		cont'd	
-13.975	4257	55.876	100666
-11.019	5076	56.646	103344
-8.106	6005	60.963	119433
-4.982	7186	64.859	135602
-1.388	8691	69.512	157101
0.288	9497	73.943	180024
1.972	10376	77.724	201571
2.007	10391	25.0	30806
5.493	12417		
5.511	12432	eq. 3	P/kPa
9.077	14840	A	6.25478
9.093	14851	B	1216.689
12.473	17480	C	-42.875
16.928	21525		
20.717	25544		
25.045	30867	Ambrose et al 1975a	
29.275	36912		
33.720	44267	bp/°C	56.067
28.601	53675		
42.834	63079	eq. 3	P/kPa
47.320	74449	A	6.25632
52.170	88536	B	1217.904
		C	-42.692
		equation for vapor pressures below 200 kPa	
		$\Delta H_v / (\text{kJ mol}^{-1}) =$	
		at 25°C	31.3
		at bp	29.6

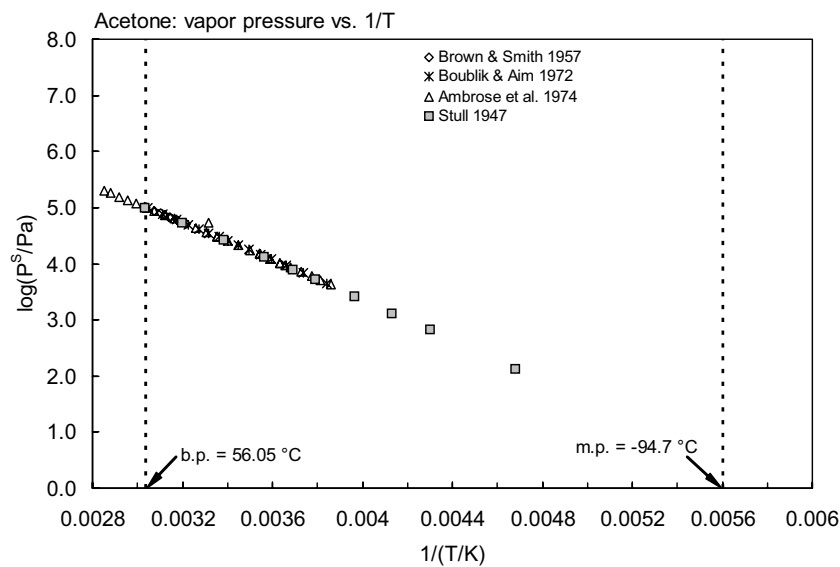


FIGURE 12.1.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for acetone.

TABLE 12.1.2.1.2
Reported Henry's law constants of acetone at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$
$$\ln (1/K_{AW}) = A - B/(T/K)$$
$$\ln (k_H/\text{atm}) = A - B/(T/K)$$
$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$
$$\log (1/K_{AW}) = A - B/(T/K)$$
$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

$$(1)$$
$$(2)$$
$$(3)$$
$$(4)$$
$$(5)$$

$$(1a)$$
$$(2a)$$
$$(4a)$$

1.

Snider & Dawson 1985		Zhou & Mopper 1990				Betterton 1991	
gas stripping-GC/FID		gas stripping-HPLC/UV		gas stripping-HPLC/UV		gas stripping-GC/FID	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
		fresh water		sea water			
0	0.908	10	1.421	10	1.735	14.9	2.303
25	3.935	17	-	17	2.356	25	3.070
		25	2.846	25	3.311	25	3.269
		30	3.658	30	4.037	25	3.897
enthalpy of transfer		35	4.585	35	4.825	25	3.753
ΔH =	37.24 kJ/mol	40	-	40	5.537	25	3.958
		45	6.178	45	6.846	35.1	7.794
						44.9	11.92
		eq. 1a	K _H '/(M/atm)	eq. 1a	k _H '/(M/atm)		
		A	-5.00	A	-3.60		
		B	-1977	B	-1518		

TABLE 12.1.2.1.2 (Continued)

2.

Benkelberg et al. 1995

equilibrium vapor phase concentration-headspace GC

t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
	deionized water		rain water
0.51	0.7222	−28.0	0.742
9.0	1.260	25.0	3.735
16.61	2.0445	39.51	8.328
31.0	5.313		
38.51	7.514		artificial sea water
		0	0.757
for deionized and rain water:		14.51	2.189
eq. 3	k _H /atm	30.0	6.639
A	18.4 ± 0.3	39.51	10.305
B	5286 ± 100		

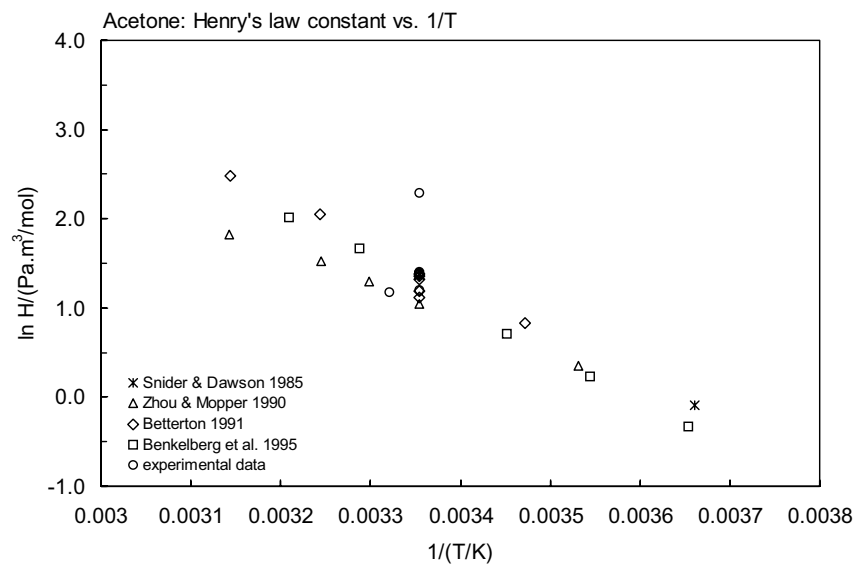


FIGURE 12.1.2.1.2 Logarithm of Henry's law constant versus reciprocal temperature for acetone.

12.1.2.2 2-Butanone (Methyl ethyl ketone)



Common Name: Methyl ethyl ketone

Synonym: 2-butanone, butan-2-one, MEK

Chemical Name: 2-butanone, methyl ethyl ketone

CAS Registry No: 78-93-3

Molecular Formula: C_4H_8O , $CH_3CH_2COCH_3$

Molecular Weight: 72.106

Melting Point ($^{\circ}C$):

−86.64 (Lide 2003)

Boiling Point ($^{\circ}C$):

79.59 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8054 (Weast 1982–83)

0.7997 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

89.9 (calculated-density, Rohrschneider 1973)

96.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

14.7 (pK_a , Riddick et al. 1986)

−7.2 (pK_{BH}^+ , Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

8.439 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

240000 ($20^{\circ}C$, synthetic method, Jones 1929; quoted, Palit 1947; Dean 1985; Riddick et al. 1986)

255700* (shake flask-volumetric method, measured range 20 – $30^{\circ}C$ Ginnings et al. 1940)

343550 (shake flask-volumetric, Ginnings et al. 1940)

228020 (estimated, McGowan 1954)

12420 ($20^{\circ}C$, Amidon et al. 1975)

136280 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

353000 ($20^{\circ}C$, Verschuereen 1983)

249000 (selected, Yaws et al. 1990)

276000*, 235000 ($19.3^{\circ}C$, $29.7^{\circ}C$, shake flask-GC, measured range 0 – $70.2^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

12954* (interpolated-regression of tabulated data, temp range -48.3 to $79.6^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.22200 - 1343.6/(230 + t/^{\circ}C)$, (Antoine eq., Dreisbach & Martin 1949)

16500* ($31.84^{\circ}C$, ebulliometry, measured range 31.84 – $79.5^{\circ}C$, Dreisbach & Shrader 1949)

25158* ($41.46^{\circ}C$, flow calorimetry, measured range 41.46 – $79.5^{\circ}C$, Nickerson et al. 1961)

26568* ($42.778^{\circ}C$, ebulliometry, measured range 42.778 – $88.444^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.06376 - 1261.455/(221.982 + t/^{\circ}C)$; temp range 42.778 – $88.444^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 19.48322 - 2328.0/(T/K) - 3.92657 \cdot \log(T/K)$; temp range 42.778 – $88.444^{\circ}C$ (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = [-0.2185 \times 8149.5/(T/K)] + 7.959295$; temp range -48.3 to $79.6^{\circ}C$ (Antoine eq., Weast 1972–73)

- 12079* (ebulliometry, Ambrose et al. 1975a; quoted, Riddick et al. 1986; Howard 1990)
 12000, 12060, 12640 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.02273 - 1167.861/(211.199 + t/^{\circ}\text{C})$; temp range 41.46–97.42°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.18397 - 1258.948/(221.725 + t/^{\circ}\text{C})$; temp range 42.78–86.44°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.18838 - 1261.297/(222.964 + t/^{\circ}\text{C})$; temp range 42.79–88.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 12020 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.06356 - 1261.34/(221.97 + t/^{\circ}\text{C})$; temp range 43–88°C (Antoine eq., Dean 1985, 1992)
 12700 (Howard et al. 1986; quoted, Banerjee et al. 1990)
 12120 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.24715 - 1294.53/(-47.442 + T/\text{K})$; temp range 294–352 K (Antoine eq.-I., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.18479 - 1259.519/(-51.359 + T/\text{K})$; temp range 315–363 K (Antoine eq.-II., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.22518 - 1286.794/(-47.766 + T/\text{K})$; temp range 353–403 K (Antoine eq.-III., Stephenson & Malanowski 1987)
 5425 (calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 47.706 - 3.0965 \times 10^3/(T/\text{K}) - 15.184 \cdot \log(T/\text{K}) + 7.4846 \times 10^{-3} \cdot (T/\text{K}) - 1.7084 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 186–536 K (vapor pressure eq., Yaws 1994)
 12071* (static method-manometry, measured range 0–50°C, Garriga et al. 1996)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 4.710 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
 4.723 (quoted, exptl., Hine & Mookerjee 1975)
 5.549, 4.408 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 3.87 (headspace-GC, Vitenberg et al. 1975)
 6.191, 4.215 (calculated- γ -P, calculated-MW, Rathbun & Tai 1982)
 0.987, 5.76 (0, 25°C, gas stripping-GC, Snider & Dawson 1985)
 13.17* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = -26.32 - 5214/(T/\text{K})$, temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)
 5.210 (gas stripping-HPLC/UV, Zhou & Mopper 1990)
 5.117* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)
 $\ln[K_H'/(M/\text{atm})] = -6.03 + 2184/(T/\text{K})$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
 $\ln[K_H'/(M/\text{atm})] = -5.97 + 2138/(T/\text{K})$, temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1 l), Zhou & Mopper 1990)
 18.28* (45°C, equilibrium headspace-GC, measured range 45–80°C, Ettre et al. 1993)
 $\log(1/K_{AW}) = -3.7973482 + 1889.5294/(T/\text{K})$, temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)
 3.85 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 3.95 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 4.764 - 2213/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 5.04 – 3.54 (27°C, equilibrium headspace-GC, solute concn 10.01–85.10 mg/L, measured range 300–315 K, Cheng et al. 2003)
 5.04* (27°C, equilibrium headspace-GC, measured range 27–42°C, Cheng et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.26 (shake flask-CR, Collander 1957)
 0.28 (shake flask-UV, Fujita et al. 1964, Hansch & Leo 1979)
 0.32 ± 0.01 (shake flask-UV, calculated, Iwasa et al. 1965)
 0.29 (shake flask-UV, GC, Hansch & Anderson 1967; Hansch et al. 1968; Leo et al. 1969, 1971)
 0.28 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

0.69	(generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
0.26	(shake flask-GC, Tanii et al. 1986)
0.62	(calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
0.29	(recommended, Sangster 1989, 1993)
0.29	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.77	(head-space GC, Abraham et al. 2001)
------	--------------------------------------

Bioconcentration Factor, $\log BCF$:

0.00	(estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)
------	--

Sorption Partition Coefficient, $\log K_{OC}$:

1.53	(soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)
1.47 ± 0.55 , 1.53 ± 0.88 ; 1.50	(Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
0.070	(predicted- K_{OW} , Walton et al. 1992)
-0.03	(calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on lab. data for evaporation relative to the reaeration rate of 0.27 (Mackay et al. 1982; Rathbun & Tai 1982; quoted, Howard 1990) and typical reaeration rates of rivers and lakes (Mill et al. 1982; quoted, Howard 1990),

$t_{1/2} = 3$ d for evaporation from a river and $t_{1/2} = 12$ d from lake (Howard 1990).

Photolysis: rate constant $k = 1.4 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carrier et al. 1986); calculated lifetime $\tau \sim 4$ d in air (Atkinson 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 48.8 - 81.4$ yr, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 2.4 - 24$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976)

$k_{OH} = (0.20 \pm 0.06) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

$k < 2.0 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation with singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 00$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 1.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 2.9$ d (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{OH} = (0.95 \pm 0.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at (295 ± 2) K in air (relative rate technique to ethene Cox et al. 1981; quoted, Atkinson 1985)

$k_{OH} = (1.20 \pm 0.20) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K in air (flash photolysis-resonance fluorescence, Zetzsch 1982; quoted, Atkinson 1985)

$k = (0.12 \pm 0.02) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 20–300 mM *t*-BuOH as scavenger at pH 2 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 1.38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 0.97 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 24°C with an atmospheric lifetime $\tau = 12$ d (Edney et al. 1986)

$k_{OH} = 1.15 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K and $k(\text{soln}) = 1.50 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the aqueous-phase reaction with OH radical in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

$k_{OH}^* = 1.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

photooxidation $t_{1/2} = 64.2 - 642$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Howard et al. 1991)

$k_{OH}(\text{calc}) = 1.65 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: first-order hydrolysis $t_{1/2} > 0$ yr, based on nonreactive hydrolysis from pH 5 to 9 at 15°C (Kollig et al. 1987; selected, Howard et al. 1991).

Biodegradation:

$k = 0.021 - 0.025 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b)

$t_{1/2}(\text{aq. aerobic}) = 24 - 168 \text{ h}$, based on unacclimated grab sample of aerobic freshwater (Dojlido 1979; selected, Howard et al. 1991) and aerobic aqueous screening test data (Takemoto et al. 1981; selected, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 96 - 672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4 - 24 \text{ h}$ in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 9.8 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976)

$t_{1/2} = 2.3 \text{ d}$ for the atmospheric reaction with photochemically produced hydroxyl radical (Cox et al. 1981; quoted, Howard 1990);

photooxidation $t_{1/2} = 64.2 - 642 \text{ h}$, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991);

calculated atmospheric lifetime $\tau = 12 \text{ d}$ due to reaction with OH radical (Edney et al. 1986) atmospheric transformation lifetime $\tau < 1 \text{ d}$ (estimated, Kelly et al. 1994);

calculated lifetime $\tau = 10 \text{ d}$ for reaction with OH radical (Atkinson 2000).

Surface water: photooxidation $t_{1/2} = 48.8 - 81.4 \text{ yr}$, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; quoted, Howard et al. 1991); $t_{1/2} = 24 - 168 \text{ h}$, based on unacclimated grab sample of aerobic freshwater (Dojlido 1979; selected, Howard et al. 1991) and aerobic aqueous screening test data (Takemoto et al. 1981; selected, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2} = 48 - 336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: calculated $t_{1/2} = 4.9 \text{ d}$ from first-order kinetic of degradation under both sterile and nonsterile conditions (Anderson et al. 1991);

$t_{1/2} = 24 - 168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.2.2.1

Reported aqueous solubilities of 2-butanone (methyl ethyl ketone) at various temperatures

Ginnings et al. 1940		Stephenson 1992	
volumetric method		shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
20	273300	0	367000
25	255700	9.6	310000
30	240700	19.3	276000
		29.7	245000
bp/ $^{\circ}\text{C}$	80.7–80.8	39.6	220000
d ²⁵	0.8007	49.7	206000
		60.6	180000
		70.2	182000

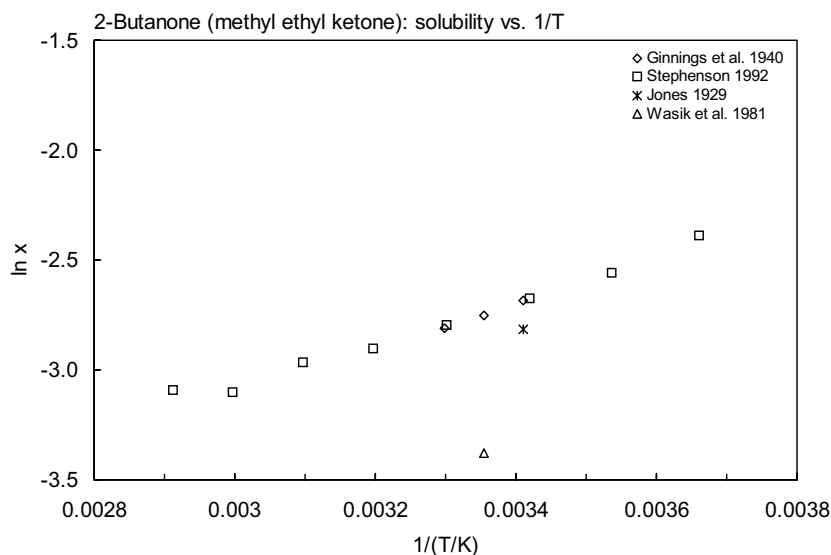


FIGURE 12.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-butanone.

TABLE 12.1.2.2.2

Reported vapor pressures of 2-butanone (methyl ethyl ketone) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Stull 1947		Dreisbach & Shrader 1949		Nickerson et al. 1961		Collerson et al. 1965	
summary of literature data		ebulliometry		flow calorimetry		ebulliometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-48.3	133.3	31.84	16500	41.46	25158	42.778	26568
-28.0	666.6	54.29	42066	65.54	63368	48.148	33024
-17.7	1333	67.36	67661	79.39	101098	53.026	39963
-6.50	2666	79.5	101325	89.43	137282	57.08	46591
6	5333			97.42	173212	60.821	53469
14	7999					64.005	59954
25	13332			eq. 4	P/mm Hg	67.009	66625
41.6	26664			A	21.78963	69.734	73184
60	53329			B	2441.9	72.343	79933
79.6	101325			C	4.70504	74.839	86849
						76.95	93063
mp/ $^{\circ}\text{C}$	-85.9					79.221	100135
						81.268	106887
						83.161	113428
						85.013	120126
						86.715	126547
						88.44	133353
						mp/ $^{\circ}\text{C}$	-86.69
						bp/ $^{\circ}\text{C}$	79.589

TABLE 12.1.2.2.2 (Continued)

Stull 1947		Dreisbach & Shrader 1949		Nickerson et al. 1961		Collerson et al. 1965	
summary of literature data		ebulliometry		flow calorimetry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						Antoine eq.	
						eq. 2	P/mmHg
						A	7.06376
						B	1261.455
						C	221.982
						Kirchhoff eq.	
						eq. 4	P/mmHg
						A	19.48322
						B	2328
						C	3.92657
						$\Delta H_v/(\text{kJ mol}^{-1}) = 31.67$	

2.

Ambrose et al. 1975(a)		Garriga et al. 1996	
comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa
25	12079	5	4277
42.778	26568	10	5644
48.137	33023	15	7334
53.016	39963	20	9435
57.07	46591	25	12071
60.812	53468	30	15281
63.996	59953	35	19110
67.001	66625	40	23682
69.726	73184	45	29132
72.335	79933	50	35540
74.832	86848		
76.944	93063	Antoine eq.	
79.215	100136	eq. 3a	P/kPa
81.262	106887	A	14.133009
83.156	113427	B	2843.871
85.009	120125	C	-53.875
86.711	126545		
88.444	133352		
bp/°C	79.583		
eq. 2	P/kPa		
A	6.18444		
B	1259.223		
C	-51.392		
$\Delta H_v/(\text{kJ mol}^{-1}) =$			
at 25°C	34.7		
at bp	31.8		

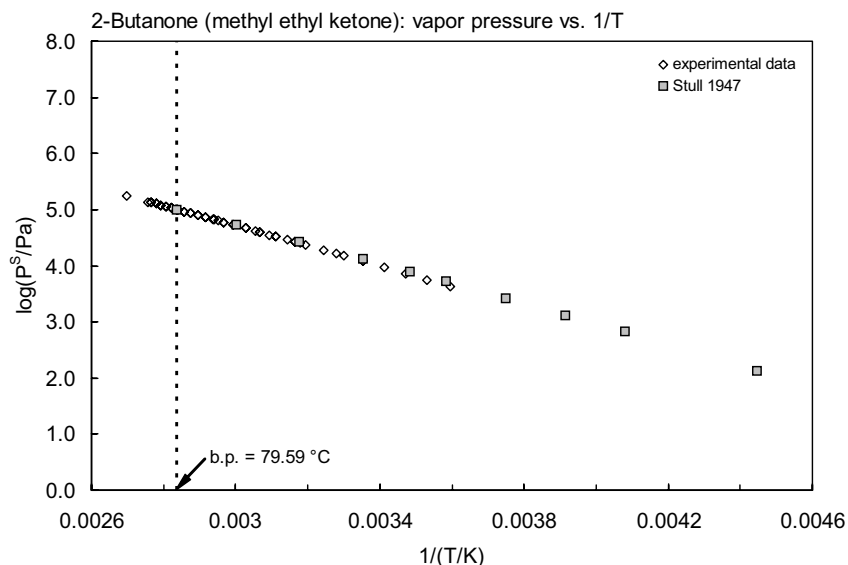


FIGURE 12.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-butanone.

TABLE 12.1.2.2.3

Reported Henry's law constants of 2-butanone (methyl ethyl ketone) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

Snider & Dawson 1985		Ashworth et al. 1988		Zhou & Mopper 1990			
gas stripping-GC		EPICS-GC		gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
0	0.9873	10	28.37	10	2.068	10	2.702
25	5.765	15	39.52	17	-	17	3.943
		20	19.25	25	5.117	25	6.666
enthalpy of transfer:		25	13.17	30	7.186	30	8.735
$\Delta H/(\text{kJ mol}^{-1}) = 46.024$		30	11.15	35	9.296	35	10.78
				40	-	40	14.07
		eq. 4a	H/(atm m ³ /mol)	45	14.27	45	18.09
		A	-26.32	eq. 1a	K _H '/(M/atm)	eq. 1a	K _H '/(M/atm)
		B	-5214	A	-6.03	A	-5.97
				B	-2184	B	-2138

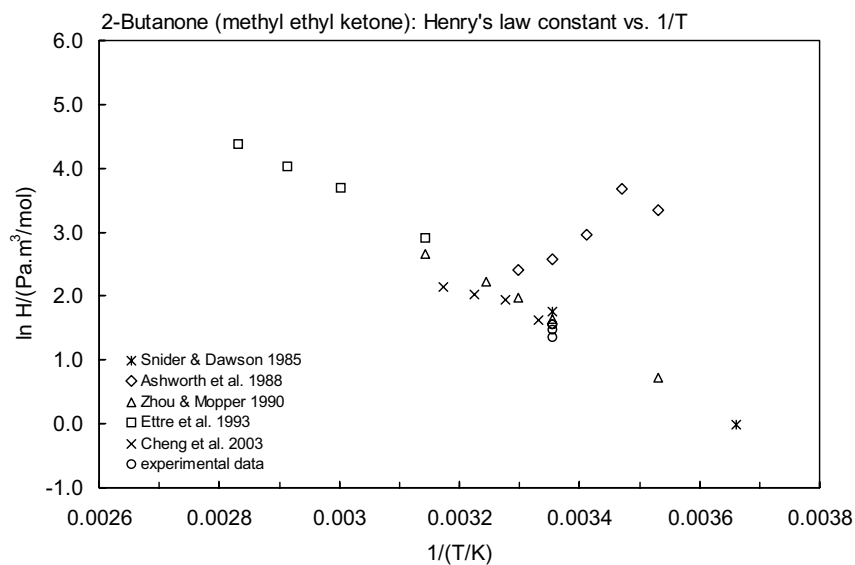
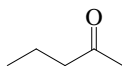


FIGURE 12.1.2.2.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-butanone.

12.1.2.3 2-Pentanone



Common Name: 2-Pentanone

Synonym: 2-pentanone, methyl propyl ketone, methyl *n*-propyl ketone, ethylacetone

Chemical Name: 2-pentanone, methyl propyl ketone

CAS Registry No: 107-87-9

Molecular Formula: C₅H₁₀O, CH₃CH₂CH₂COCH₃

Molecular Weight: 86.132

Melting Point (°C):

−77.80 (Stull 1947; Weast 1982–83; Dean 1985; Howard 1990)

−76.8 (Lide 2003)

Boiling Point (°C):

102.0 (Weast 1982–83; Verschuereen 1983)

101.7 (Dean 1985; Howard 1990)

102.26 (Lide 2003)

Density (g/cm³ at 20°C):

0.8089 (Weast 1982–83)

0.8064, 0.8015 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

118.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

2.541 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} J/mol K:

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

54268* (30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939)

30150 (30°C, Gross et al. 1939)

55100 (shake flask-volumetric, Ginnings et al. 1940)

59500 (20°C, shake flask-volumetric, Ginnings et al. 1940)

64010 (shake flask-interferometer, Donahue & Bartell 1952)

54350 (McGowan 1954; Deno & Berkheimer 1960)

43000 (Verschuereen 1977, 1983)

59500 (20°C, Riddick et al. 1986)

55400 (selected, Yaws et al. 1990)

59000* (19.7°C, shake flask-GC, measured range 0–90.5°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2088* (interpolated-regression of tabulated data, temp range −12.7 to 102.7°C, Stull 1947)

2666 (28.5°C, Stull 1947)

20440* (56.649°C, ebulliometry, measured range 56.5–111.655°C, Collerson et al. 1965)

log (P/mmHg) = 7.01753 − 1311.145/(214.693 + t/°C); temp range 56.5–111.65°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

log (P/mmHg) = 21.71880 − 2694.12/(T/K) − 4.63307·log (T/K); temp range 56.5–111.65°C (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)

log (P/mmHg) = 6.13916 − 1379.06/(221.41 + t/°C); temp range −5 to 100°C (data fitted to Antoine eq., static method-Ramsey-Young apparatus measurements, Meyer & Wagner 1966)

log (P/mmHg) = [−0.2185 × 11240.6/(T/K)] + 9.432089; temp range −12–103.3°C (Antoine eq., Weast 1972–73)

4720* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)

2133 (quoted, Verschuereen 1983)

- 1621 (quoted, Mackay & Yuen 1983)
 4648 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.14908 - 1311.372/(214.222 + t/^\circ\text{C})$, temp range 61.72–121.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = 7.02193 - 1313.85/(215.01 + t/^\circ\text{C})$, temp range 56–111°C (Antoine eq., Dean 1985, 1992)
 4702 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.14243 - 1311.145/(-58.457 + T/\text{K})$, temp range 329–386 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.1404 - 1310.269/(-58.514 + T/\text{K})$, temp range 336–422 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.47975 - 1569.596/(-24.035 + T/\text{K})$, temp range 416–501 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 18.3056 - 2.3477 \times 10^3/(T/\text{K}) - 3.6667 \cdot \log(T/\text{K}) + 7.1502 \times 10^{-4} \cdot (T/\text{K}) + 1.0912 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 196–561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 10.91 (28°C, concn. ratio-GC, Nelson & Hoff 1968)
 6.44 (partial vapor pressure-GC, Buttery et al. 1969)
 6.52 (quoted, exptl., Hine & Mookerjee 1975)
 7.66, 6.52 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 3.83 (calculated- γ -P, Rathbun & Tai 1982)
 5.876 (gas-stripping, Hawthorne 1984)
 10.13 (modified gas-stripping, Hawthorne et al. 1985)
 8.47, 6.83 (gas stripping-GC, calculated-P/C, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.91 \pm 0.03 (shake flask-UV at pH 7, Unger et al. 1978)
 0.91 (Hansch & Leo 1985)
 0.78 (shake flask-GC, Tanii et al. 1986)
 0.87 (calculated- V_1 and solvatochromic parameters, Kamlet et al. 1988)
 0.95 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 0.84 (recommended, Sangster 1989; 1993)
 0.91 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 3.19 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.477 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.869 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 15.5$ h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s, and $t_{1/2} = 14.5$ h in a wind-wave tank with a 6m/s wind speed (Howard 1990).
 Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 photooxidation $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{\text{OH}} = (4.64 \pm 0.14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(299 \pm 2) \text{ K}$ (relative rate technique to cyclohexane Atkinson et al. 1982; quoted, Atkinson 1985)

$k \sim 0.02 \text{ M}^{-1} \cdot \text{s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}}(\text{calc}) = 4.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 4.64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}} = 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K and $k(\text{soln}) = 3.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the aqueous-phase reaction with OH radical in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

$k_{\text{OH}} = 4.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 5.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}} = (4.56 \pm 0.30) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ with calculated tropospheric lifetime $\tau = 2.5 \text{ d}$ (relative rate method, Atkinson et al. 2000)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 3.5 \text{ d}$ for reactions with photochemically produced OH radical (Howard 1990);

calculated lifetime $\tau = 2.5 \text{ d}$ for reaction with OH radical (Atkinson 2000).

Surface water: volatilization $t_{1/2} = 11\text{--}17 \text{ h}$ from a model river (Howard 1990).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.3.1

Reported aqueous solubilities of 2-pentanone at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	76406	20	59500	0	87000
30	54268	25	55100	9.7	69000
50	44362	30	51800	19.7	59000
				31.0	50000
		bp/°C	102.2–102.3	39.6	46000
		d ²⁵	0.8018	49.8	42000
				60.1	40000
				70.2	40000
				80.0	38000
				90.5	34000

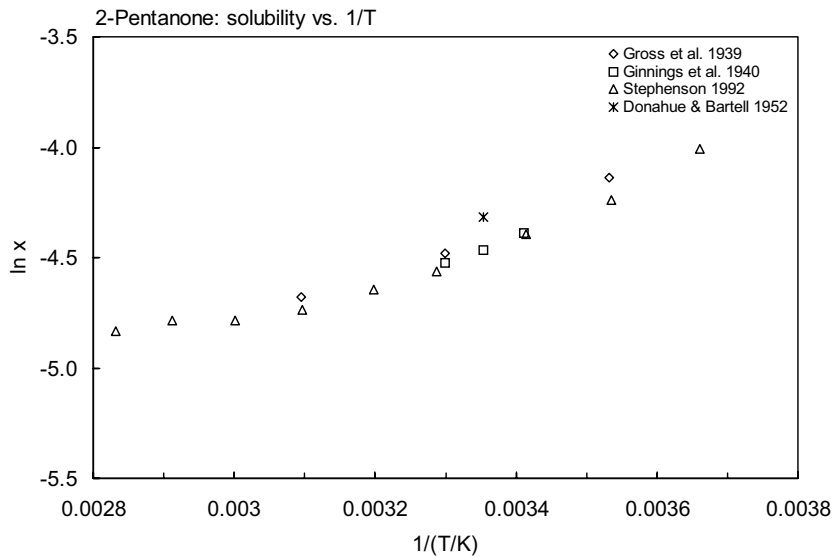


FIGURE 12.1.2.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-pentanone.

TABLE 12.1.2.3.2
Reported vapor pressures of 2-pentanone (methyl propyl ketone) at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K)$$
$$\log P = A - B/(C + t/^{\circ}\text{C})$$
$$\log P = A - B/(C + T/K)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K)$$

(1)

(2)

(3)

(4)

$$\ln P = A - B/(T/K)$$
$$\ln P = A - B/(C + t/^{\circ}\text{C})$$

(1a)

(2a)

Stull 1947		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−12.0	133.3	56.649	20440	63.175	26546
8	666.6	63.184	26546	68.889	33040
17.9	1333	68.897	33040	74.069	39992
28.5	2666	74.077	39991	78.333	46568
39.8	5333	78.34	46568	82.321	53466
47.3	7999	82.326	53466	85.703	59946
56.8	13332	85.708	59947	88.889	66611
71	26664	88.893	66527	91.832	73283
86.8	53329	91.834	73303	95.547	79906
103.3	101325	94.549	79905	97.178	86760
		97.179	86760	99.47	93107
mp/°C	−77.8	99.47	93107	101.845	100063
		101.345	100062	104.032	106831
		104.031	106831	106.116	113611
		106.114	113612	108.026	120112
		108.023	120113	109.834	126533
		109.83	126535	111.659	133292
		111.655	133283	25	4720
		mp/°C	−76.86	bp/°C	102.262
		bp/°C	102.26		

(Continued)

TABLE 12.1.2.3.2 (Continued)

Stull 1947		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		Antoine eq.		eq. 3	P/kPa
		eq. 2	P/mmHg	A	6.13925
		A	7.01753	B	1309.592
		B	1311.145	C	-58.589
		C	214.693		
		Kirchhoff eq		$\Delta H_v/(\text{kJ mol}^{-1}) =$	
		eq. 4	P/mmHg	at 25°C	38.4
		A	21.7188	at bp	33.6
		B	2594.12		
		C	4.63307		
		$\Delta H_v/(\text{kJ mol}^{-1}) = 33.64$			

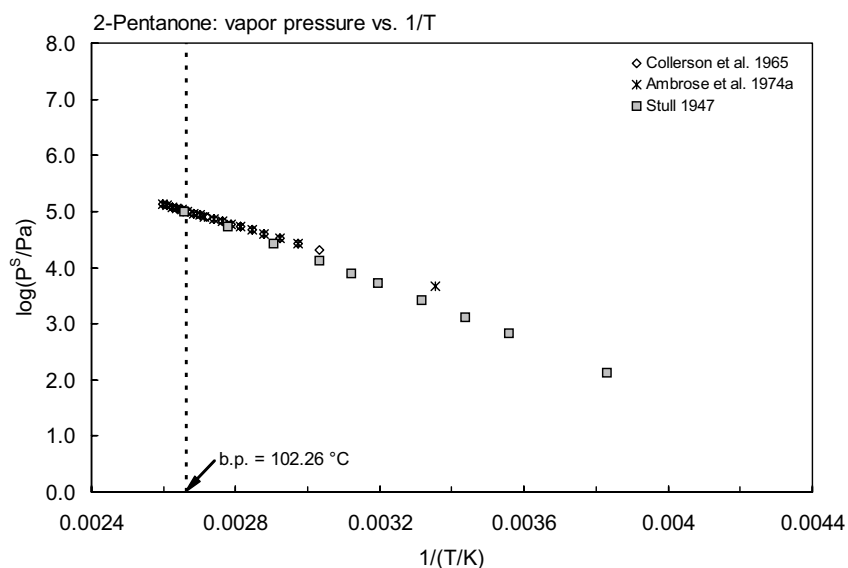
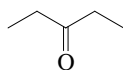


FIGURE 12.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for 2-pentanone.

12.1.2.4 3-Pentanone



Common Name: 3-Pentanone

Synonym: diethyl ketone, ethylketone, propione, *sym*-dimethylacetone

Chemical Name: 3-pentanone, diethyl ketone

CAS Registry No: 96-22-0

Molecular Formula: $C_5H_{10}O$, $CH_3CH_2COCH_2CH_3$

Molecular Weight: 86.132

Melting Point ($^{\circ}C$):

−39 (Lide 2003)

Boiling Point ($^{\circ}C$):

101.7 (Gross et al. 1933; Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8138 (Weast 1982–83)

0.8143, 0.8095 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.6 (calculated-density, Jaworska & Schultz 1993)

118.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

27.1 (pK_a , Riddick et al. 1986; Howard 1993)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

11.593 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

46900 ($30^{\circ}C$, shake flask-interferometer, Gross et al. 1933)

49617* ($30^{\circ}C$, shake flask-interferometer, measured range 10 – $50^{\circ}C$, Gross et al. 1939)

49620 ($30^{\circ}C$, shake flask-interferometer, Gross et al. 1933)

48100* (shake flask-volumetric method, measured range 20 – $30^{\circ}C$, Ginnings et al. 1940)

48100 (shake flask-volumetric, Ginnings et al. 1940)

44520 (shake flask-centrifuge, Booth & Everson 1948)

43170 (estimated, McGowan 1954)

47330 (Deno & Berkheimer 1960)

45650 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

47000, 38000 ($20^{\circ}C$, $100^{\circ}C$, Verschueren 1983)

34000 ($20^{\circ}C$, Riddick et al. 1986)

48440 (calculated-fragment solubility const., Wakita et al. 1986)

53000* ($19.3^{\circ}C$, shake flask-GC, measured range 0 – $80^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2169* (interpolated-regression of tabulated data, temp range -12.0 to $103.3^{\circ}C$, Stull 1947)

2666 ($27.9^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.25223 - 1450.0/(230 + t/^{\circ}C)$, (Antoine eq., Dreisbach & Martin 1949)

10114* ($36.36^{\circ}C$, ebulliometry, measured range 36.36 – $101.7^{\circ}C$, Dreisbach & Shrader 1949)

20441* ($56.649^{\circ}C$, ebulliometry, measured range 56.5 – $111.3^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.027427 - 1309.655/(214.118 + t/^{\circ}C)$; temp range 56.5 – $111.3^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 22.02258 - 2614.85/(T/K) - 4.72805 \cdot \log(T/K)$; temp range 56.5 – $111.3^{\circ}C$ (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/\text{mmHg}) = [-0.2185 \times 11183.0/(T/K)] + 9.406280$; temp range -12.7 – 102.7°C , (Antoine eq., Weast 1972–73)
 4723* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)
 1733 (20°C , Verschueren 1983)
 5316, 4714 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.1467 - 1307.941/(213.968 + t/^\circ\text{C})$, temp range 56.53 – 111.3°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.13703 - 1349.358/(224.351 + t/^\circ\text{C})$, temp range 36.36 – 101.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 4693 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.02529 - 1310.28/(214.19 + t/^\circ\text{C})$, temp range 56 – 111°C (Antoine eq., Dean 1985, 1992)
 4723 (Riddick et al. 1986)
 $\log(P_L/\text{kPa}) = 6.14917 - 1309.657/(-59.032 + T/K)$, temp range 329 – 384 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.14635 - 1308.327/(-59.137 + T/K)$, temp range 329 – 426 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.45505 - 1544.596/(-27.379 + T/K)$, temp range 421 – 502 K, (Antoine eq.-III, Stephenson & Malanowski 1987)
 4932 (Daubert & Danner 1989)
 $\log(P/\text{mmHg}) = 32.265 - 2.9431 \times 10^3/(T/K) - 8.5068 \cdot \log(T/K) - 4.572 \times 10^{-10} \cdot (T/K) + 2.5177 \times 10^{-6} \cdot (T/K)^2$;
 temp range 234 – 561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

3.617 (calculated- γ -P, Rathbun & Tai 1982)
 5.340 (calculated-MW, Rathbun & Tai 1982)
 8.834 (calculated-P/C, Howard 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.99 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 0.75 (calculated-activity coeff. γ , Wasik et al. 1981)
 0.67 (calculated- activity coeff. γ , Berti et al. 1986)
 1.15 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 0.82 (recommended, Sangster 1989, 1993)
 0.99 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.20 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

0.519 (estimated- K_{OW} , Lyman et al. 1990; quoted, Howard 1993)
 0.146 (estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

1.914 (soil, estimated- K_{OW} , Lyman et al. 1990; quoted, Howard 1993)
 1.08 (soil, estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated half-life from a model pond of two meter deep is 5.6 d (USEPA 1987; quoted, Howard 1993);
 based on calculated Henry's law constant, estimated $t_{1/2} \sim 12$ h from a model river of 1 m deep flowing at
 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3}
 with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 photooxidation $t_{1/2} = 2.4$ – 24 h for the gas-phase reaction with OH radical in air, based on the rate of
 disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}} = (1.82 \pm 0.33) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $299 \pm 2 \text{ K}$ in air (relative rate technique to cyclohexane Atkinson et al. 1982)

$k_{\text{OH}}(\text{calc}) = 2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.82 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}}(\text{exptl}) = 2.74 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 296 K; experimentally determined $k(\text{soln}) = 2.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

$k_{\text{OH}} = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 3.23 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: not expected to be important (Howard 1993).

Biodegradation: $t_{1/2} \sim 5$ to 10 d in acclimated cultures during screening tests (Howard 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 5.9 \text{ d}$, based on an experimentally determined rate constant for the vapor-phase reaction with OH radical in air (Wallington & Kurylo 1987; quoted, Howard 1993).

Surface water: estimated volatilization $t_{1/2} \sim 12 \text{ h}$ in a model river (1 m deep flowing at 1 m/s with a 3 m/s wind) and $t_{1/2} = 5.6 \text{ d}$ in a model environmental pond (2 m deep) (Howard 1993).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.4.1

Reported aqueous solubilities of 3-pentanone at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	67275	20	50800	0	76800
30	49617	25	48100	9.7	62500
50	39280	30	45000	19.3	53000
				30.6	42400
		bp/°C	101.6–101.9	40.3	38600
		D ²⁵	0.8116	50	36200
				60.1	34300
				70.1	33000
				80.2	31500

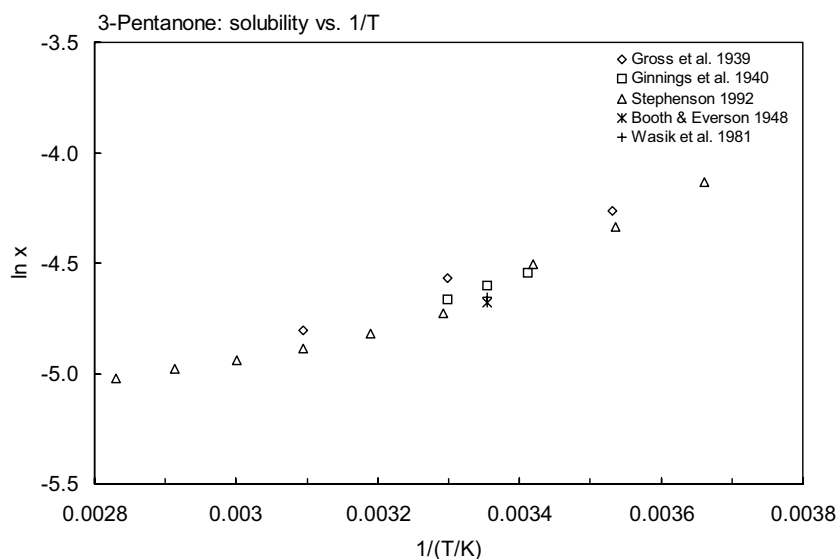


FIGURE 12.1.2.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-pentanone.

TABLE 12.1.2.4.2

Reported vapor pressures of 3-pentanone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-12.7	133.3	36.36	10114	56.544	20441	56.534	20441
7.5	666.6	51.24	16500	63.032	26530	63.023	26529
17.2	1333	76.04	42066	68.735	33041	68.727	33041
27.9	2666	88.91	67661	73.908	40009	73.901	40009
39.4	5333	101.7	101325	78.158	46590	78.152	46589
46.7	7999			82.114	53473	82.109	53473
56.2	13332			85.494	59947	85.489	59979
70.6	26664			88.612	66532	88.608	66532
86.2	53329			91.605	74147	91.602	73348
102.7	101325			94.314	79985	94.312	79985
				96.897	86752	96.896	86752
mp/ $^{\circ}\text{C}$	-42			99.177	93092	99.176	93093
				101.566	100129	101.567	100129
				103.724	106835	103.725	106834
				105.737	113413	105.739	113412
				107.682	120061	107.685	120059
				109.486	126495	109.489	126493
				111.303	133254	111.307	133252
						25	4723
				mp/ $^{\circ}\text{C}$	-38.97		
				bp/ $^{\circ}\text{C}$	101.959	bp/ $^{\circ}\text{C}$	101.96

TABLE 12.1.2.4.2 (Continued)

Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				Antoine eq		eq. 3	P/kPa
				eq. 2	P/mmHg	A	6.1457
				A	7.02427	B	1307927
				B	1309.653	C	-59.184
				C	214.118		
				Kirchhoff eq. 4, P/mmHg		ΔH_v /(kJ mol ⁻¹) =	
				A	22.02258	at 25°C	38.6
				B	2614.85	at bp	33.7
				C	4.72085		
				ΔH_v /(kJ mol ⁻¹) = 33.72			

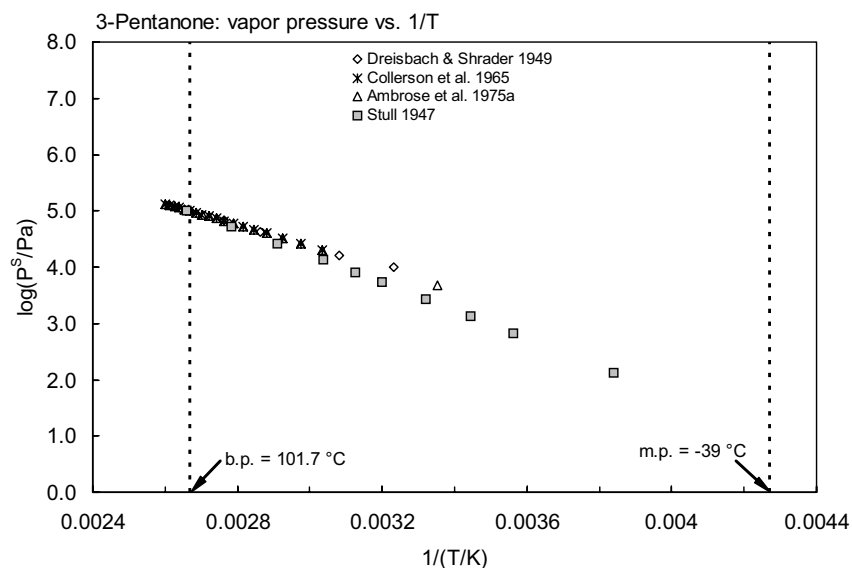
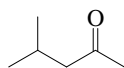


FIGURE 12.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for 3-pentanone.

12.1.2.5 Methyl isobutyl ketone (MIBK)



Common Name: Methyl isobutyl ketone

Synonym: hexone, hexanone, 4-methyl-2-pentanone, MIBK

Chemical Name: methyl isobutyl ketone, 4-methyl-2-pentanone

CAS Registry No: 108-10-1

Molecular Formula: $C_6H_{12}O$, $(CH_3)_2CHCH_2COCH_3$

Molecular Weight: 100.158

Melting Point ($^{\circ}C$):

-84 (Lide 2003)

Boiling Point ($^{\circ}C$):

116.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7978 (Weast 1982-83)

0.8010 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

125.0 ($20^{\circ}C$, calculated-density)

140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

16630* ($30^{\circ}C$, shake flask-interferometer, measured range $0-75^{\circ}C$, Gross et al. 1939)

19100* (shake flask-volumetric method, measured range $20-30^{\circ}C$, Ginnings et al. 1940)

19100 (shake flask-volumetric, Ginnings et al. 1940)

18200 (shake flask-turbidimeter, McBain & Richards 1946)

19085 (Deno & Berkheimer 1960)

17700 (shake flask-radiometric method, Lo et al. 1986)

17000 (Dean 1985; Riddick et al. 1986)

19200* ($19.4^{\circ}C$, shake flask-GC/TC, measured range $0-90.4^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* ($19.7^{\circ}C$, summary of literature data, temp range -1.40 to $119^{\circ}C$, Stull 1947)

2200* ($21.7^{\circ}C$, isoteniscope method, measured range $21.7-116.2^{\circ}C$, Fuge et al. 1952)

$\log (P/mmHg) = 31.1616 - 7.7701 \cdot \log (273.1 + t/^{\circ}C) - 3173.11/(273.11 + t/^{\circ}C)$; temp range $21.7-116.2^{\circ}C$ (isoteniscope method, Fuge et al. 1952)

$\log (P/mmHg) = [-0.2185 \times 11669.6/(T/K)] + 9.407655$; temp range: -1.4 to $119^{\circ}C$, (Antoine eq., Weast 1972-73)

800; 1333 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

2200 ($21.7^{\circ}C$, quoted exptl., Boublik et al. 1984; Howard 1990)

2587 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.81291 - 1176.833/(192.925 + t/^{\circ}C)$, temp range $21.7-116.2^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

2575 (calculated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 6.6727 - 1168.4/(191.9 + t/^{\circ}C)$, temp range $22-116^{\circ}C$ (Antoine eq., Dean 1985, 1992)

2510 (Riddick et al. 1986)

$\log (P/kPa) = 6.0976 - 1190.69/(195.45 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

2581, 2581 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.79768 - 1168.443/(-81.202 + T/\text{K})$, temp range 294–390 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.83311 - 1188.115/(-79.265 + T/\text{K})$, temp range 281–400 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

2687* (comparative ebulliometry, extrapolated-Antoine eq., measured range 309.7–416 K, Ambrose et al. 1988)

$\ln (p/\text{kPa}) = 14.07841 - 3103.029/(T/\text{K} - 61.104)$; temp range 309.7–416 K (comparative ebulliometry, Ambrose et al. 1988)

$\log (P/\text{mmHg}) = 64.1919 - 4.3577 \times 10^3/(T/\text{K}) - 19.766 \cdot \log (T/\text{K}) - 3.9997 \times 10^{-10} \cdot (T/\text{K}) + 7.102 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 189–571 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

39.5* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

$\ln [H/(\text{atm m}^3/\text{mol})] = -7.157 + 160.6/(T/\text{K})$, temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)

9.523 (calculated-P/C, Howard 1990)

47.95* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)

$\ln (1/K_{AW}) = -9.56 + 4237/(T/\text{K})$, temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

45.57 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = -1.924 + 57/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.38 (shake flask-GC, Iwasa et al. 1965)

1.09 (calculated- π constant, Hansch et al. 1968)

1.19 (Hansch & Leo, 1979)

1.39 (HPLC-RT correlation, Haky & Young 1984)

1.31 (shake flask-GC, Tanii et al. 1986)

1.38 (recommended, Sangster 1993)

1.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.301–0.699 (estimated- K_{OW} and S, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.279–2.025 (soil, estimated- K_{OW} and S, Lyman et al. 1982; quoted, Howard 1990)

0.87 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 15\text{--}33$ h from water of 1 m deep, based on lab. mass-transfer coefficient for volatilization from a stirred 557–2020 rpm water bath at 25°C (Rathbun & Tai 1982; quoted, Howard 1990).

Photolysis: direct photolysis $t_{1/2} = 15$ h in air (Howard 1990).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h for the gas-phase reaction with OH radical in air, based on the disappearance rate of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (0.9 \pm 0.3) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

$k_{OH}(\text{calc}) = 9.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 14.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 4.6\text{--}45.5$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991)

$k_{OH} = 14.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = (1.31 - 1.45) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (OH radical concn. of $8.0 \times 10^5 \text{ molecule}\cdot\text{cm}^{-3}$) at 22–27°C, estimated $t_{1/2} = 16\text{--}17 \text{ h}$ (Howard 1990)

$k_{\text{OH}}(\text{calc}) = 3.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: not expected to undergo chemical hydrolysis (Howard 1990).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aerobic aqueous screening test data (Bridie et al. 1979; Takemoto et al. 1981; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the disappearance rate of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 3.5 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976);

direct photolysis $t_{1/2} = 15 \text{ h}$ and photooxidation $t_{1/2} = 16\text{--}17 \text{ h}$ for reactions with hydroxyl radical in air (Howard 1990);

photooxidation $t_{1/2} = 4.6\text{--}45.5 \text{ h}$, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: estimated volatilization $t_{1/2} = 15\text{--}33 \text{ h}$ (Howard 1990);

$t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.2.5.1

Reported aqueous solubilities of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	30749	10	20400	0	29200
10	23137	24	19100	9.5	22100
30	16630	30	17800	19.4	19200
50	14123			30.8	16600
75	13721	bp/ $^{\circ}\text{C}$	115.6–115.7	39.6	14700
		D ²⁵	0.7969	50.1	13800
				60.4	12900
				70.2	12400
				80.1	11800
				90.4	12200

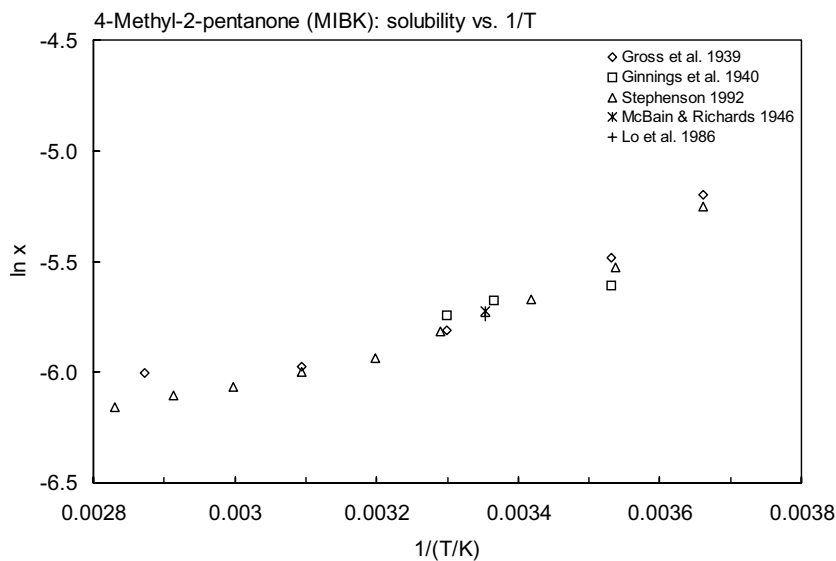


FIGURE 12.1.2.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-methyl-2-pentanone.

TABLE 12.1.2.5.2
Reported vapor pressures of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)
log P = A – B/(C + T/K)		(3)	ln P = A – B/(C + T/K)		(3a)
log P = A – B/(T/K) – C·log (T/K)		(4)			
Stull 1947		Fuge et al. 1952		Ambrose et al. 1988	
summary of literature data		isoteniscope method		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–1.40	133.3	21.7	2200	309.676	4922
19.7	666.6	32.7	3933	314.495	6239
30.0	1333	41.4	6266	318.766	7638
40.8	2666	50.2	9266	324.624	9984
52.8	5333	60.0	14999	328.196	11607
60.4	7999	70.0	21598	334.215	15105
70.4	13332	80.1	31997	339.189	18512
85.6	26664	90.9	46396	343.458	21914
102.0	53329	116.2	101325	347.213	25314
119.0	101325			352.107	30381
		bp/K	389.35 K	359.039	38940
mp/°C	–84.7			365.854	49155
		eq. 4	P/mmHg	369.784	55938
		A	31.1616	373.360	62819
		B	3173.11	379.656	76425
		C	–7.7701	383.817	86848
				389.378	101960
				400.202	137928

(Continued)

TABLE 12.1.2.5.2 (Continued)

Stull 1947		Fuge et al. 1952		Ambrose et al. 1988	
summary of literature data		isoteniscope method		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
				408.620	172120
				415.823	206364
				298.15	2687
					(extrapolated)
				eq. 3a	P/kPa
				A	14.07841
				B	3103.029
				C	-61.104

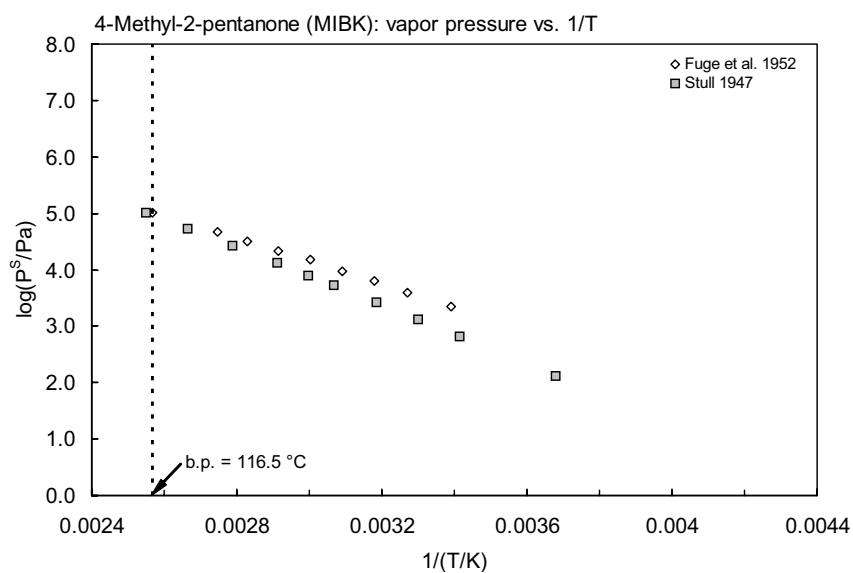


FIGURE 12.1.2.5.2 Logarithm of vapor pressure versus reciprocal temperature for 4-methyl-2-pentanone.

TABLE 12.1.2.5.3
Reported Henry’s law constants of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Ashworth et al. 1988			Kolb et al. 1992		
EPICS-GC			equilibrium headspace-GC		
t/°C	H/(Pa m³/mol)		t/°C	H/(Pa m³/mol)	
10	66.87		40	47.95	
15	37.49		60	121.5	
20	29.38		70	176	
25	39.52		80	248.8	
30	68.90				
			eq. 2	1/K _{AW}	
			A	−9.56	
eq. 4a	H/(atm·m³/mol)		B	4237	
A	−7.157				
B	160.6				

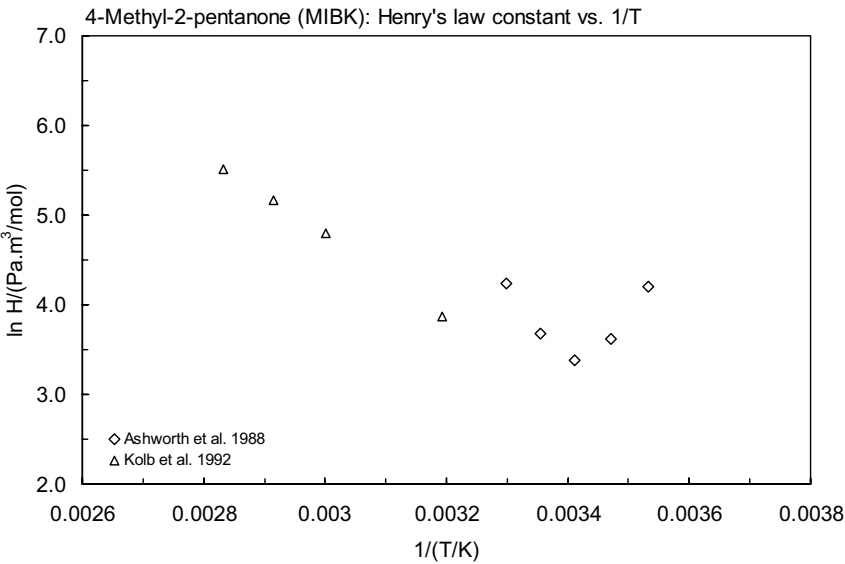
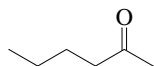


FIGURE 12.1.2.5.3 Logarithm of Henry’s law constant versus reciprocal temperature for 4-methyl-2-pentanone.

12.1.2.6 2-Hexanone (Methyl butyl ketone)



Common Name: Methyl butyl ketone

Synonym: 2-hexanone, methyl *n*-butyl ketone

Chemical Name: 2-hexanone, methylbutyl ketone

CAS Registry No: 591-78-6

Molecular Formula: C₆H₁₂O, CH₃COCH₂CH₂CH₂CH₃

Molecular Weight: 100.158

Melting Point (°C):

–55 (Lide 2003)

Boiling Point (°C):

127.6 (Lide 2003)

Density (g/cm³ at 20°C):

0.8113 (Weast 1982–83)

0.8113, 0.8067 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

124.2 (calculated-density, Hoy 1970; Amidon & Williams 1982)

140.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

–8.30 (pK_a, Riddick et al. 1986)

25.30 (pK_s, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

3.56 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

14523* (30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939)

16400* (shake flask-volumetric method, measured range 20–30°C, Ginnings et al. 1940)

16400 (shake flask-volumetric, Ginnings et al. 1940)

16000 (Erichsen 1952)

23930 (shake flask-interferometer, Donahue & Bartell 1952)

15870 (estimated, McGowan 1954)

16620 (Deno & Berkheimer 1960)

35000 (20°C, Verschueren 1983)

17500 (20°C, Riddick et al. 1986)

15100*, 13700 (19.8°C, 29.7°C, shake flask-GC, measured range 0–91.5°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

514.4* (interpolated-regression of tabulated data, temp range 7.7–212.6°C, Stull 1947)

log (P/mmHg) = [–0.2185 × 12358.3/(T/K)] + 9.642791; temp range 7.7–127.5°C, (Antoine eq., Weast 1972–73)

1549* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)

509.8 (calculated-Cox eq., Chao et al. 1983)

266.6 (20°C, Verschueren 1983)

1540 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.15217 – 1395.406/(208.946 + t/°C), temp range 34.61–154.6°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

1549 (Riddick et al. 1986)

log (P/kPa) = 6.16230 – 1401.738/(209.646 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

1715, 1540 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.4127 - 1575.5/(-43.15 + T/\text{K})$, temp range 293–411 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14816 - 1392.968/(-64.465 + T/\text{K})$, temp range 279–423 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15949 - 1399.959/(-63.704 + T/\text{K})$, temp range 310–427 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

1600 (computed-expert system SPARC, Kolling 1995)

$\log (P/\text{mmHg}) = 4.0508 - 2.6276 \times 10^3/(T/\text{K}) + 3.7783 \cdot \log (T/\text{K}) - 1.4342 \times 10^{-2} \cdot (T/\text{K}) + 8.0592 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 217–587 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

9.69 (calculated-P/C, Meylan & Howard 1991)

11.8 (calculated-bond contribution, Meylan & Howard 1991)

9.70 (calculated-P/C, Howard 1993)

8.82 (computed-expert system SPARC, Kolling 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.38 (shake flask-UV, Iwasa et al. 1965; Leo et al. 1971; Hansch & Leo 1979)

1.29 (calculated- π constant, Hansch et al. 1968)

1.39 (HPLC- k' correlation, Haky & Young 1984)

1.19 (shake flask-GC, Tanii et al. 1986)

1.38 (recommended, Sangster 1989, 1993)

1.38 (recommended, Hansch et al. 1995)

1.30 (computed-expert system SPARC, Kolling 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.68 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

0.778 (estimated- K_{OW} , Lyman et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.322 (soil, estimated- K_{OW} , Lyman et al. 1990)

2.127 (soil, estimated-S, Lyman et al. 1990)

1.10 (computed- K_{OW} , Kolling 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 135$ h from a model environmental pond of 2 m deep (USEPA 1987; quoted, Howard 1993); using Henry's law constant, $t_{1/2} \sim 12.1$ H from a model river of 1 m deep flowing at 1 m/s with a wind speed of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (6.81 \pm 0.29) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(299 \pm 2) \text{ K}$ (relative rate technique to cyclohexane, Atkinson et al. 1982; quoted, Atkinson 1985)

$k_{OH}(\text{calc}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 8.97 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 9.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 9.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C, which corresponds to a half-life of 42 h at an atmospheric OH- concn of $5 \times 10^5 \text{ molecule cm}^{-3}$ (quoted, Howard 1993)

$k_{OH}(\text{calc}) = 10.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: half-life of approximately 5 d in acclimated mixed microbial culture (Howard 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

estimated $t_{1/2} \sim 42$ h for the vapor-phase reaction with OH radical is 42 h at an atmospheric OH- concentration of 5×10^5 molecule·cm⁻³ (Atkinson 1985; quoted, Howard 1993).

Surface water: volatilization $t_{1/2} = 12.1$ h from a model river, 135 h from a model environmental pond (Howard 1993).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.6.1

Reported aqueous solubilities of 2-hexanone at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	20433	20	17500	0	24600
30	14523	25	16400	9.6	19100
50	12420	30	15300	19.8	15100
				29.7	13700
		bp/°C	127.5–127.6	39.6	12400
		d ²⁵	0.8072	50.0	11600
				60.5	11200
				70.3	11200
				80.7	11500
				91.5	11900

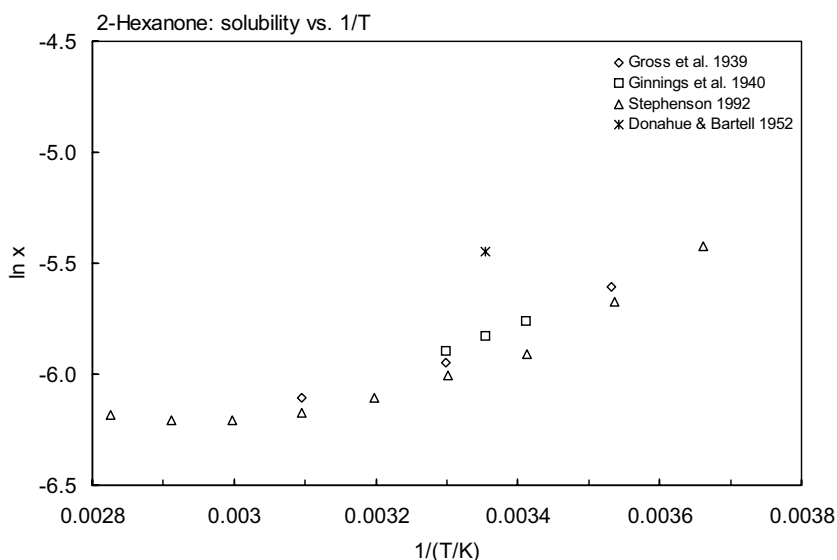


FIGURE 12.1.2.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-hexanone.

TABLE 12.1.2.6.2

Reported vapor pressures of 2-hexanone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Ambrose et al. 1975(a)			
summary of literature data		comparative ebulliometry			
t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	P/Pa
				cont'd	
7.7	133.3	34.612	2656	128.935	105328
28.8	666.6	37.070	3024	133.789	120447
38.8	1333	41.117	3737	138.034	135072
50.0	2666	44.498	4434	143.528	156043
62.0	5333	48.033	5277	149.390	181140
69.8	7999	51.799	6319	154.613	206034
79.8	13332	55.414	7476	25.0	1549
94.3	26664	59.402	8955		
111.0	53329	63.784	10853	bp/^{\circ}\text{C}	127.583
127.5	101325	67.976	12972		
		72.537	15657	Antoine eq. for full range:	
mp/^{\circ}\text{C}	-56.9	77.315	18944	eq. 3	P/kPa
		82.256	22918	A	6.16230
		86.138	26494	B	1401.738
		91.579	32278	C	-63.504
		96.410	38230	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
		101.664	45683	at 25^{\circ}\text{C}	42.9
		106.935	54287	at bp	36.0
		112.320	64383		
		117.459	75365	Antoine eq. for restricted range of	
		122.839	88399	of atmospheric pressure:	
		127.231	100312	eq. 3	P/kPa
		127.653	101527	A	6.14801
		128.362	103586	B	1392.870
				C	-64.477

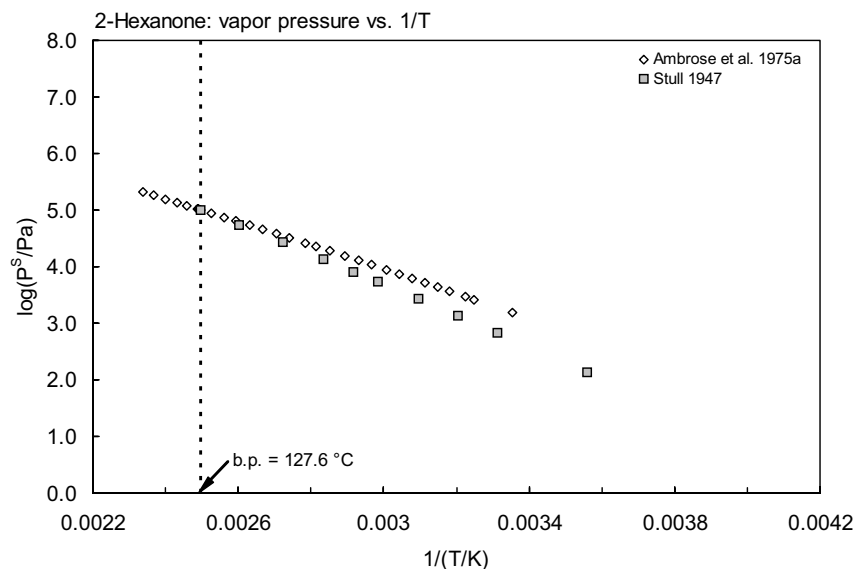
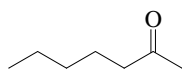


FIGURE 12.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2-hexanone.

12.1.2.7 2-Heptanone



Common Name: 2-Heptanone

Synonym: methyl *n*-amyl ketone, methyl pentyl ketone

Chemical Name: 2-heptanone

CAS Registry No: 110-43-0

Molecular Formula: $C_7H_{14}O$, $CH_3(CH_2)_4COCH_3$

Molecular Weight: 114.185

Melting Point ($^{\circ}C$):

−35 (Lide 2003)

Boiling Point ($^{\circ}C$):

151.05 (Lide 2003)

Density (g/cm^3):

0.81537, 0.81123 (20 $^{\circ}C$, 25 $^{\circ}C$, Riddick et al. 1986)

Dissociation Constant:

Molar Volume (cm^3/mol):

141.5 (30 $^{\circ}C$, Stephenson & Malanowski 1987)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

4300* (25 $^{\circ}C$, volumetric method, measured range 20–30 $^{\circ}C$, Ginnings et al. 1940)

4054* (30 $^{\circ}C$, shake flask-interferometer, measured range 10–75 $^{\circ}C$, Saylor et al. 1942)

4546 (estimated, McGowan 1954)

4300 (Riddick et al. 1986)

4360* (19.7 $^{\circ}C$, shake flask-GC/TC, measured range 0–90.5 $^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

521 (interpolated-vapor pressure eq., temp range 4–75 $^{\circ}C$, Stuckey & Saylor 1940)

$\log (P/mmHg) = 7.36537 - 1650.47/(T/K - 54.48)$; temp range 4–75 $^{\circ}C$ (Antoine eq., Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)

709* (30 $^{\circ}C$, measured range 10–75 $^{\circ}C$, Saylor et al. 1942)

133.3* (19.3 $^{\circ}C$, summary of literature data, temp range 19.3–150.2 $^{\circ}C$, Stull 1947)

$\log (P/mmHg) = 5.95166 - 1408.13/(194.84 + t/^{\circ}C)$; temp range 36 to 151 $^{\circ}C$ (data fitted to Antoine eq., static method-Ramsay-Young apparatus measurements, Meyer & Wagner 1966)

$\log (P/mmHg) = [-0.2185 \times 12478.9/(T/K)] + 9.305642$, temp range 19.3–150.2 $^{\circ}C$, (Antoine eq., Weast 1972–73)

427* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)

$\log (P/mmHg) = [1 - 400.348/(T/K)] \times 10^{\{0.934881 - 4.87941 \times 10^{-4} \cdot (T/K) + 4.16258 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 280.85–400.65 K, (Cox eq., Chao et al. 1983)

514 (Abraham 1984; Riddick et al. 1986)

504 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.14611 - 1460.276/(201.636 + t/^{\circ}C)$, temp range 94.7–179.3 $^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

469 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.07656 - 1408.73/(-78.31 + T/K)$, temp range 303–424 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15178 - 1464.092/(-71.076 + T/\text{K})$, temp range 327–457 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.56718 - 1810.283/(-26.944 + T/\text{K})$, temp range 449–580 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -13.0256 - 2.6425 \times 10^3/(T/\text{K}) + 11.879 \cdot \log (T/\text{K}) - 2.7571 \times 10^{-2} \cdot (T/\text{K}) + 1.456 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 238–612 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

14.63 (partial vapor pressure-GC, Buttery et al. 1969)

14.6; 14.94, 14.6 (exptl.; calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

5.715 (calculated-activity coefficient γ_P , Rathbun & Tai 1982)

9.120 (calculated-P/C, Mackay & Yuen 1983)

16.0 (correlated-molecular structure, Russell et al. 1992)

17.1 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.08 (calculated-activity coefficients, Wasik et al. 1981)

1.98 (generator column-HPLC, Tewari et al. 1982)

2.00 (shake flask-GC, Tani et al. 1986)

2.03 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)

1.98 (recommended, Sangster 1993)

1.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

4.15 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (8.67 \pm 8.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Wallington et al. 1987; quoted, Atkinson 1989)

$k_{OH}(\text{calc}) = 13.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{OH} = (1.17 \pm 0.11) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ with calculated tropospheric lifetime $\tau = 1.0 \text{ d}$ (relative rate method, Atkinson et al. 2000)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime $\tau = 1.0 \text{ d}$, based on gas-phase reaction with OH radical (relative rate method, Atkinson et al. 2000)

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.7.1

Reported aqueous solubilities of 2-heptanone at various temperatures

Ginnings et al. 1940		Saylor et al. 1942		Stephenson 1992	
volumetric method		shake flask-interferometer		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	4400	10	5390	0	6490
25	4300	30	4054	9.7	5350
30	4000	50	3643	19.8	4360
		60	3517	30.7	3580
bp/°C	151.2–151.3	65	3597	39.7	3430
d ²⁵	0.8115	75	3871	49.8	3360
				60.2	3330
				70.1	3140
				80.2	3480
				90.5	3530

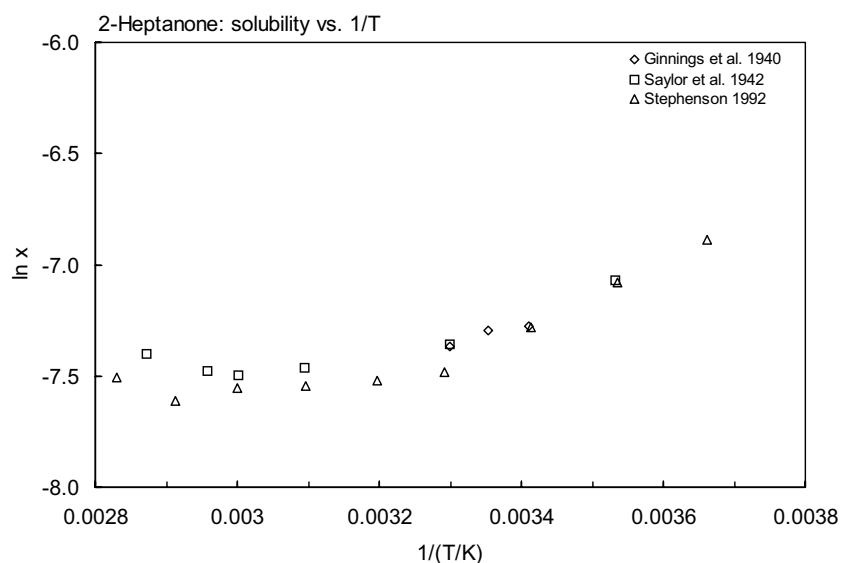
FIGURE 12.1.2.7.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-heptanone.

TABLE 12.1.2.7.2

Reported vapor pressures of 2-heptanone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stuckey & Saylor 1940		Stull 1947		Ambrose et al. 1975(a)			
static method-Hg manometer		summary of literature data		comparative ebulliometry			
t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	P/Pa
						cont'd	
data presented as		19.3	133.3	54.687	2818	151.949	103789
eq. 3	P/mmHg	43.5	666.6	57.076	3180	157.300	119605
A	7.36537	55.5	1333	60.142	3697	162.280	136005
B	1650.47	67.7	2666	64.213	4500	168.137	157388
C	-54.48	81.2	5333	67.814	5324	173.697	180116
		89.8	7999	71.989	6433	179.267	205316
		100.0	13332	71.991	6436	25.0	427
		116.1	26664	75.736	7617		
Saylor et al. 1942		133.2	53329	79.945	9127	bp/^{\circ}\text{C}	151.058
Stuckey & Saylor data		150.2	101325	84.035	10826		
10	188	mp/^{\circ}\text{C}	-	88.302	12873	Antoine eq. for full range:	
30	709			92.564	15282	eq. 3	P/kPa
50	1973			95.832	17932	A	6.15034
60	3733			102.322	21975	B	1462.981
65	4720			107.012	25997	C	-71.24
75	7413			112.377	31321	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				117.486	37167	at 25^{\circ}\text{C}	38.3
				117.629	37361	at bp	33.2
				123.186	44713		
				129.297	54129	Antoine eq. for restricted	
				134.589	63526	range of atm. pressure:	
				140.221	74904	eq. 3	P/kPa
				146.323	88989	A	6.15033
				150.976	101114	B	1463.072
						C	-71.200

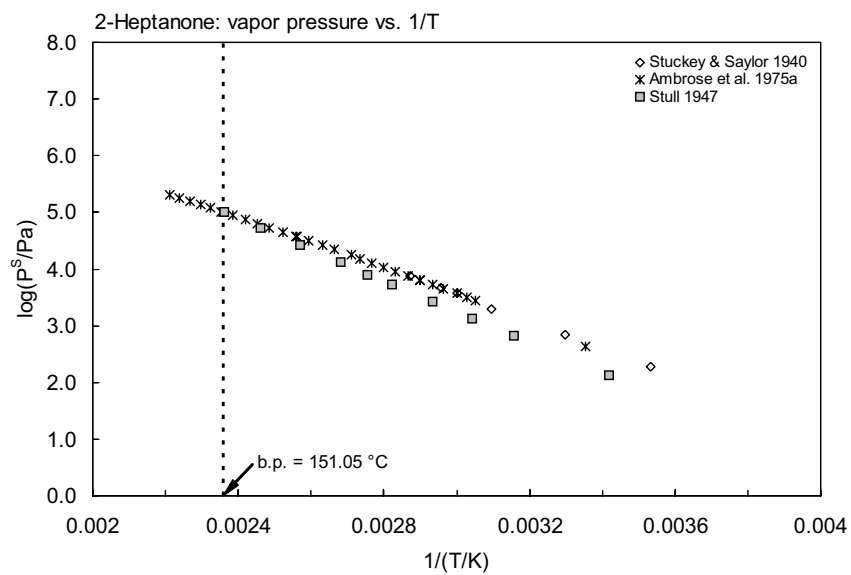
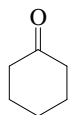


FIGURE 12.1.2.7.2 Logarithm of vapor pressure versus reciprocal temperature for 2-heptanone.

12.1.2.8 Cyclohexanone



Common Name: Cyclohexanone

Synonym:

Chemical Name: cyclohexanone

CAS Registry No: 108-94-1

Molecular Formula: C₆H₁₀O

Molecular Weight: 98.142

Melting Point (°C):

-27.9 (Lide 2003)

Boiling Point (°C):

155.43 (Lide 2003)

Density (g/cm³ at 20°C):

0.9478 (Weast 1982–83; Dean 1985)

0.9452 (Riddick et al. 1986)

Molar Volume (cm³/mol):

106.2 (calculated-density, Stephenson & Malanowski 1987)

118.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

23000 (Riddick et al. 1986)

93200 (selected, Yaws et al. 1990)

97000*, 82000 (19.5°C, 29.8°C, shake flask-GC, measured range 0–90.7°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* (26.4°C, summary of literature data, temp range 1.4–155.6°C, Stull 1947)

$\log (P/\text{mmHg}) = [-0.2185 \times 10037.6/(T/K)] + 8.019908$; temp range 1.4–155.6°C, (Antoine eq., Weast 1972–73)

533* (ebulliometry-fitted to Antoine eq., temp range 89.6–165.8°C, Meyer & Hotz 1973)

$\log (P/\text{mmHg}) = 5.978401 - 1495.511/(209.5517 + t/^{\circ}\text{C})$; temp range 89.6–165.8°C (Antoine eq. ebulliometric measurements, Meyer & Hotz 1973)

614 (interpolated-Cox eq., Chao et al. 1983)

$\log (P/\text{mmHg}) = [1 - 428.587/(T/K)] \times 10^{0.833332 - 6.42578 \times 10^{-4} \cdot (T/K) + 7.09855 \times 10^{-7} \cdot (T/K)^2}$; temp range: 274.55–438.92 K (Cox eq., Chao et al. 1983)

533 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.10133 - 1494.166/(209.399 + t/^{\circ}\text{C})$, temp range 89.29–165.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

640 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.103304 - 1495.511/(209.5517 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

620, 534 (calculated-Antoine eq.-I, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 8.434 - 2576.6/(T/K)$; temp range not specified (Antoine eq., solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.103304 - 1495.511/(-63.5983 + T/K)$, temp range 362–439 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 70.5022 - 4.412 \times 10^3/(T/K) - 23.605 \cdot \log (T/K) + 1.1205 \times 10^{-2} \cdot (T/K) - 1.5648 \times 10^{-13} \cdot (T/K)^2$; temp range 242–629 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1.216	(Hawthorne et al. 1985)
2.266	(calculated-P/C, Meylan & Howard 1991)
5.179	(estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.81	(shake flask, Hansch & Leo 1979, 1985, 1987)
0.81	(recommended, Sangster 1989, 1993)
0.81	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.39	(calculated- K_{OW} with regression eq., Lyman et al. 1982; quoted, Howard 1990)
------	---

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.00	(calculated-S, K_{OW} with regression eq., Roy & Griffin 1985; quoted, Howard 1990)
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Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 3.1$ d from a model river 1-m deep flowing 1 m s^{-1} with wind velocity of 3 m s^{-1} (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: direct sunlight photolysis rate constant of about 0.16 d^{-1} corresponding to $t_{1/2} = 4.3$ d (Mill & Davenport 1986; quoted, Howard 1990).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 24$ h to 9.9 d in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}} = 1.56 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} \sim 1$ d (Atkinson 1985; quoted, Howard 1990)

$k_{\text{OH}} = 6.39 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{\text{OH}} = 12.55 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ from Atmospheric Oxidation Program, $k_{\text{OH}}(\text{exptl}) = 6.39 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{\text{OH}}(\text{calc}) = 2.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ from Fate of Atmospheric Pollutants Program, (Meylan & Howard 1993)

$k_{\text{OH}}(\text{calc}) = 5.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation $51.5 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 24$ h to 9.9 d in air for the gas-phase reaction with hydroxyl radicals, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976);

degrade rapidly by reaction with sunlight produced hydroxyl radicals with $t_{1/2} \sim 1$ d and by direct sunlight photolysis with $t_{1/2} \sim 4.3$ d (Howard 1990).

Surface water: estimated $t_{1/2} \sim 0.003$ yr at Noordwijk (Zoeteman et al. 1981).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.8.1

Reported vapor aqueous solubilities and vapor pressures of cyclohexanone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)		
$\log P = A - B/(C + T/K)$	(3)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)				
$\log (P/\text{atm}) = A'[1 - (T_{\text{B}}/T)]$	(5)	where $A' = (a + bT + cT^2)$			
Aqueous solubility		Vapor pressure			
Stephenson 1992	Stull 1947	Meyer & Hotz 1973			
shake flask-GC/TC	summary of literature data	comparative ebulliometry			
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
0	137000	1.40	133.3	89.628	12725
9.8	115000	26.4	666.6	94.986	15528
19.5	97000	38.7	1333	100.807	19257
29.8	82000	52.5	2666	107.664	24477
40.1	75000	67.8	5333	114.303	30580
50.2	70000	77.5	7999	119.712	36416
60.5	67000	90.4	13332	125.282	43337
71.1	65000	110.3	26664	130.659	50990
80.2	68000	132.5	53329	135.774	59239
90.7	69000	155.6	101325	141.742	70181
				145.880	78656
		mp/°C	−45.0	151.916	92474
				151.969	92593
				156.917	105300
				156.988	105417
				165.769	131422
				bp/°C	155.422
				Antoine eq.	
				eq. 2	P/cmHg
				A	5.978401
				B	1495.511
				C	209.5517
				Cox eq.	
				eq. 5	P/atm
				a	0.852046
				−b × 10 ³	0.612660
				c × 10 ⁶	0.504661
				T _B /K	428.5716

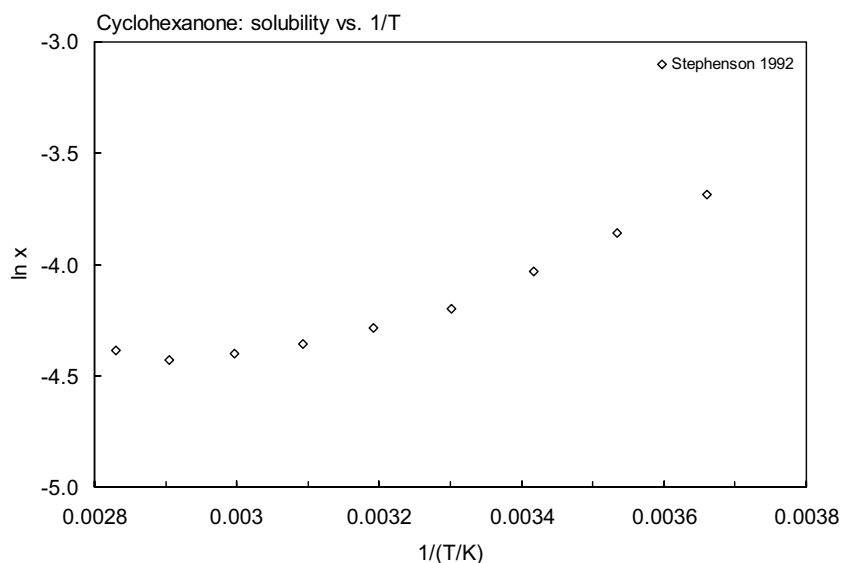
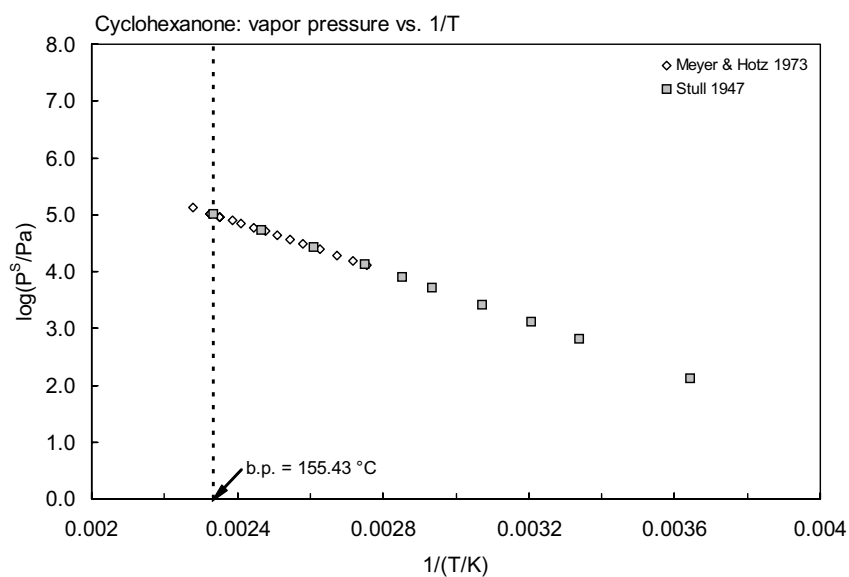
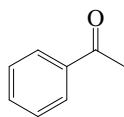


FIGURE 12.1.2.8.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cyclohexanone.



12.1.2.9 Acetophenone



Common Name: Acetophenone

Synonym: 1-phenylethanone, methyl phenyl ketone, acetylbenzene, phenylmethylketone, hyponone

Chemical Name: acetophenone, methyl phenyl ketone

CAS Registry No: 98-86-2

Molecular Formula: C_8H_8O , $C_6H_5COCH_3$

Molecular Weight: 120.149

Melting Point ($^{\circ}C$):

20.5 (Stull 1947; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

202 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0281 (Dreisbach 1955; Weast 1982–83; Riddick et al. 1986)

1.02382 ($25^{\circ}C$, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm^3/mol):

117.1 (calculated-density, Rohrschneider 1973)

140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

42.0, 53.41 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

16.65 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

42.26 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5530 (shake flask-centrifuge, Booth & Everson 1948)

6300 (shake flask-UV, Andrews & Keefer 1950)

6022 (estimated, McGowan 1954)

5540 ($24^{\circ}C$, shake flask-LSC, Means et al. 1980)

5500 (Verschuereen 1983; Dean 1985, 1992)

6130 (Southworth & Keller 1986)

5620* ($19.9^{\circ}C$, shake flask-GC/TC, measured range 19.9 – $80.1^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

266.6* ($50.2^{\circ}C$, static method-manometer, measured range 50.2 – $201.5^{\circ}C$, Kahlbaum 1898)

66.21* (extrapolated-regression of tabulated data, temp range 37.1 – $202.4^{\circ}C$, Stull, 1947)

49.53 (calculated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.15738 - 1723.46/(201.0 + t/^{\circ}C)$; temp range 102 – $330^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

41.30 (Hoy 1970)

$\log (P/mmHg) = [-0.2185 \times 11731.5/(T/K)] + 8.293248$; temp range 37.1 – $202.4^{\circ}C$ (Antoine eq., Weast 1972–73)

57.48 (extrapolated-Cox eq., Chao et al. 1983)

$\log (P/mmHg) = [1 - 474.823/(T/K)] \times 10^{0.859974 - 6.15392 \times 10^{-4} \cdot (T/K) + 6.99110 \times 10^{-7} \cdot (T/K)^2}$; temp range 310.25 – $475.55 K$ (Cox eq., Chao et al. 1983)

52.92 (Daubert & Danner 1985)

40.23 (extrapolated-Antoine eq., Dean 1985)

- log (P/mmHg) = $9.1352 - 2878.8/(T/K)$; temp range 20–100°C (Antoine eq., Dean 1985, 1992)
 49.0 (Riddick et al. 1986)
 log (P/kPa) = $6.28228 - 1723.46/(201.0 + t/°C)$, temp range not specify (Antoine eq., Riddick et al. 1986)
 45.3 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 log (P_L /kPa) = $6.28228 - 1723.46/(-72.15 + T/K)$; temp range 375–603 K (Antoine eq., Stephenson & Malanowski 1987)
 45.00 (selected, Mackay et al. 1992, 1995; quoted, Shiu & Mackay 1997)
 log (P/mmHg) = $55.5798 - 4.5101 \times 10^3/(T/K) - 17.284 \cdot \log (T/K) + 6.4184 \times 10^{-3} \cdot (T/K) + 6.5557 \times 10^{-13} \cdot (T/K)^2$;
 temp range 293–701 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1.082 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 0.784 (calculated-bond contribution, Hine & Mookerjee 1975)
 0.921* (25.1°C, gas stripping-GC, measured range 14.9–35°C, Betterton 1991)
 0.753 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 1.080, 0.982 (gas stripping-GC, calculated-P/C, Shiu & Mackay 1997)
 1.06* (EPICS-UV spectroscopy, measured range 5–25°C, Allen et al. 1998)
 $\ln K_{AW} = -9100/(T/K) + 22.47$ (EPICS-UV, temp range 5–25°C, Allen et al. 1998)
 0.560 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 7.307 - 3202/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} :

- 1.58 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1969, 1971; Hansch & Leo 1985)
 1.58 (calculated- π const., Iwasa et al. 1965)
 1.73 (shake flask-UV, Chapman et al. 1972)
 1.58 (HPLC-RT correlation, Lazare et al. 1974)
 1.68 (shake flask-UV, Holmes & Lough 1976)
 1.66 ± 0.08 (shake flask at pH 7, Unger et al. 1978)
 1.66 (Hansch & Leo 1979)
 1.59 (shake flask-GC, Khan et al 1979)
 1.59 (shake flask-LSC, Means et al. 1980)
 1.58 (shake flask-HPLC, Nahum & Horvath 1980)
 1.75 (calculated-f const., Rekker's method, Hanai et al. 1981)
 1.77, 1.56 (HPLC- k' correlation, McDuffie 1981)
 1.80 (HPLC-RT correlation, Hammers et al. 1982)
 1.83 (RP-LC-RT correlation, Hanai & Hubert 1982)
 1.56 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 1.63 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)
 1.65 (inter-laboratory studies, HPLC average, Eadsforth & Moser 1983)
 1.65; 1.68 ± 0.02 (selected best lit. value; exptl.-ALPM, Garst & Wilson 1984)
 1.59; 1.72 (HPLC-RT correlation; HPLC average, Eadsforth 1986)
 1.71 (HPLC-RT correlation, Ge et al. 1987)
 1.65 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 1.60 (shake flask-CPC, Berthod et al. 1988)
 1.58 (RP-HPLC- k' correlation, Minick et al. 1988)
 1.63 (recommended, Sangster 1989, 1993)
 1.59 (CPC centrifugal partition chromatography, Gluck & Martin 1990)
 1.56 (shake flask-UV spec., Alcorn et al. 1993)
 1.58 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 0.699–0.954 (estimated- K_{OW} and S, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, log K_{OC} :

- 1.544 (average of 3 sediments and soil samples, equilibrium sorption isotherm, Means et al. 1980)
- 1.380 (calculated, Means et al. 1980)
- 1.89 (calculated-MCI χ , Gerstl & Helling 1987)
- 1.630 (soil, quoted, Sabljic 1987)
- 1.73 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)
- 1.34–2.43 (soils and sediments, quoted exptl. and estimated values, Howard 1993)
- 1.26 (calculated- K_{OW} , Kollig 1993)
- 1.54 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.79, 1.63 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 1.61, 1.50, 1.80 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
- 1.56, 1.55 (sediments: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on calculated Henry's law constant, $t_{1/2} \sim 3.8$ d from a model river of 1-m deep flowing at 1 m s^{-1} with a wind velocity of 3 m s^{-1} (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$$k_{OH} = (2.74 \pm 0.15) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1989)}$$

$k_{OH}(\text{calc}) = 1.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated from Atmospheric Oxidation Program; $k_{OH}(\text{exptl}) = 2.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated from Fate of Atmospheric Pollutants Program with OH radical in vapor phase (Meylan & Howard 1993)

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 2.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation: biodegradation rate constant $k = 0.029\text{--}0.042 \text{ h}^{-1}$ in 30 mg L^{-1} activated sludge after a time lag of 15–20 h (Urano & Kato 1986b);

rate constants: $k = 0.022 \text{ d}^{-1}$ in ground water, $k = 0.083 \text{ d}^{-1}$ in river waters and $k = 0.155 \text{ d}^{-1}$ in Superior harbor waters (Vaishnav & Babeu 1987).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated photooxidation $t_{1/2} \sim 22$ d in atmosphere, based on the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson 1988; quoted, Howard 1993); atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: biodegradation $t_{1/2} = 8$ d in river water and $t_{1/2} = 4.5$ d in lake water (Vaishnav & Babeu 1986, 1987; quoted, Howard 1993) and $t_{1/2} = 4$ d in Superior harbor waters (Vaishnav & Babeu 1987).

Ground water: biodegradation $t_{1/2} = 32$ d (Vaishnav & Babeu 1986, 1987; quoted, Howard 1993); estimated $t_{1/2} \sim 0.01$ yr at Noordwijk (Zoeteman et al. 1981).

Sediment:

Soil:

Biota:

TABLE 12.1.2.9.1
Reported aqueous solubilities and Henry’s law constants of acetophenone at various temperatures

Aqueous solubility		Henry’s law constant			
Stephenson 1992		Betterton 1991		Allen et al. 1998	
shake flask-GC/TC		gas stripping-GC		EPICS-UV	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
19.9	5620	14.9	0.582	15	0.263
29.5	7100	25.1	0.921	17.5	0.362
39.5	8330	35.0	2.068	20	0.463
49.8	8140	45.0	4.053	25	1.065
60.1	8880	$\Delta H/(\text{kJ mol}^{-1}) = -50.5$		$\ln K_{\text{AW}} = A - B/(T/\text{K})$ eq. 1 K_{AW} A -9100 B 22.47 $\Delta H/(\text{kJ mol}^{-1}) = -75.6$ $\Delta S/(\text{J K}^{-1} \text{mol}^{-1}) = 186.9$	
70.2	9920				
80.1	12040				

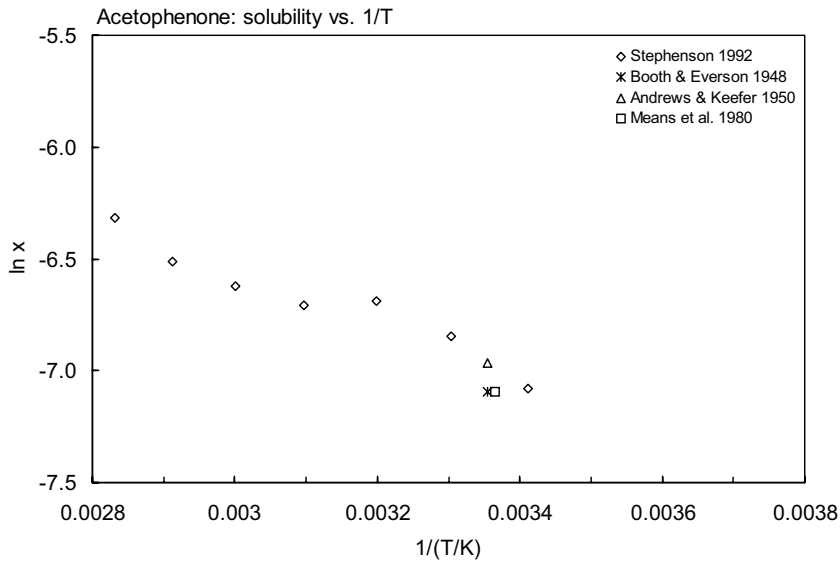


FIGURE 12.1.2.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for acetophenone.

TABLE 12.1.2.9.2

Reported vapor pressures of acetophenone at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Kahlbaum 1898		Stull 1947	
static method-manometer*		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
50.2	266.6	37.1	133.3
56.0	400.0	64.0	666.6
61.0	533.3	78.0	1333
65.0	666.6	92.4	2666
79.0	1333.2	109.4	5333
87.3	1999.8	119.8	7999
93.4	2666.4	133.6	13332
102.4	3999.7	154.2	26664
109.7	5332.9	178.0	53329
114.7	6666.1	202.4	101325
125.2	9999.2		
133.2	13332	mp/°C	20.5
154.1	26664		
167.6	39997		
177.7	53329		
185.7	66661		
192.5	79993		
198.5	93326		
201.5	101325		

*complete list see [ref.](#)

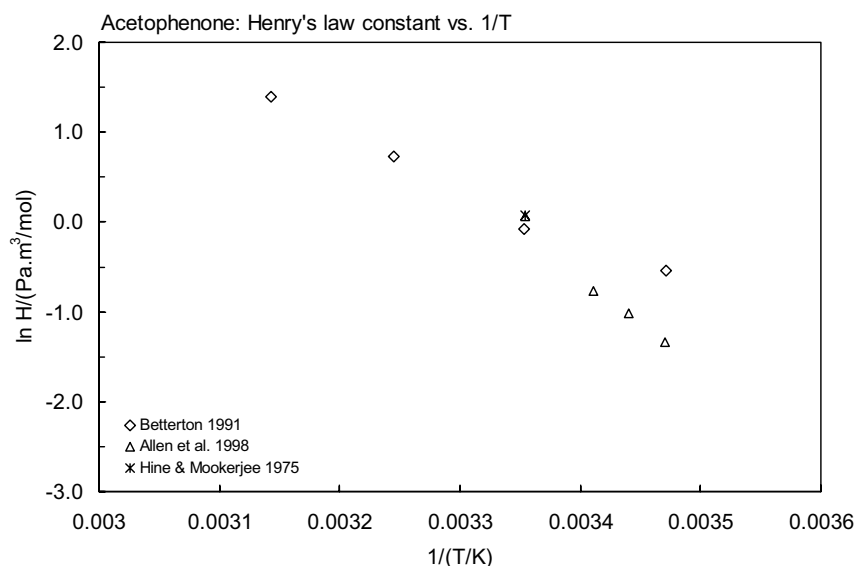


FIGURE 12.1.2.9.2 Logarithm of Henry's law constant versus reciprocal temperature for acetophenone.

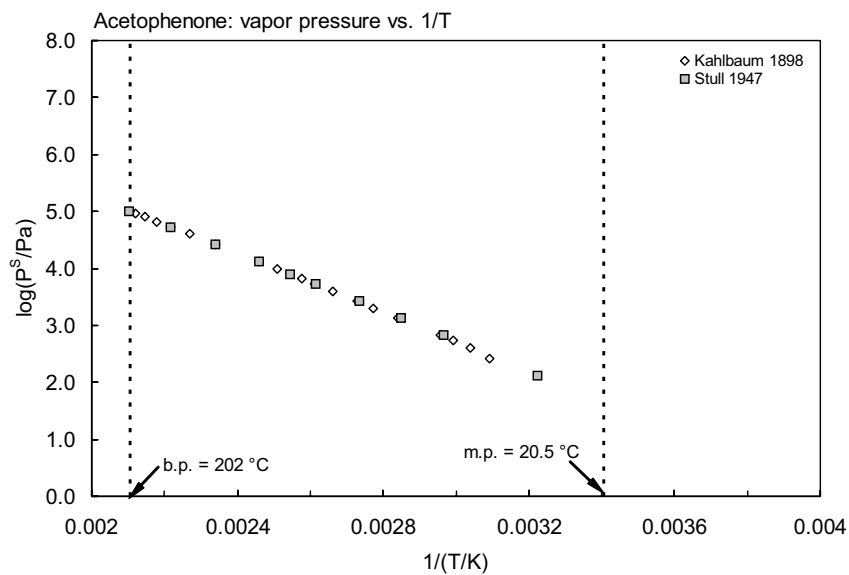
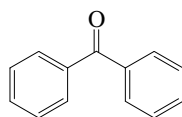


FIGURE 12.1.2.9.3 Logarithm of vapor pressure versus reciprocal temperature for acetophenone.

12.1.2.10 Benzophenone



Common Name: Benzophenone

Synonym: diphenyl ketone, diphenyl methanone

Chemical Name: benzophenone, diphenyl ketone

CAS Registry No: 119-61-9

Molecular Formula: $C_{13}H_{10}O$, $C_6H_5COC_6H_5$

Molecular Weight: 182.217

Melting Point ($^{\circ}C$):

48.1 (α , Weast 1982–83; Dean 1985)

26.0 (β , Weast 1982–83; Dean 1985)

47.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

305.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.6077 (α , $19^{\circ}C$, Weast 1982–83)

1.6059 (β , $23^{\circ}C$, Weast 1982–83)

1.111 ($18^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

206.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Vaporization, ΔH_v (kJ/mol):

53.38, 81.90 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

16.99 (Dreisbach 1955)

13.36 (Yalkowsky & Valvani 1980)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.596 (mp at $47.9^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

20720, 21000 (calculated- ΔS_{fus} and mp, estimated, Yalkowsky & Valvani 1980)

276 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)

77.7 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

33330* ($257.15^{\circ}C$, temp range 257.15 – $302.85^{\circ}C$, Jaquerod & Wassher 1904; quoted, Boublik et al. 1984)

0.617* (extrapolated-regression tabulated data, temp range 108.3 – $305.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.81086 - 2643.0/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

6287* ($200.50^{\circ}C$, ebulliometry, measured range 200.50 – $306.1^{\circ}C$, Dreisbach & Shrader 1949)

1.242 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.28937 - 2144.6/(181.0 + t/^{\circ}C)$; temp range 1980 – $600^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 14725.4/(T/K)] + 8.456678$; temp range 108.2 – $305.4^{\circ}C$ (Antoine eq., Weast 1972–73)

3.146* ($55.9^{\circ}C$, effusion method, measured range 55.9 – $71.2^{\circ}C$, DePablo 1976)

0.086, 0.0115 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.2931 - 2056.386/(173.545 + t/^{\circ}C)$, temp range 200.5 – $306.1^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.37814 - 2127.915/(181.209 + t/^{\circ}C)$, temp range 257.1 – $302.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.080 (extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.34966 - 2331.4/(195.0 + t/^{\circ}\text{C})$, temp range 48–202°C (Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.16294 - 2051.855/(173.074 + t/^{\circ}\text{C})$; temp range 200–306°C (Antoine eq., Dean 1985, 1992)

0.086, 0.095 (interpolated-eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 12.44989 - 4924.329/(T/\text{K})$; temp range 293–318 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 11.736 - 4698/(T/\text{K})$; temp range 298–318 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.41427 - 2144.6/(-92.15 + T/\text{K})$; temp range 433–673 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 16.4144 - 3.8064 \times 10^3/(T/\text{K}) - 2.3984 \cdot \log (T/\text{K}) - 7.4544 \times 10^{-4} \cdot (T/\text{K}) + 2.9345 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 321–816 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.18 (shake flask-UV, Leo et al. 1971)

3.58 (shake flask-UV, Holmes & Lough 1976)

3.10 (shake flask-UV, Unger & Chiang 1981)

3.02 (HPLC- k' correlation, McDuffie 1981)

3.03 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)

3.18 (recommended, Sangster 1989, 1993)

3.18 (recommended, Hansch et al. 1995)

3.09 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

3.32 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

2.63 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 12.1.2.10.1

Reported vapor pressures of benzophenone at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Jaquerod & Wassher 1904		Stull 1947		Dreisbach & Shrader 1949		DePablo 1976	
in Boublik et al. 1984#		summary of lit. data		ebulliometry		effusion method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
257.15	33330	108.2	133.3	200.50	6287	55.9	3.146
260.05	35997	141.7	666.6	206.42	7605	60.7	4.280
265.56	41330	157.6	1333	211.76	8851	66.9	7.146
270.65	46663	175.8	2666	215.46	10114	71.2	9.533
275.23	51996	195.7	5333	231.57	16500		
280.40	58662	208.2	7999	266.87	42066		
285.11	65328	224.4	13332	287.23	67661		
290.26	73327	249.8	26664	306.1	101325		
295.00	81326	276.8	53329				
300.11	91992	305.4	101325				
302.85	95992						
complete data set see ref.		mp/°C	48.5	Antoine eq. given by Dreisbach & Martin 1949			
eq. in Boublik et al. 1984				Eq. 2	P/mmHg		
eq. 2				A	7.81086		
A				B	2643.0		
B				C	230		
C				bp/°C	306.10		
bp/°C				mp/°C	47.93		

Jaquerod, A. Wassher, E. Ber. 3, 2531 (1904)

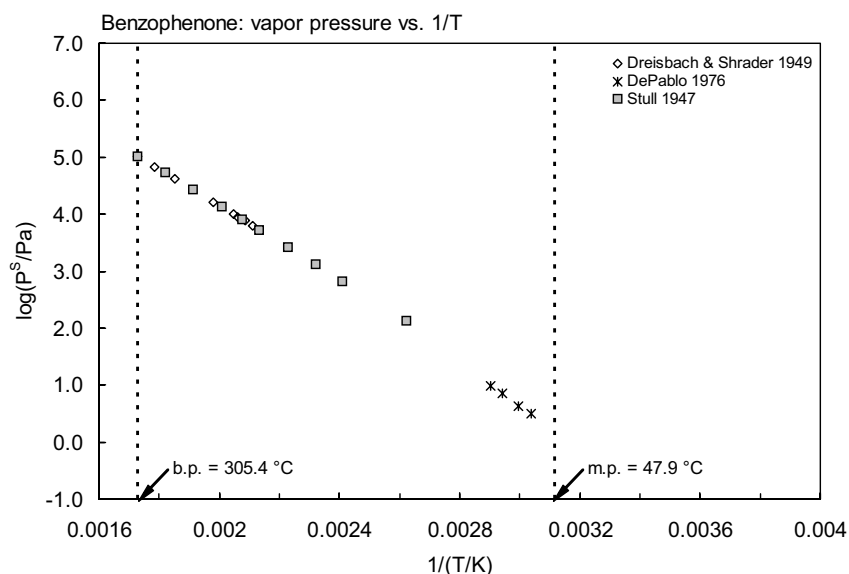


FIGURE 12.1.2.10.1 Logarithm of vapor pressure versus reciprocal temperature for benzophenone.

12.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 12.2.1

Summary of physical properties of aldehydes and ketones

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm³/mol	
							MW/ρ at 20°C	Le Bas cm³/mol
Aldehydes:								
Methanal (Formaldehyde)	50-00-0	HCHO	30.026	−92	−19.1	1		29.6
Ethanal (Acetaldehyde)	75-07-0	CH ₃ CHO	44.052	−123.37	20.1	1	56.23#	51.8
Propanal (Propionaldehyde)	123-38-6	C ₂ H ₅ CHO	58.079	−80	48	1	72.87	74.0
Butanal (<i>n</i> -Butyraldehyde)	123-72-8	C ₃ H ₇ CHO	72.106	−96.86	74.8	1	89.95	96.2
Isobutyraldehyde	78-84-2	<i>i</i> C ₃ H ₇ CHO	72.106	−65.9	64.5	1	91.38	96.2
Pentanal (<i>n</i> -Valeraldehyde)	110-62-3	C ₄ H ₉ CHO	86.132	−91.5	103	1	106.40	118.4
Hexanal	66-25-1	C ₅ H ₁₁ CHO	100.158	−56	131	1	120.17	140.6
Heptanal	111-71-7	C ₆ H ₁₃ CHO	114.185	−43.4	152.8	1	140.41**	162.8
Octanal	124-13-0	C ₇ H ₁₅ CHO	128.212		171	1	156.15	185.0
2-Propenal (Acrolein)	107-02-8	H ₂ C=CHCHO	56.063	−87.7	52.6	1	66.83	66.6
2-Butenal	123-73-9	CH ₃ CH=CHCHO	70.090	−76	102.2	1	82.30	88.8
Furfural (2-Furaldehyde)	98-01-1	C ₅ H ₄ O ₂	96.085	−38.1	161.7	1	82.83	92.1
Benzaldehyde	100-52-7	C ₆ H ₅ CHO	106.122	−57.1	178.8	1	101.59	118.2
Ketones:								
Acetone	67-64-1	CH ₃ COCH ₃	58.079	−94.7	56.05	1	73.53	74.0
2-Butanone (Methyl ethyl ketone)	78-93-3	C ₂ H ₅ COCH ₃	72.106	−86.64	79.59	1	89.53	96.2
2-Pentanone	107-87-9	C ₃ H ₇ COCH ₃	86.132	−76.8	102.26	1	106.81	118.4
3-Pentanone	96-22-0	CH ₃ CH ₂ COCH ₂ CH ₃	86.132	−39	101.7	1	105.77	118.4
Methyl isobutyl ketone (MIBK)	108-10-1	(CH ₃) ₂ CHCH ₂ COCH ₃	100.158	−84	116.5	1	125.04	140.6
2-Hexanone	591-78-6	C ₄ H ₉ COCH ₃	100.158	−55	127.6	1	123.45	140.6
2-Heptanone	110-43-0	CH ₃ (CH ₂) ₄ COCH ₃	114.185	−35	151.05	1	140.04	162.8
2-Octanone	111-13-7	C ₇ H ₁₆ CO	128.212	−16	172.5	1	156.36	185.0
Cyclopentanone	120-92-3	C ₄ H ₈ CO	84.117	−51.90	130.57	1	88.67	99.5
Cyclohexanone	108-94-1	C ₅ H ₁₀ CO	98.142	−27.9	155.43	1	103.83	118.2
Acetophenone	98-86-2	C ₆ H ₅ COCH ₃	120.149	20.5	202	1	116.87	140.4
Benzophenone	119-61-9	C ₆ H ₅ COC ₆ H ₅	182.217	47.9	305.4	0.596	164.01#	206.8

* Assuming ΔS_{fus} = 56 J/mol K; # at 18°C; ** at 25°C.

TABLE 12.2.2
Summary of selected physical-chemical properties of aldehydes and ketones at 25°C

Compound	Selected properties					Henry's law constant H/(Pa·m³/mol)				
	Solubility		Vapor pressure		log K _{OW}	calcd P/C	exptl (a)	exptl (b)	exptl (c)	exptl (c)
	S/(g/m³)	C _L /(mol/m³)	P _S /Pa	P _L /Pa						
Aldehydes:										
Methanal	miscible	miscible	517000	517000	0.35			0.0298		0.0341
Ethanal	miscible	miscible	121300	121300	0.45		6.69	6.80	8.00	8.90
Propanal	310000	5338	42400	42400	0.59	7.944	7.44	8.40	7.51	
Butanal	71000	984.7	15200	15200	0.88	15.44	11.65	11.65		
<i>n</i> -Valeraldehyde			2180	2180			14.87	15.59		
Hexanal	5020	50.12			1.78		21.57	19.49		
2-Propenal (Aroclein)	208000	3710	36500	36500	−0.10	9.838	13.37		13.17	
2-Butenal	15600	222.6	5100	5100		22.91				
Furfural	79400	826.4	310	310	0.41	0.3751				
Benzyldehyde	3000	28.27	174	174	1.48	6.155	2.28			2.71
Ketones:										
Acetone	miscible	miscible	30806	30800	−0.24		3.97		3.93	3.07
2-Butanone	240000	3328.4	12100	12100	0.29	3.635	9.71		5.76	
2-Pentanone	59500	690.8	4720	4720	0.84	6.833	6.44			
3-Pentanone	34000	394.7	4700	4700	0.82	11.91				
Methyl isobutyl ketone	17000	169.7	2600	2600		15.32				
2-Hexanone	17500	174.7	1600	1600	1.38	9.157				
2-Heptanone	4300	37.66	500	500	2.08	13.28	14.73			
2-Octanone	1130	8.814	180	180	2.37	20.42	19.09			
Cyclopentanone			1540	1540						
Cyclohexanone	23000	234.4	620	620	0.81	2.646				
Acetophenone	5500	45.78	45	45	1.63	0.983				0.92
Benzophenone	276	2.541	0.09	0.151	3.18	0.059				

(a) Butler et al. 1935, Buttery et al. 1969; (b) Zhou & Mopper 1990; (c) Snider & Dawson 1985; (d) Betterton & Hoffmann 1988.

TABLE 12.2.3

Suggested half-life classes for aldehydes and ketones at various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aldehydes:				
Methanal (Formaldehyde)	1	3	3	4
Ethanal (Acetaldehyde)	1	3	3	4
Propanal (Propionaldehyde)	1	3	3	4
Butanal (<i>n</i> -Butyraldehyde)	1	3	3	4
2-Propenal (Acrolein)	1	3	3	4
2-Butenal	1	3	3	4
Furfural (2-Furaldehyde)	1	3	3	4
Benzaldehyde	1	3	3	4
Ketones:				
Acetone	4	3	4	5
2-Butanone (Methyl ethyl ketone)	4	3	3	5
2-Pentanone	3	4	4	5
3-Pentanone	3	4	4	5
Methyl isobutyl ketone (MIBK)	3	4	4	5
2-Hexanone	3	4	4	5
2-Heptanone	3	4	4	5
Cyclohexanone	3	4	4	5
Acetophenone	5	4	4	5
Benzophenone	5	4	4	5

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

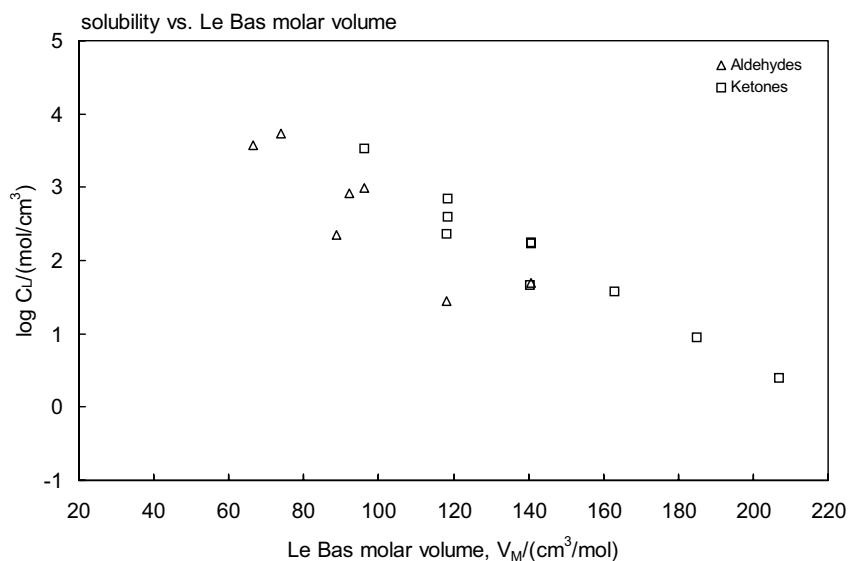


FIGURE 12.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for aldehydes and ketones.

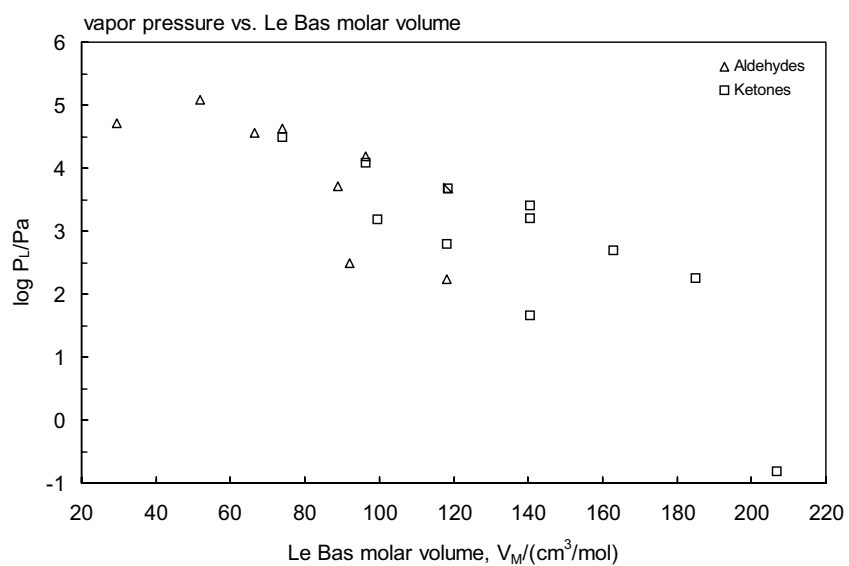


FIGURE 12.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for aldehydes and ketones.

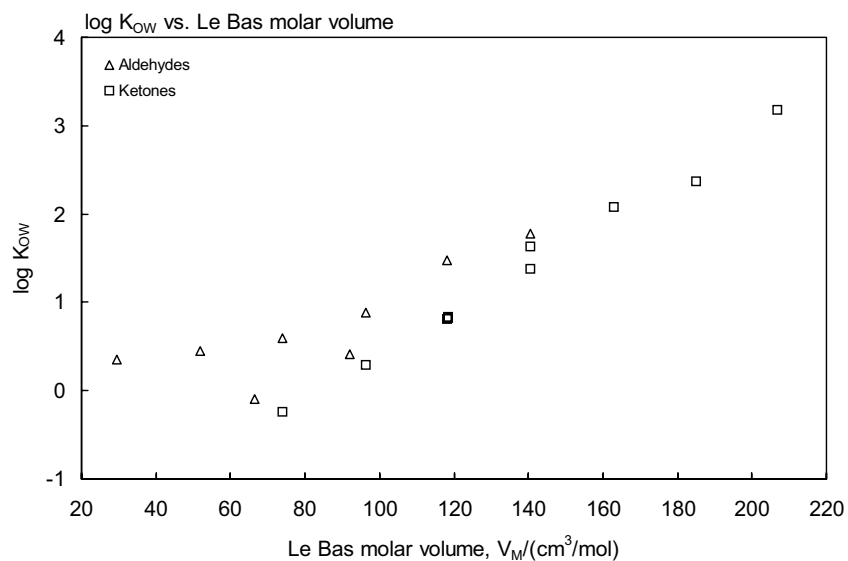


FIGURE 12.2.3 Octanol-water partition coefficient versus Le Bas molar volume for aldehydes and ketones.

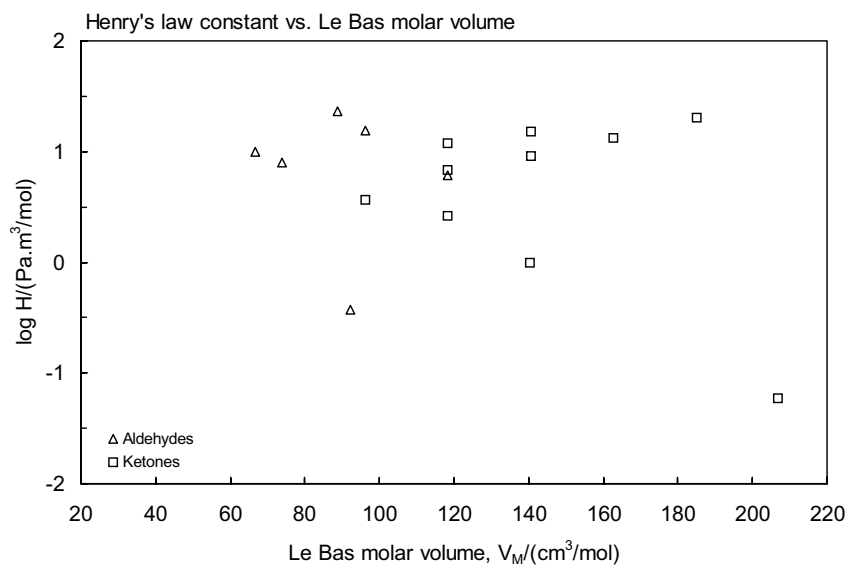


FIGURE 12.2.4 Henry's law constant versus Le Bas molar volume for aldehydes and ketones.

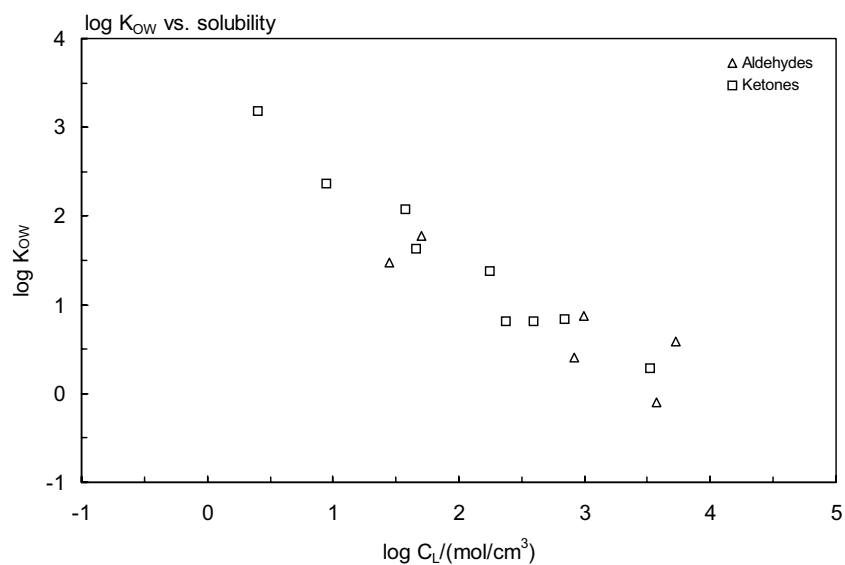


FIGURE 12.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for aldehydes and ketones.

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13 Carboxylic Acids

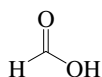
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13.1 LIST OF CHEMICALS AND DATA COMPILATIONS

13.1.1 ALIPHATIC ACIDS

13.1.1.1 Formic acid



Common Name: Formic acid

Synonym: methanoic acid

Chemical Name: formic acid

CAS Registry No: 64-18-6

Molecular Formula: CH_2O_2 , HCOOH

Molecular Weight: 46.026

Melting Point ($^{\circ}\text{C}$):

8.3 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

101 (Lide 2003)

Density (g/cm^3 at 20°C):1.21961, 1.21328 (20°C , 25°C , Dreisbach & Martin 1949)

1.2200 (Weast 1982–83; Dean 1985)

1.2141 (25°C , Riddick et al. 1986)Molar Volume (cm^3/mol):

37.7 (calculated-density, Stephenson & Malanowski 1987)

46.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :3.751 (pK_a , Dean 1985)3.752 (pK_a , Riddick et al. 1986)3.740 (pK_a , Sangster 1989)

3.800 (Kollig 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.68 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 13.5 \text{ J}/\text{mol K}$), F: 1.0Water Solubility (g/m^3 or mg/L at 25°C):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4344* (24.6°C , temp range 21.8 – 100.6°C , Kahlbaum 1894)5333* (24°C , compiled and evaluated data, temp range -20 to 100.6°C , Stull 1947) $\log(P/\text{mmHg}) = 7.15689 - 1414.1/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)10114* (37.75°C , ebulliometry, measured range 37.75 – 100.7°C , Dreisbach & Shrader 1949) $\log(P/\text{mmHg}) = [-0.2185 \times 9896.5/(T/\text{K})] + 8.779337$; temp range -20 to 100.6°C (Antoine eq., Weast 1972–73)4666, 7198 (20°C , 30°C , Verschuereen 1983)

5720, 5744, 4420 (calculated-Antoine eq., Boublik et al. 1984)

 $\log(P/\text{kPa}) = 4.09278 - 539.775/(136.826 + t/^{\circ}\text{C})$; temp range 0.5 – 34.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984) $\log(P/\text{kPa}) = 6.69157 - 1689.096/(259.726 + t/^{\circ}\text{C})$; temp range 37.35 – 100.7°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984) $\log(P/\text{kPa}) = 3.7279 - 295.021/(70.7 + t/^{\circ}\text{C})$; temp range 21 – 100.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- 5744 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.5818 - 1699.2/(260.7 + t/^{\circ}\text{C})$; temp range: 37–101°C (Antoine eq., Dean 1985, 1992)
 5750 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.50280 - 1563.28/(247.06 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 5733* (comparative ebulliometry, measured range 299.8–393 K, Ambrose & Ghiassee 1987)
 $\ln (P/\text{kPa}) = 15.40560 - 3894.764/[(T/\text{K}) - 13.0]$; temp range 299.8–393 K (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghiassee 1987)
 5711 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.611 - 3160/(T/\text{K})$; temp range 268–281 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.5028 - 1563.28/(-26.09 + T/\text{K})$; temp range 283–384 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
 5680, 67850 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 27.9278 - 2.5976 \times 10^3/(T/\text{K}) - 7.2489 \cdot \log (T/\text{K}) + 6.411 \times 10^{-10} \cdot (T/\text{K}) + 3.9421 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 282–580 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

- 0.0181 (calculated, Keene & Galloway 1986)
 0.0274 (calculated, Jacob 1986)
 0.017 (pH 4, Gaffney et al. 1987)
 0.112 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
 0.0076, 0.0098, 0.0178 (24°C, bubble column technique, concn: of 1, 10, 10⁵ ppm, Servant et al. 1991)
 0.0281 (Betterton 1992)
 0.018 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)
 $\ln [k_H/(\text{mol kg}^{-1} \text{atm}^{-1})] = -10.31 + 5634/(T/\text{K})$, temp range 178.15–308.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0183 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)
 0.018–0.028 (calculated-thermodynamic data, Johnson et al. 1996)
 0.0118, 0.00921 (counter-flow packed column technique-ion chromatography; "best" exptl. value, Johnson et al. 1996)
 $\ln [k_H/(\text{M/atm})] = -11.04 + 6100/(T/\text{K})$; temp range 2–35°C (counter-flow packed column measurements, Johnson et al. 1996)
 0.0137 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 0.0107 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 2.914 - 2425/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- −0.54 (shake flask-titration, Collander 1951; quoted, Leo et al. 1971; Hansch et al. 1972; Hansch & Leo 1979)
 −0.54 (shake flask-titration, Whitehead & Geankoplis 1955)
 −0.46 (calculated-f const., Rekker & de Kort 1979)
 −0.54 (recommended, Sangster 1989)
 −0.54 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

- −0.27 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = (3.2 \pm 1.0) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982)

$k = (100 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ at pH 8; $(5 \pm 5) \text{ M}^{-1} \text{ s}^{-1}$ for protonated species; $(100 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2.0–4.0 and 20–23°C (Hoigné & Bader 1983b)

$k_{\text{OH}}^* = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–430 K (flash photolysis-resonance fluorescence, Wine et al. 1985)

$k_{\text{OH}} = (2.95 \pm 0.07) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance absorption, Jolly et al. 1986)

$k_{\text{OH}} = (3.7 \pm 0.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-RF, Dagaut et al. 1988)

$k_{\text{OH}}^* = (2.69 \pm 0.17) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $4.47 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 297–445 K (laser photolysis-resonance absorption, Singleton et al. 1988)

$k_{\text{OH}} = 3.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k(\text{soln}) = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}}^* = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 7.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.1.1.1

Reported vapor pressures of formic acid at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3) \quad \ln (P/\text{Pa}) = A - B/(C + T/K) \quad (3a)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Kahlbaum 1894		Stull 1947		Dreisbach & Shrader 1949		Ambrose & Ghiassie 1987	
Ber. 16, 2476		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
21.8	3312	−20.0	133	37.75	10114	299.789	6188
22.6	3688	−5.0	666.6	48.79	16500	302.006	6876
24.6	4344	2.10	1333	73.55	42066	307.578	8881
27.9	5520	10.3	2666	87.82	67661	308.389	9230
30.5	6621	24.0	5333	100.7	101325	310.035	9896
37.8	9938	32.4	7999			313.764	11668
100.6	101325	43.8	13332	bp/°C	100.7	316.803	13293
		61.4	26664			319.729	15031
		80.3	53329			324.842	18432
		100.6	101325			326.895	20105
						329.030	21830
		mp/°C	8.2			332.807	25236
						336.159	28640
						342.086	35456
						344.582	38845
						346.997	43226
						349.134	45630

TABLE 13.1.1.1.1 (Continued)

Kahlbaum 1894		Stull 1947		Dreisbach & shrader 1949		Ambrose & Ghiassee 1987	
Ber. 16, 2476		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
						350.313	47321
						353.362	52449
						355.215	55868
						↓	↓
						392.654	172035
						298.15	5733
						Antoine eq.	
						eq. 3a	P/kPa
						A	15.40560
						B	3894.764
						C	−13.0
						bp/K	374.04

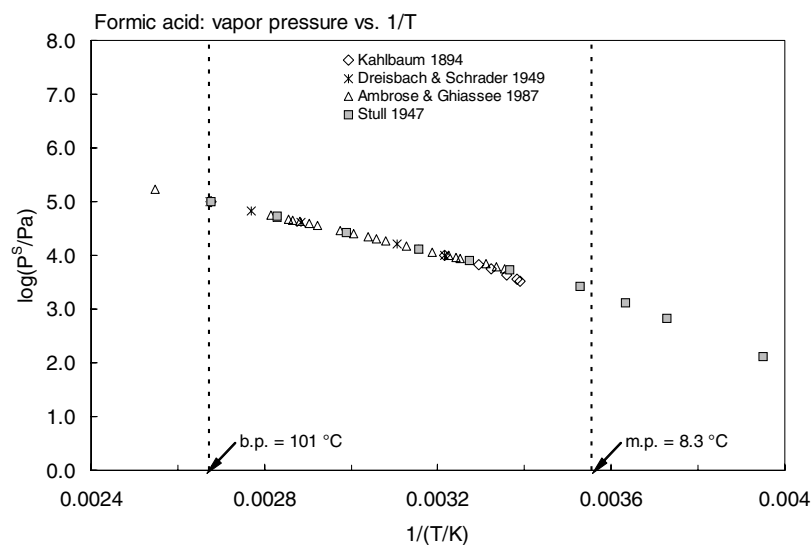


FIGURE 13.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for formic acid.

13.1.1.2 Acetic acid



Common Name: Acetic acid

Synonym: ethanoic acid, methanecarboxylic acid, glacial acetic, vinegar acid

Chemical Name: acetic acid

CAS Registry No: 64-19-7

Molecular Formula: CH_3COOH

Molecular Weight: 60.052

Melting Point ($^{\circ}\text{C}$):

16.64 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

117.9 (Weast 1982–83; Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at 20°C):

1.04923, 1.04365 (20°C , 25°C , Dreisbach & Martin 1949)

1.0492 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

57.1 (calculated-density, Rohrschneider 1973)

68.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.733 (pK_a , Korman & La Mer 1936)

4.760 (pK_a , Fieser & Fieser 1958; Sangster 1989)

4.750 (pK_a , Weast 1982–83; Howard 1990)

4.756 (pK_a , Dean 1985; Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.72 (Ambrose et al. 1977; Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

miscible (Dean 1985; Riddick et al. 1986)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2040* (interpolated-regression of tabulated data, temp range -17.2 – 118°C , Stull 1947)

$\log(P/\text{mmHg}) = 7.45144 - 1589.3/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

10114* (55.75°C , ebulliometry, measured range 55.75 – 117.72°C , Dreisbach & Shrader 1949)

2666* (29.8°C , static method-manometer, measured range 29.8 – 126.45°C , Potter & Ritter 1954)

8297* (52.36°C , ebulliometry, measured range 52.36 – 118.14°C , McDonald et al. 1959)

$\log(P/\text{mmHg}) = 7.55716 - 1642.54/(233.386\text{C} + t/^{\circ}\text{C})$; temp range 52 – 118°C (ebulliometry, McDonald et al. 1959)

2105 (calculated by formula, Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.18807 - 1416.7/(211 + t/^{\circ}\text{C})$, temp range 36 – 170°C , (Antoine eq. for liquid state, Dreisbach 1961)

2030 (Hoy 1970)

$\log(P/\text{mmHg}) = [-0.2185 \times 9963.9/(T/\text{K})] + 8.50200$; temp range -35 to 10°C (Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 9486.6/(T/\text{K})] + 8.142405$; temp range -17.2 to 312.5°C (Antoine eq., Weast 1972–73)

2079* (ebulliometry, fitted to Antoine eq., measured range 304.065 – 415.041 K , Ambrose et al. 1977)

$\log(P/\text{kPa}) = 6.66686 - 1633.288/[(T/\text{K}) - 40.626]$; temp range 351.347 – 415.041 K (Antoine eq.-I, ebulliometry, Ambrose et al. 1977)

- $\log (P/\text{kPa}) = 6.59795 - 1587.182/\{(T/\text{K}) - 45.392\}$; temp range 304.065–415.041 K (Antoine eq.-II, ebulliometry, Ambrose et al. 1977)
 1520, 2666 (20°C, 30°C, Verschuereen 1983)
 2088 (extrapolated average-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.5039 - 1527.764/(221.742 + t/^{\circ}\text{C})$, temp range 29.8–126.45°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.72515 - 1670.427/(236.091 + t/^{\circ}\text{C})$, temp range 52.36–118.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 2050 (calculated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.38782 - 1533.313/(222.309 + t/^{\circ}\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
 2079 (Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.66686 - 1633.288/(232.885 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 2076 (comparative ebulliometry data, Ambrose & Ghassee 1987)
 $\ln (P/\text{kPa}) = 15.19234 - 3654.622/[(T/\text{K}) - 45.392]$ (Antoine eq. Ambrose & Ghassee 1987)
 2114 (calculated-Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 7.672 - 2177/(T/\text{K})$, temp range: 238–283 K, (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 9.9268 - 2847/(T/\text{K})$; temp range 243–289 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.68206 - 1642.54/(-39.764 + T/\text{K})$; temp range 289–392 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.39226 - 2258.22/(2762 + T/\text{K})$; temp range 391–550 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.5729 - 1572.32/(-46.777 + T/\text{K})$; temp range 290–396 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.82561 - 1748.572/(-28.259 + T/\text{K})$; temp range 391–447 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.22638 - 2010.805/(12.244 + T/\text{K})$; temp range 437–535 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.44129 - 3628.409/(182.674 + T/\text{K})$; temp range 525–593 K (Antoine eq.-VIII, Stephenson & Malanowski 1987)
 1520, 32660 (measured, calculated-solvatochromic parameters., Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 28.3756 - 2.9734 \times 10^3/(T/\text{K}) - 7.032 \cdot \log (T/\text{K}) - 1.5051 \times 10^{-9} \cdot (T/\text{K}) + 2.1806 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 290–593 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$) at 25°C and reported temperature dependence equations):

- 0.0303 (partial pressure, Butler & Ramchandani 1935)
 0.0305 (exptl., Hine & Mookerjee 1975)
 0.0300, 0.0280 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.0115 (calculated, Keene & Galloway 1986)
 0.0101 (effective Henry's law constant, pH 4, Gaffney et al. 1987)
 0.0254 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 0.121 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
 0.0101, 1.01×10^{-4} (at pH 4, pH 7, Howard 1990)
 0.0109, 0.00905, 0.0158 (23°C, bubble column technique, concn: 1, 10, 10^5 ppm. Servant et al. 1991)
 0.0184 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)
 $\ln [K_H/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -25.67 + 8322/(T/\text{K})$, temp range 278.15–303.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0285 (calculated-bond contribution, Brimblecombe et al. 1992)
 0.0431 (calculated-molecular structure, Russell et al. 1992)
 0.0182 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)
 0.0115–0.0195 (calculated-thermodynamic data, Johnson et al. 1996)
 0.0245, 0.0145 (counter-flow packed column technique-ion chromatography; "best" exptl value, Johnson et al. 1996)

$\ln [K_H/(M/atm)] = -12.5 + 6200/(T/K)$, temp range 2–35°C (counter-flow packed column measurements, Johnson et al. 1996)

0.0130 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.0154 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 3.650 - 2596/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

-0.30 (shake flask-titration, Leonard et al. 1948)

-0.31 (shake flask-titration, Collander 1951)

-0.29; -0.17 (calculated-fragment const.; calculated- π const., Rekker 1977)

-0.29 (shake flask-radiochemical method, pH 1, Wolfenden 1978)

-0.17, -0.31 (Hansch & Leo 1979)

-0.17 (shake flask, Log P Database, Hansch & Leo 1987)

-0.17 (recommended, Sangster 1989, 1993)

-0.17 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

4.31 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

< 0.0 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

no detectable sorption (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)

0.00 (soil, quoted exptl., Meylan et al. 1992)

-0.21 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

0.00 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (0.6 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 26.7 \text{ d}$ for the vapor-phase reaction with 5×10^5 hydroxyl radical/cm³ in air at 25°C (flash photolysis-resonance fluorescence technique, Zetzsch & Stuhl 1982; quoted, Atkinson 1985)

$k(aq.) \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water; $k \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2.0–5.5 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH}^* = (7.4 \pm 0.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-resonance fluorescence, Dagaut et al. 1988)

$k_{OH} = 7.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air, and $k(soln) = 2.70 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH} = 7.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{OH}(calc) = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996).

Hydrolysis:

Biodegradation: > 90% degradation in 3 d using an activated sludge inoculum; in 24 h in batch aeration in sewage and 14 d using sediment from the Rhine river as inocula (Howard 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 26.7 \text{ d}$, based on measured rate constant of $0.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radicals/cm³ in air at 25°C (Atkinson 1985; quoted, Howard 1990).

Surface water: $t_{1/2} = 26\text{--}46 \text{ yr}$, based on OH radical concn. in sunlit natural water of $1 \times 10^{-17} \text{ mol/L}$ (Howard 1990).

Groundwater:

Sediment: > 90% degradation in 14 d using Rhine River sediment as inocula (Kool 1984; quoted, Howard 1990).

Soil:

Biota:

TABLE 13.1.1.2.1

Reported vapor pressures of acetic acid at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Dreisbach & Shrader 1949		Potter & Ritter 1954		McDonald et al. 1959	
summary of literature data		ebulliometry		static method-manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−17.2	133	55.75	10114	29.8	2666	52.36	8297
6.3	666.6	66.07	16500	40.25	4693	55.63	9998
17.5	1333	91.13	42066	51.08	8013	67.20	16517
29.9	2666	117.72	101325	55.54	9866	91.49	42302
43	5333			60.93	12599	105.49	68210
51.7	7999	bp/°C	100.79	65.50	15332	115.51	94156
63	13332			71.04	19345	116.83	98175
80	26664			75.70	23105	117.27	99584
99	53329			80.41	28038	117.71	110901
118.1	101325			85.69	34224	118.14	102318
				90.59	40930		
mp/°C	16.7			95.66	48982	eq. 2	P/mmHg
				100.29	57488	A	7.55716
				105.45	68314	B	1642.54
				110.0	79193	C	233.386
				115.12	92992		
				118.41	102978	mp/°C	16.34
				122.44	116137		
				123.86	121256		
				126.45	130669		
				Antoine eq.			
				eq. 2	P/mmHg		
				A	7.4275		
				B	1558.03		
				C	224.79		

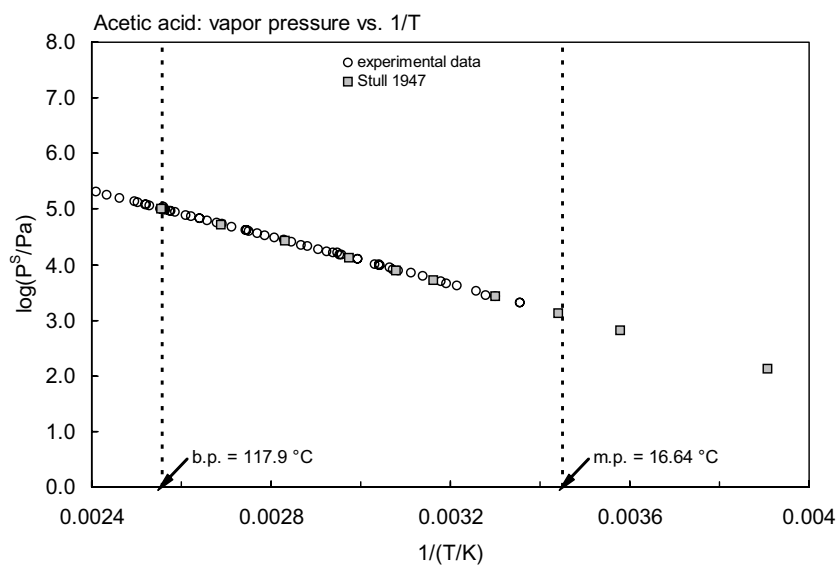
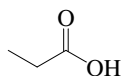


FIGURE 13.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for acetic acid.

13.1.1.3 Propionic acid



Common Name: Propionic acid

Synonym: methylacetic acid, propanoic acid

Chemical Name: propanoic acid, propionic acid

CAS Registry No: 79-09-4

Molecular Formula: $C_3H_6O_2$, CH_3CH_2COOH

Molecular Weight: 74.079

Melting Point ($^{\circ}C$):

−20.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

141.15 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.99336, 0.98797 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

0.9930 (Weast 1982–83)

Molar Volume (cm^3/mol):

74.6 ($20^{\circ}C$, calculated-density)

90.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

−6.80 (pK value, Perrin 1972)

4.874 (Dean 1985; Riddick et al. 1986)

4.870 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.66 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

550* (interpolated-regression of tabulated data, temp range 4.6 – $141.4^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.92234 - 1869.4/(230 + t/^{\circ}C)$, (Antoine eq., Dreisbach & Martin 1949)

7605* ($72.39^{\circ}C$, ebulliometry, measured range 72.39 – $140.80^{\circ}C$, Dreisbach & Shrader 1949)

446 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.35027 - 1497.775/(194.12 + t/^{\circ}C)$, temp range 60 – $185^{\circ}C$ (Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 12454.4/(T/K)] + 9.647835$; temp range 4.6 – $238^{\circ}C$ (Antoine eq., Weast 1972–73)

435* (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.64344 - 1594.723/[(T/K) - 70.545]$; temp range 328 – $438\ K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

500, 442 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.84202 - 1736.007/(218.032 + t/^{\circ}C)$, temp range 72.39 – $128.34^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.67457 - 1615.227/(204.788 + t/^{\circ}C)$, temp range 55.11 – $164.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

257 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.403 - 950.2/(130.3 + t/^{\circ}C)$, temp range 56 – $139.5^{\circ}C$ (Antoine eq., Dean 1985, 1992)

451 (Riddick et al. 1986)

$\log(P/kPa) = 6.64334 - 1594.273/(202.605 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

452 (comparative ebulliometry, Ambrose & Ghiassee 1987)

$\ln (P/\text{kPa}) = 15.29686 - 3670.949/[(T/\text{K}) - 70.545]$, (Antoine eq., Ambrose & Ghiassaei 1987)

$\log (P_L/\text{kPa}) = 6.60267 - 1577.96/(-79.844 + T/\text{K})$, temp range 343–419 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 9.24101 - 12835.99/(-23.07 + T/\text{K})$, temp range 414–511 K (Antoine eq.-II, Stephenson & Malanowski 1987)

453, 8758 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 20.2835 - 3.1165 \times 10^3/(T/\text{K}) - 3.6015 \cdot \log (T/\text{K}) - 1.3892 \times 10^{-3} \cdot (T/\text{K}) + 7.1801 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 252–604 K (vapor pressure eq., Yaws 1994)

14560* (88.37°C, VLE still-manometry, measured range 88.37–140.59°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 18.105654 - 5640.3443/[(t/^\circ\text{C}) + 277.46143]$; temp range 88.37–140.59°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.0445 (partial pressure, Butler & Ramchandani 1935)

0.0450 (exptl., Hine & Mookerjee 1975)

0.0420, 0.0430 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.0298 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

0.0163, 0.00151, 0.0289 (23.1°C, bubble column technique, concn: 1, 10, 10^5 ppm. Servant et al. 1991)

0.0180 (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0431 (calculated-bond contribution, Brimblecombe et al. 1992)

0.0177 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.25 (shake flask-titration, Collander 1951)

0.23, 0.24 (calculated- π const., calculated-fragment const., Rekker 1977)

0.33, 0.25 (Hansch & Leo 1979)

0.27 (shake flask-titration, Umland 1983)

0.33 (recommended, Sangster 1989; 1994)

0.33 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.6 \pm 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982; quoted, Atkinson 1985)

$k = 2.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water, $k \leq 4.0 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k = (1 \pm 0.5) \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2–5 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH}^* = (1.22 \pm 0.12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-RF, Dagaut et al. 1988)

$k_{OH} = 1.22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air and $k(\text{soln}) = 1.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH} = (1.22 - 1.60) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 1.35 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.1.3.1

Reported vapor pressures of propionic acid at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log P = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log P = A – B/(C + T/K)		(3)		ln P = A – B/(C + T/K)		(3a)	
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Ambrose et al. 1981		Clifford et al. 2004	
summary of literature data		ebulliometry		comparative ebulliometry		VLE still-Hg manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
4.60	133.3	72.39	7605	55.174	2891	88.37	14560
28.0	666.6	76.75	8851	57.414	3274	95.22	19580
39.7	1333	79.68	10114	60.143	3787	105.80	29650
52.0	2666	90.73	16500	63.850	4594	113.59	39730
65.8	5333	114.62	42066	67.094	5417	119.78	49790
74.1	7999	128.34	67661	70.860	6529	125.94	59860
85.8	13332	140.80	101325	74.311	7713	129.50	69920
102.5	26664			78.096	9217	133.65	79990
122.0	53329			81.787	10917	137.18	90070
141.5	101325			85.630	12961	138.82	95100
				89.553	15372	140.59	101210
mp/°C	–22			93.303	18022		
				98.207	22058	Antoine eq.	
				102.401	26085	eq. 3a	P/kPa
				107.174	31400	A	18.105654
				111.847	37437	B	56403343
				116.747	44780	C	277.46143
				122.130	54180		
				126.788	63579	data also fitted to Wagner eq.	
				131.723	74946		
				137.045	89022		
				141.105	101143		
				25.0	451		
				eq. 3	P/kPa		
				A	6.64334		
				B	1594.273		
				C	–70.545		
				data also fitted to Chebyshev and Wagner equations			
				bp/K	436.868		

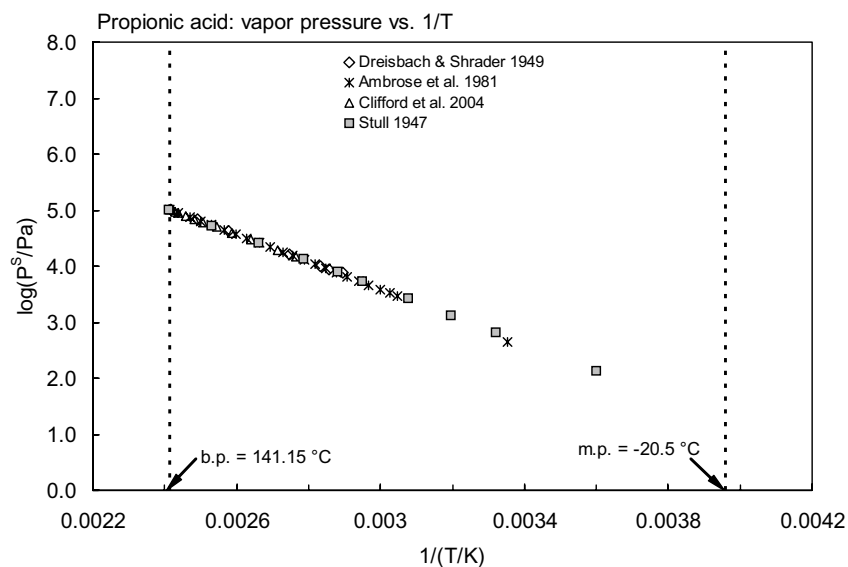
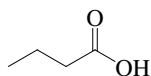


FIGURE 13.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for propionic acid.

13.1.1.4 Butyric acid



Common Name: Butyric acid

Synonym: butanoic acid, *n*-butyric acid, ethylacetic acid

Chemical Name: *n*-butyric acid, butyric acid

CAS Registry No: 107-92-6

Molecular Formula: $C_4H_8O_2$, $CH_3CH_2CH_2COOH$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

−5.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

163.75 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.95767, 0.95273 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

0.9582 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.0 ($20^{\circ}C$, calculated-density)

112.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.817 (Dean 1985)

4.822 (Riddick et al. 1986)

4.820 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.6 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($25.5^{\circ}C$, temp range 25.5 – $163.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 8.19524 - 2089.9/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

4716* ($90.92^{\circ}C$, ebulliometry, measured range 90.92 – $163.25^{\circ}C$, Dreisbach & Shrader 1949)

95.77 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.38423 - 1542.6/(179.0 + t/^{\circ}C)$, temp range 82 – $210^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 11881.2/(T/K)] + 8.773450$; temp range 25.5 – $352^{\circ}C$ (Antoine eq., Weast 1972–73)

83.95* (comparative ebulliometry, fitted to Antoine eq., measured range 340 – $452 K$, Ambrose et al. 1981)

$\log(P/kPa) = 6.55643 - 1563.444/[(T/K) - 93.307]$; temp range 339.7 – $452 K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

104, 92 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.8682 - 1766.906/(200.097 + t/^{\circ}C)$, temp range 90.2 – $163.25^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.67596 - 1642.683/(188.013 + t/^{\circ}C)$; temp range 76.53 – $178.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

104.3 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.7399 - 1764.7/(199.9 + t/^{\circ}C)$; temp range 90 – $163^{\circ}C$ (Antoine eq., Dean 1985, 1992)

102.0 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.55643 - 1563.444/(179.843 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

- 101 (comparative ebulliometry, Ambrose & Ghassee 1987)
 $\ln(P/\text{kPa}) = 15.09674 - 3599.963/[(T/\text{K}) - 93.307]$, (Antoine eq. from previous comparative ebulliometry measurements, Ambrose & Ghassee 1987)
 $\log(P_L/\text{kPa}) = 6.50913 - 1542.6/(-94.15 + T/\text{K})$; temp range 355–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.3554 - 2180.05/(-29.337 + T/\text{K})$; temp range 437–592 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 11.53324 - 5291.631/(128.778 + T/\text{K})$; temp range 301–358 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 8.0847 - 3.3219 \times 10^3/(T/\text{K}) + 2.4312 \cdot \log(T/\text{K}) - 1.1734 \times 10^{-2} \cdot (T/\text{K}) + 5.7992 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 268–628 K (vapor pressure eq., Yaws 1994)
 14560* (110.4°C, VLE still-manometry, measured range 110.4–162.9°C, Clifford et al. 2004)
 $\ln(P/\text{kPa}) = 14.511627 - 3164.4707/[(t/^\circ\text{C}) + 156.56122]$; temp range 110.4–162.9°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.0542 (partial pressure, Butler & Ramchandani 1935)
 0.0542; 0.0590; 0.0650 (exptl.; calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
 0.0375 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 0.0222 (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0654 (calculated-bond contribution, Brimblecombe et al. 1992)
 0.358 (calculated-molecular structure, Russell et al. 1992)
 0.0211 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.79 (shake flask-TN, Collander 1951)
 0.94 (calculated-TSA, Iwase et al. 1985)
 0.824, 0.70 (calculated-CLOGP, calculated-M.O., Bodor et al. 1989)
 0.79 (recommended, Sangster 1993)
 0.79 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (2.4 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K was determined using (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982; quoted, Atkinson 1985, 1989)

$k(\text{apparent}) \leq 4 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water, $k \leq 6.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k \leq 6.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2–4 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH} = 1.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air and $k(\text{soln}) = 3.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH}(\text{calc}) = 3.11 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

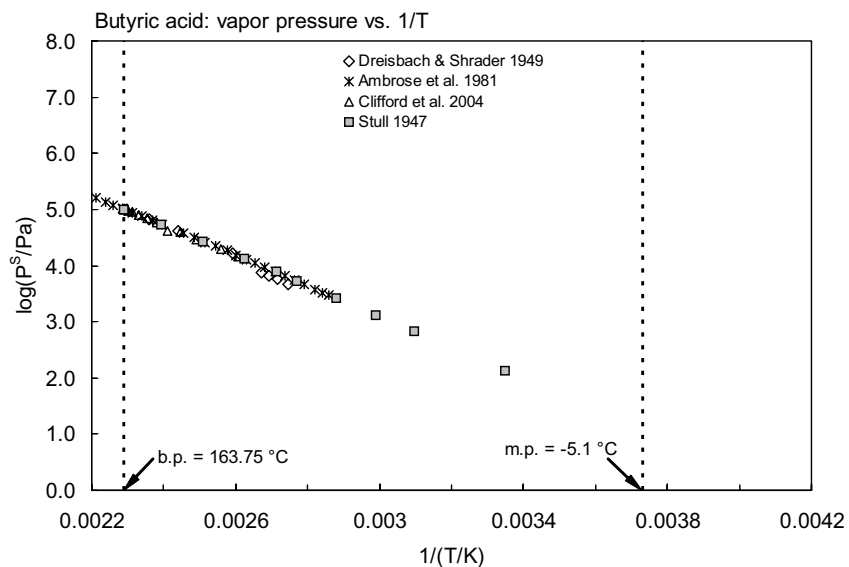
Soil:

Biota:

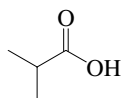
TABLE 13.1.1.4.1

Reported vapor pressures of butyric acid at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)	ln P = A – B/(C + T/K)		(3a)		
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Ambrose et al. 1981	Clifford et al. 2004		
summary of literature data		ebulliometry		comparative ebulliometry	VLE still-manometry		
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
25.5	133.3	90.92	4716	76.524	2939	110.4	14560
49.8	666.6	95.01	5704	78.773	3305	117.72	19580
61.5	1333	98.35	6639	81.494	3818	128.17	29650
74.0	2666	101.32	7586	85.202	4614	135.85	39720
88.0	5333	112.57	16500	88.517	5443	141.84	40790
95.5	7999	136.57	42066	92.350	6558	147.07	59860
108.0	13332	150.70	67661	95.880	7754	151.66	69920
125.5	26664	163.25	101326	99.708	9255	155.81	79990
144.5	53329			103.451	10955	159.46	90070
163.5	101325			107.241	13000	161.36	95100
				111.319	15409	162.90	100040
mp/°C	–4.70			115.124	18601		
				120.102	22098	Antoine eq.	
				124.357	26126	eq. 3a	P/kPa
				129.207	31448	A	14.511627
				133.944	37489	B	3164.4707
				144.392	54256	C	156.56122
				149.125	63651		
				154.135	75000	data also fitted to Wagner eq.	
				159.367	89123		
				163.687	101252		
				164.110	102558		
				164.553	103927		
				169.357	120015		
				173.698	136172		
				178.873	157694		
				Antoine eq.			
				eq. 3	P/kPa		
				A	6.55643		
				B	1563.444		
				C	–1563.444		
				data also fitted to Chebyshev and Wagner equations			



13.1.1.5 Isobutyric acid



Common Name: Isobutyric acid

Synonym: isobutanoic acid, *i*-butyric acid, 1-butyric acid, dimethylacetic acid, 2-methylpropionic acid, isopropylformic acid

Chemical Name: *i*-butyric acid, isobutyric acid

CAS Registry No: 79-31-2

Molecular Formula: $C_4H_8O_2$, $(CH_3)_2CHCOOH$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

−46.0 (Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

154.45 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9490 (Verschuereen 1983)

0.9682 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.7 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

112.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.860 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.02 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

228000 ($20^{\circ}C$, synthetic method, Jones 1929)

200000 ($20^{\circ}C$, quoted, Verschuereen 1983)

170000 (Dean 1985)

228000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

273.8* (interpolated-regression of tabulated data, temp range 14.7 – $154.5^{\circ}C$, Stull 1947)

185 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.40246 - 1529.2/(185.0 + t/^{\circ}C)$, temp range 73 – $190^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 11182.8/(T/K)] + 8.55228$; temp range 14.7 – $336^{\circ}C$ (Antoine eq., Weast 1972–73)

185.0 (Riddick et al. 1986)

184* (comparative ebulliometry, measured range 344.3 – 445.6 K, Ambrose & Ghassee 1987)

$\ln(P/kPa) = 15.31143 - 3695.332/[(T/K) - 82.0]$; temp range 344.3 – 447 K (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghassee 1987)

257.2 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.20794 - 2023.52/(-38.649 + T/K)$; temp range 288 – 428 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.11635 - 2006.61/(-35.297 + T/K)$, temp range 428 – 562 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 11.3037 - 3.1625 \times 10^3/(T/K) + 0.7263 \cdot \log(T/K) - 8.9331 \times 10^{-3} \cdot (T/K) + 4.8215 \times 10^{-6} \cdot (T/K)^2$; temp range 227 – 609 K (vapor pressure eq., Yaws 1994)

14550* ($102.6^{\circ}C$, VLE still-manometer, measured range 102.6 – $153.01^{\circ}C$, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 15.176238 - 3527.8614/[(t/^{\circ}\text{C}) + 180.5140]$; temp range 102–153.01°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.0178, 0.0289, 0.0633 (23.7°C, bubble column technique, concn: 1, 10, 10⁵ ppm. Servant et al. 1991)

0.0897 (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0899 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.50, 1.13 (calculated, Verschueren 1983)

0.94 (recommended, Sangster 1993)

1.10 (at pH 3.5, quoted, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}^* = (2.0 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-RF, Dagaut et al. 1988; Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 1.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.1.5.1

Reported vapor pressures of isobutyric acid (2-methyl propanoic acid) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)	$\ln P = A - B/(C + T/K)$		(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Ambrose & Ghiassie 1987		Clifford et al. 2004	
summary of literature data		comparative ebulliometry		VLE still-manometry	
$t/^{\circ}\text{C}$	P/Pa	T/K	P/Pa	$t/^{\circ}\text{C}$	P/Pa
14.7	133.3	344.287	3425	102.06	14550
39.3	666.6	347.850	4128	108.99	18580
51.2	1333	350.797	4801	118.62	29650
64.0	2666	355.776	6153	126.28	39720
77.8	5333	357.992	6852	132.29	49790
86.3	7999	360.006	7548	137.60	59850
98.0	13332	361.903	8260	142.36	69920
115.8	26664	365.785	9886	146.62	79990

TABLE 13.1.1.5.1 (Continued)

Stull 1947		Ambrose & Ghiasee 1987		Clifford et al. 2004	
summary of literature data		comparative ebulliometry		VLE still-manometry	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
134.5	53329	369.394	11370	150.21	90070
154.5	101325	375.207	15006	151.71	95100
mp/°C	−47	380.090	18440	153.01	100590
		384.218	21842	Antoine eq. eq. 3(a)	P/kPa
		387.840	25241		
		392.544	30312		
		399.095	38759		
		405.577	48959		
		409.363	55877	A	15.176238
		412.692	62629	B	3527.8614
		↓	↓	C	180.5140
		445.602	172068	data also fitted to Wagner eq.	
		298.15	184		
Antoine eq.					
eq. 3(a)	P/kPa				
A	15.31143				
B	3695.332				
C	−82.0				
bp/K	427.57				
		data also fitted to Wagner eq.			

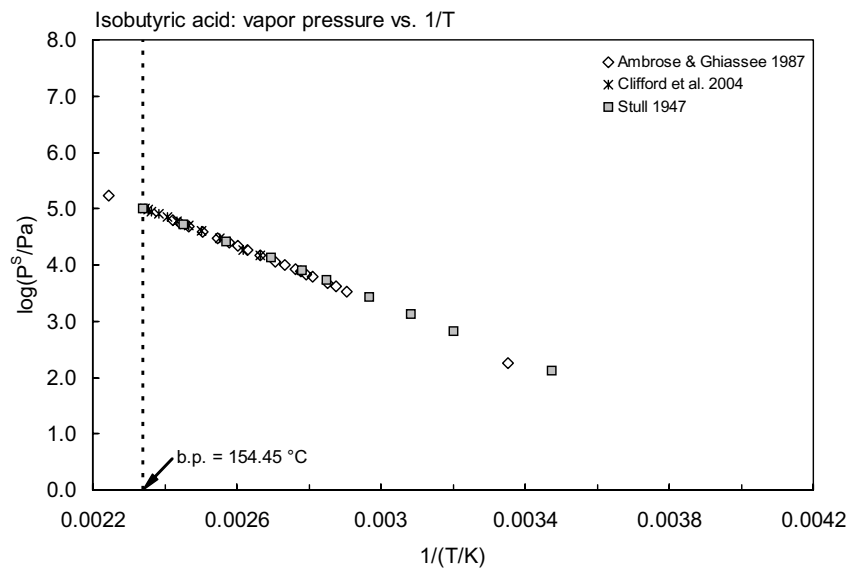
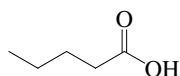


FIGURE 13.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for isobutyric acid.

13.1.1.6 *n*-Valeric acid

Common Name: *n*-Valeric acid

Synonym: pentanoic acid, valeric acid

Chemical Name: *n*-valeric acid, valeric acid

CAS Registry No: 109-52-4

Molecular Formula: $C_5H_{10}O_2$, $CH_3CH_2CH_2CH_2COOH$

Molecular Weight: 102.132

Melting Point ($^{\circ}C$):

−33.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

186.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9391 (Weast 1982–83)

0.9390 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

108.4 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

135.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.820 ($18^{\circ}C$, Weast 1982–83)

4.860 (Riddick et al. 1986)

4.830 (Sangster 1989, 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.17 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 1.0$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

26000 ($20^{\circ}C$, quoted, Amidon et al. 1975)

24000 (Verschuereen 1983; Dean 1985)

24000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

39.6* (extrapolated-regression of tabulated data, temp range 42.2 – $184.4^{\circ}C$, Stull 1947)

18.75 (calculated by formula, Dreisbach 1961)

$\log (P/mmHg) = 7.57366 - 1694.37/(175.0 + t/^{\circ}C)$, temp range 102 – $250^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = [-0.2185 \times 13370.3/(T/K)] + 9.271178$; temp range 42.2 – $184.4^{\circ}C$ (Antoine eq., Weast 1972–73)

20.0 ($20^{\circ}C$, Verschuereen 1983)

4.33, 6.37 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 4.58366 - 609.613/(62.754 + t/^{\circ}C)$; temp range 72.4 – $173.7^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 5.0835 - 878.669/(95.711 + t/^{\circ}C)$; temp range 81.1 – $116.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/mmHg) = 5.412 - 591/(60 + t/^{\circ}C)$; temp range 72 – $174^{\circ}C$ (Antoine eq., Dean 1985, 1992)

19.0 (Riddick et al. 1986)

$\log (P/kPa) = 6.7818 - 1777.2/(186.6 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

21.0* (comparative ebulliometry, measured range 372.5 – $465.3\ K$, Ambrose & Ghassee 1987)

$\ln (P/kPa) = 15.25555 - 3811.202/[(T/K) - 101.0]$, temp range 372.5 – $456.3\ K$ (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghassee 1987)

16.9 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.69856 - 1694.37/(-98.15 + T/\text{K})$, temp range 375–523 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 15.3454 - 3.9024 \times 10^3/(T/\text{K}) - 0.024353 \cdot \log (T/\text{K}) - 1.1099 \times 10^{-2} \cdot (T/\text{K}) + 5.6315 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 239–651 K (vapor pressure eq., Yaws 1994)

14560 (130°C, VLE still-manometer, measured range 130–178.77°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 36.410366 - 30029.229/(t/^\circ\text{C}) + 760.44819$; temp range 130–178.77°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.0478 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

$\ln [K_H' / (\text{mol kg}^{-1} \text{ atm}^{-1})] = -15.37 + 6879/(T/\text{K})$; temp range 278.15–308.15 K. (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0618, 0.0989 (calculated-P/C, calculated-bond contribution, Brimblecombe et al. 1992)

0.0448* (equilibrium partial pressure, pH 5.4, measured range 5–35°C, Khan et al. 1995)

$\ln [K_H' / (\text{mol kg}^{-1} \text{ atm}^{-1})] = -14.3371 + 6582.96/(T/\text{K})$; temp range 5–35°C (equilibrium partial pressure measurements, Khan et al. 1995)

0.0310 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.030 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 4.861 - 2865/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.42 (Scherrer & Howard 1979)

0.99, 1.69 (calculated, Verschueren 1983)

1.39 (recommended, Sangster 1993)

1.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 13.1.1.6.1

Reported vapor pressures and Henry's law constants of n-valeric acid at various temperatures

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Vapor pressure				Henry's law constant			
Stull 1947		Ambrose & Ghiassie 1987		Clifford et al. 2004		Khan et al. 1995	
summary of literature data		comparative ebulliometry		VLE still-manometry		gas stripping	
t/^{\circ}\text{C}	P/Pa	T/K	P/Pa	t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	H/(Pa m^3/mol)
42.2	133.3	372.543	3410	130.0	14560	5	0.00823
67.7	666.6	376.278	4112	137.56	19590	15	0.018
79.8	1333	379.415	4801	143.92	24630	25	0.0448
93.1	2666	384.489	6125	149.04	29650	35	0.0878

(Continued)

TABLE 13.1.1.6.1 (Continued)

Vapor pressure						Henry's law constant		
Stull 1947		Ambrose & Ghiassee 1987		Clifford et al. 2004		Khan et al. 1995		
summary of literature data		comparative ebulliometry		VLE still-manometry		gas stripping		
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³/mol)	
116.6	7999	398.670	11637	163.33	49780	ln H = A - B/(T/K)		
128.3	13332	404.759	15006	168.74	59850	H/(mol kg ⁻¹)		
146.0	26664	414.079	21807	173.30	69920	A	-14.3371	
165.0	53329	422.753	30285	175.33	74960	B	6582.96	
184.4	101325	429.637	55786	17720	79990			
		443.796	62659	17877	86030			
mp/°C	-34.5	449.980	76308					
		454.060	86528	Antoine eq.				
		460.052	101592	eq. 2a	P/Pa			
		405.378	120678	A	36.410366			
				B	30029.229			
				C	760.44819			
				Antoine eq.				
				eq. 2a	P/kPa			
				A	15.2555	data also fitted to Wagner eq.		
				B	3811.202			
		C	-101.0					
				data also fitted to Wagner eq.				

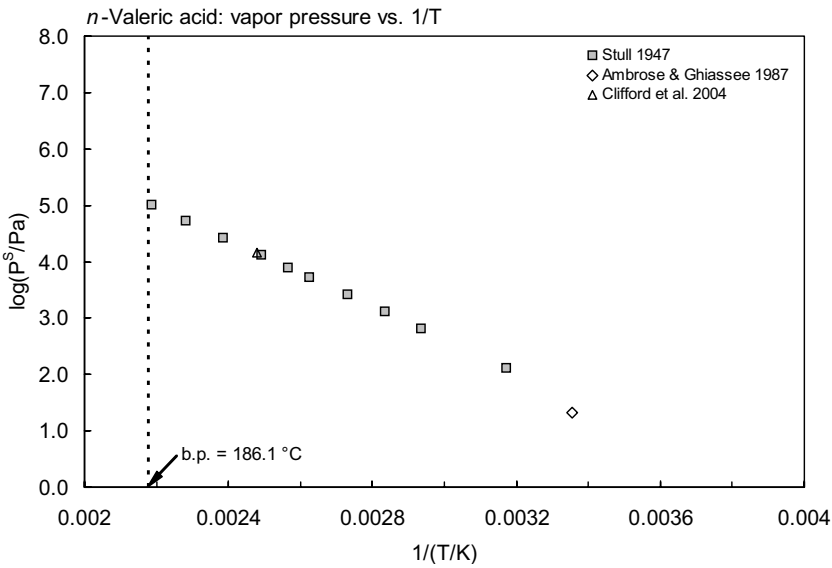


FIGURE 13.1.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-valeric acid.

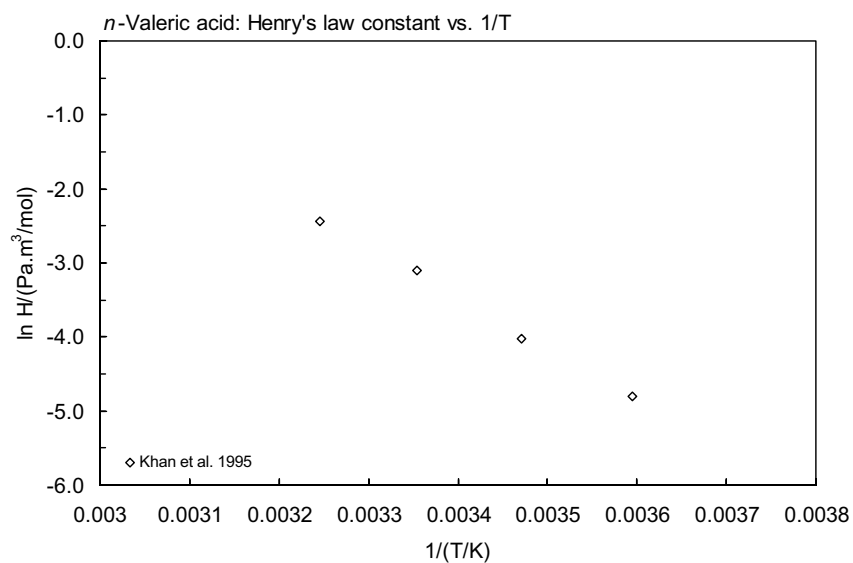
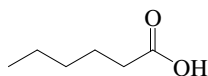


FIGURE 13.1.1.6.2 Logarithm of Henry's law constant versus reciprocal temperature for *n*-valeric acid.

13.1.1.7 Hexanoic acid (Caproic acid)



Common Name: Hexanoic acid

Synonym: butylacetic acid, caproic acid, *n*-hexanoic acid

Chemical Name: butylacetic acid, hexanoic acid, *n*-hexanoic acid

CAS Registry No: 142-62-1

Molecular Formula: $C_6H_{12}O_2$, $CH_3(CH_2)_4COOH$

Molecular Weight: 116.158

Melting Point ($^{\circ}C$):

−3 (Lide 2003)

Boiling Point ($^{\circ}C$):

205.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

125.0 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

157.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.850 (Dean 1985; Bintein & Devillers 1994)

4.879 (Riddick et al. 1986)

4.870 (Sangster 1989, 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.4 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9887 (Valvani et al. 1981)

11000 (Verschuereen 1983)

10816 (Windholz 1983)

6391 (calculated-activity coefficient γ from UNIFAC, Banerjee 1985)

9580 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($71.4^{\circ}C$, summary of literature data, temp range 71.4 – $202^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 16189.4/(T/K)] + 10.431464$; temp range 71.4 – $202^{\circ}C$ (Antoine eq., Weast 1972–73)

4.40 (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.76323 - 1789.425/(T/K) - 101.930$; temp range: 386.3 – $441.8 K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

26.7 ($20^{\circ}C$, Verschuereen 1983)

9.92, 1.65 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.74777 - 1779.677/(178.361 + t/^{\circ}C)$, temp range 113.1 – $168.6^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose et al. 1981, Boublik et al. 1984)

$\log(P/kPa) = 6.06182 - 1347.897/(127.391 + t/^{\circ}C)$, temp range 98.1 – $179.1^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.9249 - 1340.8/(126.6 + t/^{\circ}C)$, temp range 98 – $179^{\circ}C$ (Antoine eq., Dean 1985, 1992)

5.00 (Riddick et al. 1986)

$\log(P/kPa) = 6.76323 - 1789.425/(171.22 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

6.0 (calculated from Wagner eq. derived from experimental data, Ambrose & Ghassee 1987)

$\ln(P/kPa) = 15.30352 - 3957.396/[(T/K) - 108]$ (Antoine eq., Ambrose & Ghassee 1987)

$\log(P_L/kPa) = 7.08241 - 2009.93/(-82.69 + T/K)$; temp range 335 – $487 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 55.7058 - 5.6602 \times 10^3/(T/K) - 15.458 \cdot \log (T/K) + 1.0823 \times 10^{-9} \cdot (T/K) + 1.8718 \times 10^{-13} \cdot (T/K)^2$;
temp range 270–667 K (vapor pressure eq., Yaws 1994)

9520 (140.25°C, VLE still-manometer, measured range 140.25–178.28°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 13.46595 - 2642.198/[t/^\circ\text{C} + 95.20133]$; temp range 140.25–178.28°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0768 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

$\ln [K_H/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -12.69 + 5988/(T/K)$; temp range 278.15–303.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0873, 0.149 (calculated-P/C, calculated-bond contribution, Brimblecombe et al. 1992)

0.0720* (equilibrium partial pressure, pH 5.4, measured range 5–35°C, Khan et al. 1995)

$\ln [K_H'/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -13.9424 + 6303.73/(T/K)$; temp range 5–35°C (equilibrium partial pressure measurements, Khan et al. 1995)

0.0583 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.0556 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 3.955 - 2520/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.88 (Scherrer & Howard 1979)

1.87 (HPLC-RT correlation, D'Amboise & Hanai 1982)

1.92 (shake flask-titration, Umland 1983)

2.09 (shake flask-fluorescence, Nishimura et al. 1985)

1.32 (calculated-activity coefficient γ from UNIFAC, Banerjee & Howard 1988)

2.03 ± 0.01 (potentiometric titration, Hersey et al. 1989)

1.92 (recommended, Sangster 1989, 1993)

1.92 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.38; 1.42; 1.57 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)

1.46; 0.88 (soil, quoted exptl.; calculated-MCI χ and fragment contribution, Meylan et al. 1992)

1.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 13.1.1.7.1
Reported vapor pressures and Henry’s law constants of hexanoic acid (caproic acid) at various temperatures

Vapor pressure						Henry’s law constant	
Stull 1947		Ambrose et al. 1981		Clifford et al. 2004		Khan et al. 1995	
summary of literature data		comparative ebulliometry		VLE still-manometer		gas stripping	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³/mol)
71.4	133.3	386.270	2952	140.25	9520	5	0.0167
89.5	666.6	388.571	3314	149.73	14560	15	0.036
99.5	1333	391.485	3831	156.77	19590	25	0.072
111.8	2666	395.428	4638	162.47	24630	35	0.150
125.0	5333	398.865	5459	166.88	29640		
133.3	7999	402.913	6576	171.11	34680	ln H = A – B/(T/K)	
144.0	13332	406.610	7762	174.73	39720		H/(mol kg ⁻¹)
160.8	26664	410.665	9267	178.28	44750	A	–13.9424
181.0	53329	414.581	10963			B	6303.73
202.0	101325	418.705	13001	Antoine eq.			
		422.887	15422	eq. 2a	P/Pa		
mp/°C	–1.5	432.157	22112	A	13.46595		
		441.779	31458	B	2642.198		
				C	95.20133		
		eq. 2	P/kPa				
		A	6.76323	data also fitted to Wagner eq.			
		B	1789.425				
		C	–101.930				
data also fitted to Wagner eq.							

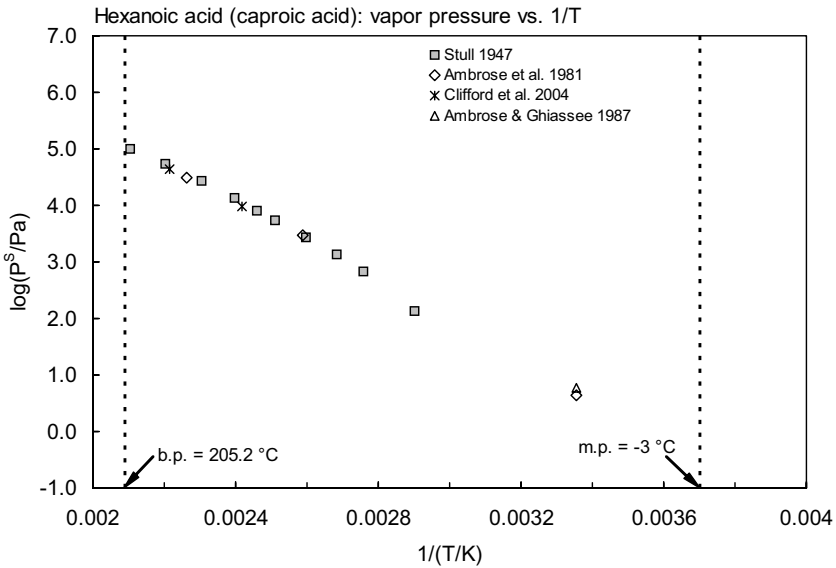


FIGURE 13.1.1.7.1 Logarithm of vapor pressure versus reciprocal temperature for hexanoic acid.

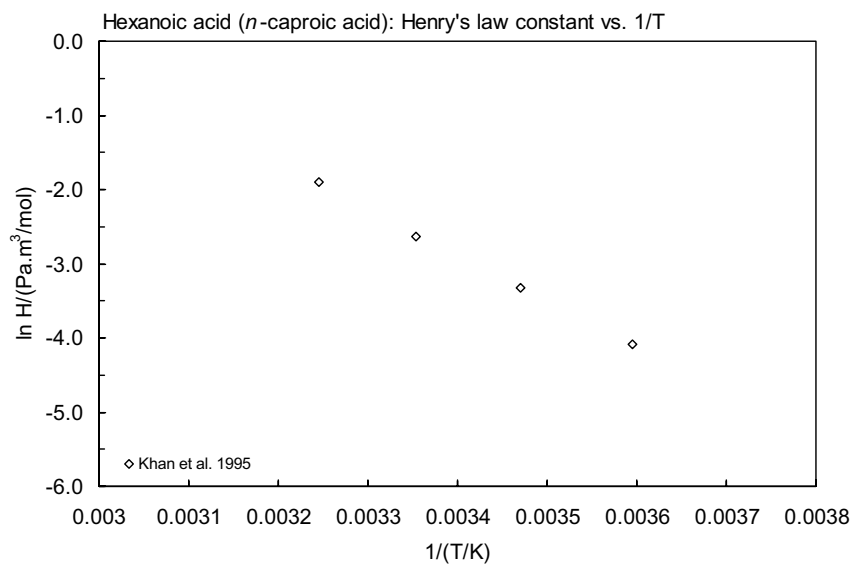
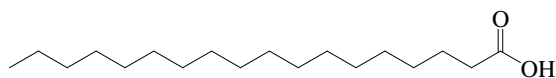


FIGURE 13.1.1.7.2 Logarithm of Henry's law constant versus reciprocal temperature for hexanoic acid.

13.1.1.8 Stearic acid (Octadecanoic acid)



Common Name: Stearic acid

Synonym: octadecanoic acid

Chemical Name: stearic acid, octadecanoic acid, *n*-octadecylic acid

CAS Registry No: 57-11-4

Molecular Formula: $C_{18}H_{36}O_2$, $CH_3(CH_2)_{16}COOH$

Molecular Weight: 284.478

Melting Point ($^{\circ}C$):

69.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

350 (dec., Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9408 (Weast 1982–83)

Molar Volume (cm^3/mol):

335.9 ($70^{\circ}C$, Stephenson & Malanowski 1987)

423.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.50 (estimated, Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

39.57; 43.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.368 (mp at $69.3^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

340 (Verschuereen 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

133.3 ($173.7^{\circ}C$, summary of literature data, temp range: 173.7 – $370^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 19306.6/(T/K)] + 9.457471$; temp range: 173.7 – $370^{\circ}C$, (Antoine eq., Weast 1972–73)

1.69×10^{-12} (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.17126 - 2157.5/(-153.78 + T/K)$; temp range 349 – $415 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.85188 - 1717.93/(-201.829 + T/K)$; temp range 447 – $649 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -40.3638 - 4.7724 \times 10^3/(T/K) + 24.502 \cdot \log(T/K) - 3.7665 \times 10^{-2} \cdot (T/K) + 1.4595 \times 10^{-5} \cdot (T/K)^2$; temp range 343 – $799 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.23 (HPLC-RT correlation, D'Amboise & Hanai 1982)

8.23 (recommended, Sangster 1989, 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

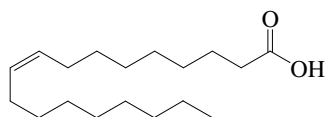
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

13.1.1.9 Oleic acid



Common Name: Oleic acid

Synonym: *cis*-9-octadecenoic acid, (Z)-9-octadecenoic acid

Chemical Name: oleic acid

CAS Registry No: 112-80-1

Molecular Formula: $C_{18}H_{34}O_2$, $CH_3(CH_2)_7CH=CH(CH_2)_6CH_2COOH$

Molecular Weight: 282.462

Melting Point ($^{\circ}C$):

13.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

360 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8870 ($25^{\circ}C$, Riddick et al. 1986)

0.8935 (Lide 2003)

Molar Volume (cm^3/mol):

314.7 (Stephenson & Malanowski 1987)

416.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

5.02 (Riddick et al. 1986)

4.50 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

insoluble (McBain & Richards 1946; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

133 ($178.5^{\circ}C$, summary of literature data, temp range 176.5 – $360^{\circ}C$, Stull 1947)

0.00144 (extrapolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 20326.7/(T/K)] + 9.930301$; temp range 176.5 – $360^{\circ}C$ (Antoine eq., Weast 1972–73)

0.00113 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.22018 - 3711.59/(-36.125 + T/K)$; temp range 444 – 635 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 78.6973 - 8.8227 \times 10^3/(T/K) - 22.472 \cdot \log(T/K) + 4.8353 \times 10^{-11} \cdot (T/K) + 2.6578 \times 10^{-6} \cdot (T/K)^2$; temp range 287 – 633 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.64 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)

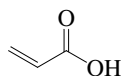
7.64 (recommended, Sangster 1989, 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

13.1.1.10 Acrylic acid (2-Propenoic acid)



Common Name: Acrylic acid

Synonym: acroleic acid, ethylenecarboxylic acid, 2-propenoic acid, propenoic acid

Chemical Name: acrylic acid, 2-propenoic acid, propenoic acid

CAS Registry No: 79-10-7

Molecular Formula: $C_3H_4O_2$, $CH_2=CHCOOH$

Molecular Weight: 72.063

Melting Point ($^{\circ}C$):

12.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

141 (Lide 1003)

Density (g/cm^3 at $20^{\circ}C$):

1.0511 (Weast 1982–83; Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

68.9 (calculated-density, Stephenson & Malanowski 1987)

83.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

–4.41 (Perrin 1972)

4.25 (pK_a , Weast 1982–83)

4.26 (pK_a , Dean 1985)

4.255 (pK_a , Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.13 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

570.8 (interpolated-regression of tabulated data, temp range 3.5 – $141^{\circ}C$, Stull 1947)

506.5 (Hoy 1970)

570 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 10955.1/(T/K)] + 8.659704$; temp range 3.5 – $141^{\circ}C$ (Antoine eq., Weast 1972–73)

426.6 ($20^{\circ}C$, Verschueren 1983)

$\log(P/mmHg) = 5.65204 - 648.629/(154.683 + t/^{\circ}C)$; temp range 20 – $70^{\circ}C$ (Antoine eq., Dean 1985, 1992)

533.0 (Howard et al. 1986)

1030 ($20^{\circ}C$, Riddick et al. 1986)

581.7 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.93296 - 1827.9/(-43.15 + T/K)$; temp range 341 – $414\ K$ (Antoine eq., Stephenson & Malanowski 1987)

533, 12530 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/mmHg) = 23.0607 - 3.1347 \times 10^3/(T/K) - 4.8813 \cdot \log(T/K) + 4.369 \times 10^{-4} \cdot (T/K) - 4.9161 \times 10^{-13} \cdot (T/K)^2$; temp range 287 – $615\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.042 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 0.43 (Leo et al. 1971)
- 0.31, 0.43 (calculated, Verschueren 1983)
- 0.35 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} t_{1/2} = 2.5\text{--}23.8$ h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; selected, Howard et al. 1991)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous screening test data (Dore et al. 1975; Sasaki 1978; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672\text{--}4320$ h, based on unacclimated anaerobic reactor test data (Chou et al. 1979; selected, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 28$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.5\text{--}23.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; selected, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 28$ d in natural waters (Capel & Larson 1995)

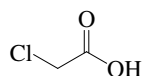
Groundwater: $t_{1/2} = 48\text{--}4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

13.1.1.11 Chloroacetic acid



Common Name: Chloroacetic acid

Synonym:

Chemical Name: chloroacetic acid (α or β)

CAS Registry No: 79-11-8

Molecular Formula: $\text{C}_2\text{H}_3\text{ClO}_2$, ClCH_2COOH

Molecular Weight: 94.497

Melting Point ($^{\circ}\text{C}$):

61.2 (α , Stull 1947; Yalkowsky & Valvani 1980)

56.0 (β , Yalkowsky & Valvani 1980)

56–63 (Weast 1982–83; Dean 1985)

63 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

189.3 (Lide 2003)

Density (g/cm^3 at 20°C):

1.4043 (40°C , Weast 1982–83)

Molar Volume (cm^3/mol):

68.8 (63°C , Stephenson & Malanowski 1987)

89.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.85 (Weast 1982–83)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

56 (estimated, Yalkowsky & Valvani 1980)

36.73, 42.22 (observed for α , observed for β , Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.424 (mp at 63°C)

Water Solubility (g/m^3 or mg/L at 25°C):

120835 (α , calculated- ΔS_{fus} and mp, calculated-mp, Yalkowsky & Valvani 1980)

107200 (β , calculated- ΔS_{fus} and mp, calculated-mp, Yalkowsky & Valvani 1980)

109000 (shake flask-titrimetric assay, Bowden et al. 1998)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

39.70* (extrapolated-regression of tabulated data, temp range 43.0 – 189.5°C , Stull 1947)

$\log (P/\text{mmHg}) = 8.28534 - 2263.7/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

6301* (112.8°C , ebulliometry, measured range 112.8 – 187.55°C , Dreisbach & Shrader 1949)

4141* (104.47°C , ebulliometry, measured range 104.47 – 190.27°C , McDonald et al. 1959)

$\log (P/\text{mmHg}) = 7.56597 - 1733.96/(180.996 + t/^{\circ}\text{C})$; temp range: 104 – 190°C (Antoine eq. from ebulliometry measurement, McDonald et al. 1959)

$\log (P/\text{mmHg}) = [-0.2185 \times 13134.5/(T/\text{K})] + 9.099371$; temp range 43 – 189°C (Antoine eq., Weast 1972–73)

18.52, 12.9 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.67559 - 1723.714/(180.01 + t/^{\circ}\text{C})$; temp range 104 – 190.27°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.29612 - 1468.443/(154.397 + t/^{\circ}\text{C})$; temp range 123.19 – 187.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

18.52 (extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.55016 - 1723.365/(179.98 + t/^{\circ}\text{C})$; temp range 104 – 190°C (Antoine eq., Dean 1985, 1992)

8.51, 11.5 (extrapolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.69087 - 1733.96/(-92.154 + T/K)$; temp range 336–463 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.67975 - 1727.293/(-97.742 + T/K)$; temp range 377–464 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 42.6726 - 4.597 \times 10^3/(T/K) - 11.348 \cdot \log (T/K) - 2.8515 \times 10^{-10} \cdot (T/K) + 1.7995 \times 10^{-6} \cdot (T/K)^2$; temp range 333–686 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

0.000938 (partial pressure equilibrium, Bowden et al. 1998)

$\ln [(K_H'/(\text{mol kg}^{-1} \text{ atm}^{-1}))] = -21.087 + 9742.6/(T/K)$, temp range $5\text{--}35^\circ\text{C}$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000536 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 7.343 - 4104/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.22 (shake flask, Hansch & Leo 1987; recommended, Hansch et al. 1995)

0.22 (recommended, Sangster 1993)

0.22 (calculated-fragment const. with correction factors in multiCASE program, Dambrosky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: aqueous photolysis $t_{1/2} = 1900\text{--}19000$ h, based on experimental photolysis data utilizing an artificial light source (Draper & Crosby 1983; quoted, Howard et al. 1991);

atmospheric photolysis $t_{1/2} = 1900\text{--}19000$ h, based on estimated aqueous photolysis half-life (Howard et al. 1991);

photocatalyzed mineralization by the presence of TiO_2 with the rate of 5.5 ppm/min per gram of catalyst (Ollis 1985).

Hydrolysis: first-order hydrolysis $t_{1/2} = 23000$ h, based on losses in dark control tests during photolysis experiments (Draper & Crosby 1983; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 230\text{--}2300$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on river die-away tests using radio-labeled material (Boethling & Alexander 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 230\text{--}2300$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 5 d (Kelly et al. 1994).

Surface water: aqueous photolysis $t_{1/2} = 1900\text{--}19000$ h, based on experimental photolysis data utilizing an artificial light source (Draper & Crosby 1983; quoted, Howard et al. 1991); $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 13.1.1.11.1

Reported vapor pressures of chloroacetic acid at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959	
summary of literature data		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
43.0	133	112.8	6301	104.47	4141
68.3	666.6	123.19	10114	114.60	6675
81.0	1333	134.67	16468	128.32	12103
94.2	2666	159.95	42066	146.78	25198
109.2	5333	174.44	67661	167.51	38583
118.3	7999	187.55	101325	187.59	97205
130.7	13332			189.35	102165
140.0	26664			190.27	104738
169.0	53329				
189.5	101325			mp/°C	62.65
mp/°C	61.2			eq. 2	P/mmHg
				A	7.56597
				B	1733.96
				C	180.996

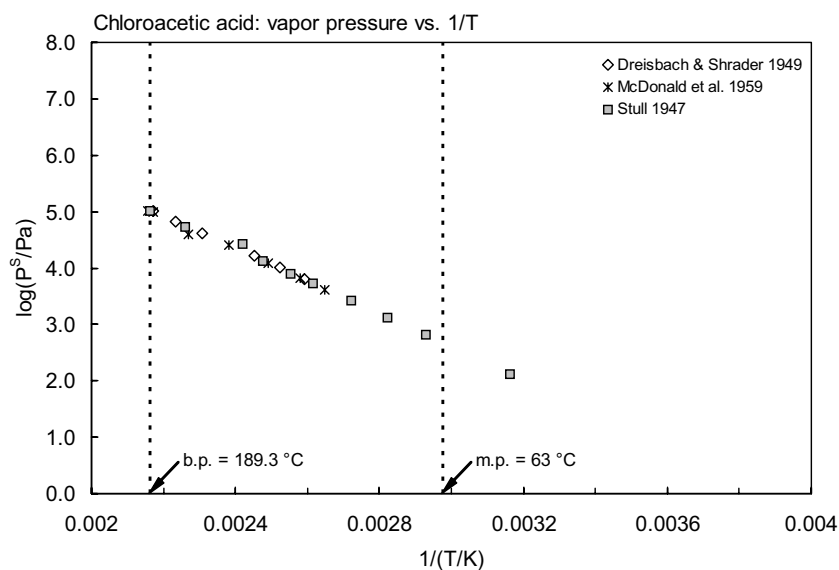
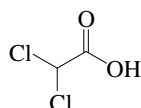


FIGURE 13.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for chloroacetic acid.

13.1.1.12 Dichloroacetic acid



Common Name: Dichloroacetic acid

Synonym: dichloroethanoic acid

Chemical Name: dichloroacetic acid

CAS Registry No: 79-43-6

Molecular Formula: $C_2H_2Cl_2O_2$, $Cl_2CHCOOH$

Molecular Weight: 128.942

Melting Point ($^{\circ}C$):

13.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

194.0 (Weast 1982–83; Verschueren 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5634 (Weast 1982–83)

1.5630 (Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

82.50 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

110.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

1.26 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

37.94* (extrapolated-regression of tabulated data, temp range 44 – $194.4^{\circ}C$, Stull 1947)

133.3 ($44^{\circ}C$, Stull 1947; quoted, Verschueren 1983)

$\log(P/mmHg) = [-0.2185 \times 12952.9/(T/K)] + 8.946605$; temp range 44 – $194.4^{\circ}C$ (Antoine eq., Weast 1972–73)

34.3 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.47122 - 2385.6/(-31.197 + T/K)$, temp range 317 – $468\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -7.2806 - 3.3706 \times 10^3/(T/K) + 9.3771 \cdot \log(T/K) - 2.0832 \times 10^{-2} \cdot (T/K) + 9.5091 \times 10^{-6} \cdot (T/K)^2$; temp range 287 – $686\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.00085 (partial pressure equilibrium, Bowden et al. 1998)

$\ln[(K_H'/(mol\ kg^{-1}\ atm^{-1}))] = -15.1776 + 8010.6/(T/K)$; temp range 5 – $35^{\circ}C$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000536 ($20^{\circ}C$, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 4.776 - 3352/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.92 (shake flask, Log P Database, Hansch & Leo 1987)

0.92 (recommended, Sangster 1993)

0.92 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 8.5 ppm/min per gram catalyst (Ollis 1985).

Half-Lives in the Environment:

TABLE 13.1.1.12.1

Reported vapor pressures of dichloroacetic acid at various temperatures

Stull 1947

summary of literature data

$t/^{\circ}C$	P/Pa
44.0	133
69.8	666.6
82.6	1333
96.3	2666
111.8	5333
121.5	7999
134.0	13332
152.3	26664
173.7	53329
194.4	101325
mp/ $^{\circ}C$	9.7

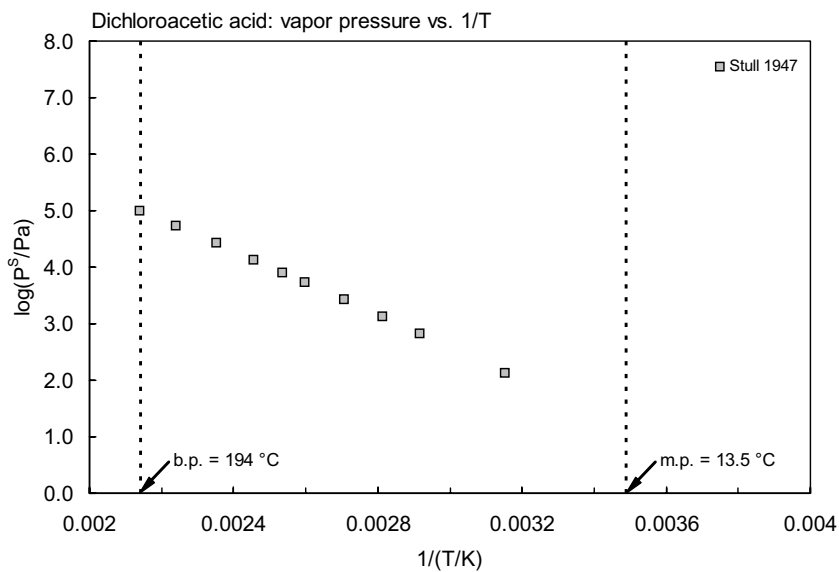
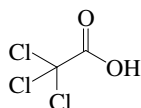


FIGURE 13.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for dichloroacetic acid.

13.1.1.13 Trichloroacetic acid



Common Name: Trichloroacetic acid

Synonym: TCA

Chemical Name: trichloroacetic acid (α or β)

CAS Registry No: 76-03-9

Molecular Formula: Cl_3CCOOH

Molecular Weight: 163.39

Melting Point ($^{\circ}\text{C}$):

59.2 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

196.5 (Lide 2003)

Density (g/cm^3 at 20°C):

1.620 (25°C , Weast 1982–83)

Molar Volume (cm^3/mol):

100.3 (61°C , Stephenson & Malanowski 1987)

131.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

0.70 (Weast 1982–83)

0.52 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

17.78, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 0.462 (mp at 59.2°C)

Water Solubility (g/m^3 or mg/L at 25°C):

114550 (calculated- ΔS_{fus} and mp, Yalkowsky & Valvani 1980)

191860 (calculated-mp, Yalkowsky & Valvani 1980)

13000 (Verschuereen 1983)

1200000 (120 in 100 parts solvent, Dean 1985)

38300 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

21.88* (extrapolated-regression of tabulated data, temp range 51 – 195.6°C , Stull 1947)

4620* (112.62°C , ebulliometry, measured range 112.62 – 197.93°C , McDonald et al. 1959)

$\log(P/\text{mmHg}) = 7.31057 - 1618.97/(167.882 + t/^{\circ}\text{C})$; temp range 112.6 – 197.94°C (Antoine eq. from ebulliometry measurement, McDonald et al. 1959)

$\log(P/\text{mmHg}) = [-0.2185 \times 13817.0/(T/\text{K})] + 9.341430$; temp range 51 – 195.6°C (Antoine eq., Weast 1972–73)

10.63 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.4026 - 1597.434/(165.711 + t/^{\circ}\text{C})$; temp range 112.6 – 197.93°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

66.14 (extrapolated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 7.2730 - 1594.3/(165.4 + t/^{\circ}\text{C})$; temp range 112 – 198°C (Antoine eq., Dean 1985, 1992)

133.3 (Howard et al. 1986; quoted, Banerjee et al. 1990)

11.01 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.43547 - 1618.97/(-105.268 + T/\text{K})$; temp range 326 – 473 K (Antoine eq., Stephenson & Malanowski 1987)

133.3, 491 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 63.4449 - 3.6769 \times 10^3/(T/\text{K}) - 21.13 \cdot \log(T/\text{K}) + 1.0777 \times 10^{-2} \cdot (T/\text{K}) + 4.8481 \times 10^{-12} \cdot (T/\text{K})^2$; temp range 258 – 491 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.000137 (partial pressure equilibrium, Bowden et al. 1998)

$\ln [(K_H'/(\text{mol kg}^{-1} \text{ atm}^{-1}))] = -17.836 + 8660.09/(T/K)$; temp range $5\text{--}35^\circ\text{C}$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000834 (20°C , selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 5.931 - 3634/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.33 (shake flask, Log P Database, Hansch & Leo 1987)

1.33 (recommended, Sangster 1993)

1.33 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: no photocatalyzed mineralization by the presence of TiO_2 as compared to both dichloroacetic acid and trichloroacetic acid (Ollis 1985).

Half-Lives in the Environment:

TABLE 13.1.1.13.1

Reported vapor pressures of trichloroacetic acid at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$	(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)		
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)		
Stull 1947		McDonald et al. 1959		
summary of literature data		ebulliometry		
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	
51.0	133	112.62	4620	
76.0	666.6	118.13	5949	
88.2	1333	122.75	7326	
101.8	2666	129.99	9998	
116.3	5333	168.75	42302	
125.9	7999	183.92	68210	
137.8	13332	194.91	94156	
155.4	26664	196.49	98175	
175.2	53329	197.02	99584	
195.6	101325	197.48	100901	
		197.93	102318	
mp/ $^\circ\text{C}$	57.0	mp/ $^\circ\text{C}$	59.16	
		eq. 2	P/mmHg	
		A	7.31057	
		B	1618.97	
		C	167.882	

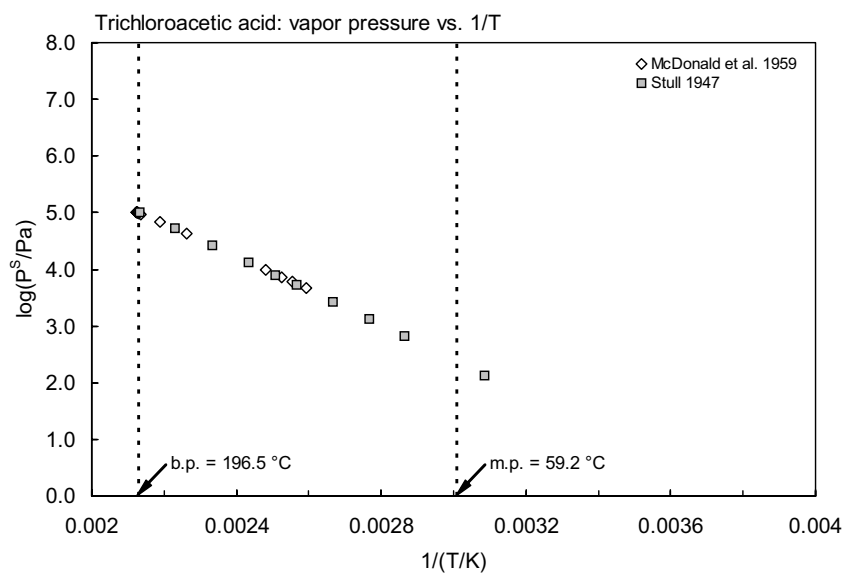
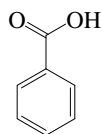


FIGURE 13.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for trichloroacetic acid.

13.1.2 AROMATIC ACIDS**13.1.2.1 Benzoic acid**

Common Name: Benzoic acid

Synonym:

Chemical Name: benzoic acid

CAS Registry No: 65-85-0

Molecular Formula: $C_7H_6O_2$, C_6H_5COOH

Molecular Weight: 122.122

Melting Point ($^{\circ}C$):

122.35 (Lide 2003)

Boiling Point ($^{\circ}C$):

249.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2659 ($15^{\circ}C$, Weast 1982–83)

1.0800 (Dean 1985)

Molar Volume (cm^3/mol):

113.6 ($130^{\circ}C$, Stephenson & Malanowski 1987)

134.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.20 (McDaniel & Brown 1958)

4.33 ± 0.02 , 4.38 ± 0.03 (HPLC, Unger et al. 1978)

4.08 (shake flask-TN, Clarke 1984)

4.05 ± 0.01 (equilibrium titration, Clarke & Cahoon 1987)

4.204 (Dean 1985; Lee et al. 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

69.2 (395.2 K, de Kruif & Block 1982)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

94.5 ($25^{\circ}C$, average value, Malaspina et al. 1973)

90.6 (Colomina et al. 1982)

90.51 (Ribeiro da Silva et al. 1995)

89.71 (Li et al. 2002)

90.1 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.0 (Tsonopoulos & Prausnitz 1971)

18.2 (395.2 K, de Kruif & Block 1982)

Entropy of Fusion, ΔS_{fus} (J/mol K):

45.61 (Tsonopoulos & Prausnitz 1971)

43.81 (Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.111 (mp at $122.35^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3340* ($24.6^{\circ}C$, shake flask-synthetic method, Ward & Cooper 1930)

3298* (shake flask-thermostatic and synthetic methods, measured range 25 – $88.6^{\circ}C$, Morrision 1944)

4200 (shake flask-liquid scintillation counting, Lu & Metcalf 1975)

3600 (shake flask-UV, Yalkowsky et al. 1983)

3416* (shake flask-weight titration, measured temp range 5 – $65^{\circ}C$, Strong et al. 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 799.9* (122.2°C, static method-manometer, measured range 122.2–249.0°C, Kahlbaum 1898)
 6.893* (60.1°C, isoteniscope method, measured range 60.1–247°C, Klosky et al. 1927)
 $\log(P_s/\text{mmHg}) = 11.956 - 4409/(T/K)$; temp range 61–121°C (solid, isoteniscope, Klosky et al. 1927)
 $\log(P_L/\text{mmHg}) = 30.172 - 4714/(T/K) - 6.720 \cdot \log(T/K)$; temp range 128–247°C (liquid, isoteniscope, Klosky et al. 1927)
 0.840* (extrapolated-regression of tabulated data, temp range 96–227°C, Stull 1947)
 12.35* (70.48°C, transpiration method, measured range 70.48–114.11°C, Davies & Jones 1954)
 $\log(P/\text{mmHg}) = 12.8699 - 4775.7/(T/K)$, temp range 70.48–114.11°C (transpiration, Davies & Jones 1954)
 0.160* (298.3 K, Knudsen effusion, measured range 290.4–315.5 K, Wiedemann 1971)
 $\log(P/\text{mmHg}) = [-0.2185 \times 15253.3/(T/K)] + 9.03300$; temp range 60–110°C (Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 16295.1/(T/K)] + 9.741362$; temp range 96–249.2°C (Antoine eq., Weast 1972–73)
 0.160* (Knudsen effusion weight-loss method, fitted to Antoine eq., measured range 65.05–110.25°C, Malaspina et al. 1973)
 $\log(P/\text{mmHg}) = (12.175 \pm 0.040) - (4501 \pm 17)/(T/K)$; temp range 338–383 K (Antoine eq., Knudsen effusion, Malaspina et al. 1973)
 0.108* (effusion method, measured range 25–70.5°C, DePablo 1976)
 16.8* (71.25°C, isoteniscope method, measured range 344.4–393.8 K, Sachinidis & Hill 1980)
 $\log(P/\text{mmHg}) = 12.45 - 4605/(T/K)$; temp range 344.4–393.8 K (isoteniscope method, Sachinidis & Hill 1980)
 0.070*, 0.050* (20°C, gas saturation method, vapor pressure balance, OECD 1981)
 0.112* (25.25°C, Knudsen effusion method, temp range 20.25–40.25°C, Colomina et al. 1982)
 $\log(P/\text{Pa}) = (14.87 \pm 0.02) - (4719.6 \pm 7.1)/(T/K)$; temp range 293.4–313.4 K (Antoine eq., Knudsen effusion, Colomina et al. 1982)
 0.0907 (20°C, evaporation method, Gückel et al. 1982)
 0.105* (diaphragm manometer/torsion mass-loss effusion, extrapolated from measured range 316–391 K, de Kruif & Block 1982)
 0.109 ± 0.005 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
 0.9505 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 9.033 - 3333.3/(T/K)$, temp range 60–110°C (Antoine eq., Dean 1985, 1992)
 0.105 (solid P_s , interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_s/\text{kPa}) = 15.94025 - 7420.596/(74.333 + T/K)$; temp range 294–321 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log(P_s/\text{kPa}) = 11.8285 - 4719.5/(T/K)$; temp range 343–373 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)
 0.772 (liquid P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.80911 - 2776.12/(-43.978 + T/K)$; temp range 405–523 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
 0.600 (20°C, OECD 1981; quoted, Howard 1989)
 $\log(P/\text{mmHg}) = -140.0388 + 80.479/(T/K) + 62.611 \cdot \log(T/K) - 6.5321 \times 10^{-2} \cdot (T/K) + 2.4596 \times 10^{-5} \cdot (T/K)^2$; temp range 396–751 K (vapor pressure eq., Yaws 1994)
 0.13* (26°C, Knudsen effusion, measured range 26–50°C, Li et al. 2002)
 $\ln(P/\text{Pa}) = (34.031 \pm 0.30) - (10790 \pm 93)/(T/K)$; temp range 299–323 K (Knudsen effusion technique, Li et al. 2002)
 $\ln(P/\text{Pa}) = 34.320 - 10866/(T/K)$; temp range 304–317 K (regression eq. of Ribeiro da Silva et al. 1995 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (34.181 \pm 0.446) - (10836 \pm 140)/(T/K)$; temp range 299–328 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C):

- 0.00709 (Howard 1989)
 0.00575; 0.0110 (calculated-P/C, calculated-bond contribution, Meylan & Howard 1991)
 0.00415 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 1.87 (shake flask-UV, Fujita et al. 1964)
- 1.68 (shake flask-UV, Halmekoski & Hannikainen 1964)
- 1.85 \pm 0.01 (shake flask-UV, Iwasa et al. 1965)
- 2.03 (shake flask-LSC, Lu & Metcalf 1975)
- 1.78 \pm 0.01, 1.77 \pm 0.01 (HPLC- k' correlation, Unger et al. 1978)
- 1.79 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
- 1.86, 1.87 (calculated-fragment const., Rekker 1977)
- 1.94 (RP-HPLC correlation, Hanai & Hubert 1982)
- 1.95 (HPLC- k' correlation; Miyake & Terada 1982)
- 1.87 (microelectrometric titration, Clarke 1984)
- 2.18 \pm 0.03; 2.03 (exptl.-ALPM, selected best lit. value, Garst & Wilson 1984)
- 1.44, 1.87 (HPLC- k' correlation, Haky & Young 1984)
- 1.88 (shake flask-UV at pH 0.5, Nishimura et al. 1985)
- 1.97 (microelectrometric titration, Clarke & Cahoon 1987)
- 1.94 (shake flask-radiochemical method, at pH 0.5, Laznicek et al. 1987)
- 1.93 (HPLC- k' correlation, Miyake et al. 1987)
- 1.88 (CPC, Berthod et al. 1988)
- 1.85 \pm 0.04 ("Filter Chamber"-UV, Hersey et al. 1989)
- 1.87 (recommended, Sangster 1989, 1993)
- 1.88 (back flashing-CPC centrifugal partition chromatography, Menges et al. 1990)
- 1.87 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

- 1.32, 2.00, 2.14 (fish, algae, mosquito, Lu & Metcalf 1975)
- 3.26, 3.45 (daphnia, snail, Lu & Metcalf 1975)
- 0.48 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
- 1.43 (alga *Chlorella fusca*, calculated- K_{ow} , Geyer et al. 1984)
- < 1.0 (golden ide, Freitag et al. 1985)
- < 1.0 (algae, Freitag et al. 1985)
- 3.11 (activated sludge, Freitag et al. 1985)
- 1.15 (trout muscle, calculated- K_{ow} , Branson 1978)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.26; 1.86; 0.602 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
- 1.50 (soil, quoted exptl., Meylan et al. 1992)
- 1.16 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 1.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: rate of evaporation $k = 1.89 \times 10^{-8} \text{ mol cm}^{-2} \text{ h}^{-1}$ at 20°C determined by evaporation method (Gückel et al. 1982).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.0 \text{ d}$, based on estimated vapor-phase reaction with hydroxyl radical in air (Howard 1989).

Hydrolysis: $k = 4.3 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ for reactions of hydroxyl radical in aqueous solution (Buxton et al. 1986)

$k = 1.15 \times 10^{13} \text{ M}^{-1} \text{ h}^{-1}$ (Mabury & Crosby 1996);

$k(\text{exptl}) = 1.2 \times 10^{13} \text{ M}^{-1} \text{ h}^{-1}$ for reaction with hydroxy radical (Armbrust 2000)

Biodegradation: completely degraded by a soil microflora after 24 h (Alexander & Lustigman 1966; quoted, Verschueren 1983);

completely degraded for 16 mg/L concn. within one day by soil and by wastewater (Haller 1978);

$t_{1/2} \sim 0.2\text{--}3.6$ d if released into water, should readily biodegrade (Howard 1989);
average $k(\text{exptl}) = 0.11533 \text{ h}^{-1}$ compared to group method predicted $k = 0.0993 \text{ h}^{-1}$ (nonlinear) and $k = 0.0263 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993).

Biotransformation: degradation $k = 6.84 \times 10^{-17} \text{ mol cell}^{-1} \text{ h}^{-1}$ in pure culture system (Banerjee et al. 1984).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} \sim 2.0$ d for reactions with photochemically produced hydroxyl radical (Howard 1989).
Surface water: if released into water, should readily biodegrade with an estimated $t_{1/2} = 0.2\text{--}3.6$ d (Howard 1989).
Groundwater:
Sediment:
Soil:
Biota:

TABLE 13.1.2.1.1
Reported aqueous solubilities of benzoic acid at various temperatures

Ward & Cooper 1930		Morrison 1944		Strong et al. 1989	
shake flask-synthetic method		thermostatic and synthetic		shake flask-weight titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
24.6	3340	25.0	3298	5	1830
42.4	6280	35.0	4641	15	2482
57.8	10930	45.0	6167	25	3416
74.1	20670	55.4	10137	35	4776
83.1	31300	60.2	12213	45	6656
88.3	39660	64.6	14533	55	9629
		68.5	16976	65	14325
		75.1	22838		
		79.3	26991		
		82.1	31021		
		88.6	43356		

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 23.29$
25°C

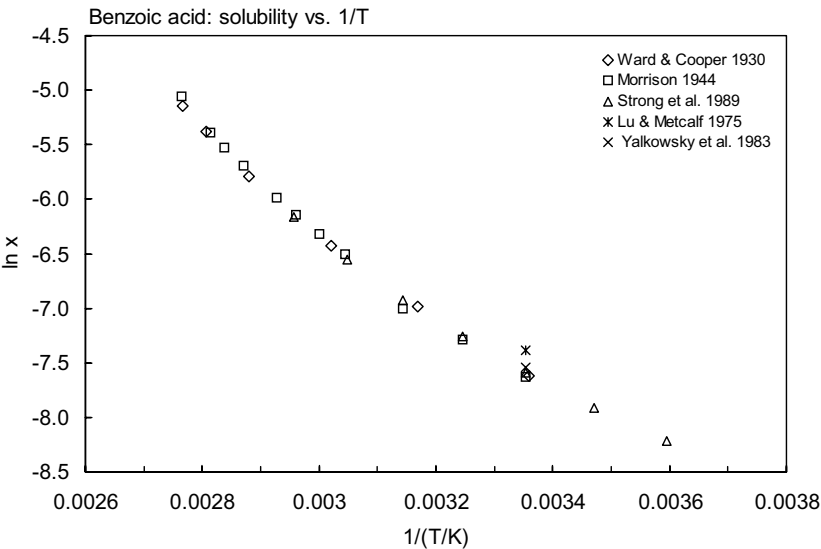


FIGURE 13.1.2.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzoic acid.

TABLE 13.1.2.1.2

Reported vapor pressures of benzoic acid at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & & \end{aligned}$$

1.

Kahlbaum 1898		Klosky et al. 1927		Stull 1947		Davies & Jones 1954	
static method-manometer*		isoteniscope method		summary of literature data		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
solid							
122.2	799.9	60.1	6.893	96.0	133.3	70.48	12.35
132.5	1333	80.4	41.06	119.5	666.6	75.14	19.33
146.5	2666	100.2	190.1	132.1	1333	80.43	31.02
155.5	4000	121.0	777.3	146.7	2666	84.47	44.0
161.9	5333			162.6	5333	89.88	68.66
167.2	6666	eq. 1	P/mmHg	172.8	7999	95.35	108.9
178.5	9999	A	11.956	186.2	13332	100.59	149.2
185.9	13332	B	4409	205.8	26664	105.05	230.8
196.5	19998			227.0	53329	109.85	341.0
204.9	26664		liquid	249.2	101325	114.11	458.1
211.5	33331	128.6	1120				
217.0	39997	134.5	1573	mp/°C	121.7	eq. 1	P/mmHg
225.8	53329	148.0	2960			A	12.8699
233.8	66661	158.2	4533			B	4775.7
239.8	79993	172.8	8506				
245.5	93326	187.6	14772			$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 91.42$	
249.0	101325	199.7	22238			at 365.5 K	
		216.2	38224			$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 94.37$	
		233.0	63835			at 298.15 K	
		247.0	95739				
		eq. 4	P/mmHg				
		A	30.172				
		B	4714				
		C	6.720				

*complete list see [ref.](#)

2.

Wiedemann 1971		Malaspina et al. 1973		Sachinidis & Hill 1980		OECD 1981	
Knudsen effusion		Knudsen effusion		isoteniscope-manometer		gas saturation/effusion	
T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
gas saturation							
290.4	0.0613	65.05	9.879	344.4	16.80	10	0.02
294.4	0.118	71.35	16.72	352.8	37.73	20	0.07
298.3	0.160	74.65	23.91	373.7	167.6	30	0.24
299.8	0.205	77.95	29.69	393.8	733.5	40	0.76
300.5	0.244	85.25	55.02			50	2.20
301.1	0.220	89.15	76.1	eq. 1	P/mmHg	vapor pressure balance	
304.4	0.337	94.05	112.5	A	12.45	10	0.012
315.5	1.173	99.75	169.2	B	4605	20	0.05

TABLE 13.1.2.1.2 (Continued)

Wiedemann 1971		Malaspina et al. 1973		Sachinidis & Hill 1980		OECD 1981	
Knudsen effusion		Knudsen effusion		isoteniscope-manometer		gas saturation/effusion	
T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
293.36	0.0889*	105.05	255.3	$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 88.1$		30	0.17
293.56	0.0907*	110.25	362.7			40	0.56
293.36	0.0893*					50	1.70
eq. 1	P/mmHg	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.92$ at 298.15 K		<div>DePablo 1976</div> <div>effusion method</div>			
A	12.2937	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.18$					
B	4530.02	at 360.8 K					
$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 86.61$		eq. 1	P/mmHg				
*different orifice areas of Knudsen effusion cell		A	12.175	25	0.108		
		B	4501	45	1.03		
		temp range 338.2–383.4 K		70.25	11.92		
		calculated average value					
		$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 94.5$ at 298 K					

3.

Colomina et al. 1982		de Kruif & Block 1982		Li et al. 2002	
Knudsen effusion		manometer/effusion		Knudsen effusion	
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
293.4	0.0604	316.4	0.89	299.15	0.13
293.67	0.063	321.01	1.44	303.25	0.22
295.5	0.0781	321.25	1.48	308.15	0.38
295.75	0.0814	323.58	1.9	313.15	0.66
296.59	0.09	328.73	3.25	318.15	1.13
298.38	0.112	329.01	3.34	323.15	1.86
298.95	0.119	335.67	6.44		
301.19	0.157	338.66	8.6	eq. 1a	P/Pa
301.71	0.167	344.64	14.74	A	34.031
304.47	0.23	347.6	19.6	B	10790
305.15	0.25	350.01	24.17		
307.6	0.334	353.14	31.79		
308.11	0.354	359.05	52.37		
308.34	0.365	361.41	63.5		
310.14	0.445	364.96	84.69		
311.17	0.503	367.77	106.4		
311.29	0.508	368.43	111.9		
313.38	0.64	383.04	334.8		
		390.93	588.4		
eq. 1		Data fitted to 3-parameter vapor-pressure eq. see ref. at 395.52K			
A	14.87				
B	4719.6				
$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 90.6 \pm 0.2$		$\Delta H_{\text{v}}/(\text{kJ/mol}) = 69.2$			
temp range 293–313 K		$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 87.4$			
		$\Delta H_{\text{fus}}/(\text{kJ/mol}) = 18.0$			

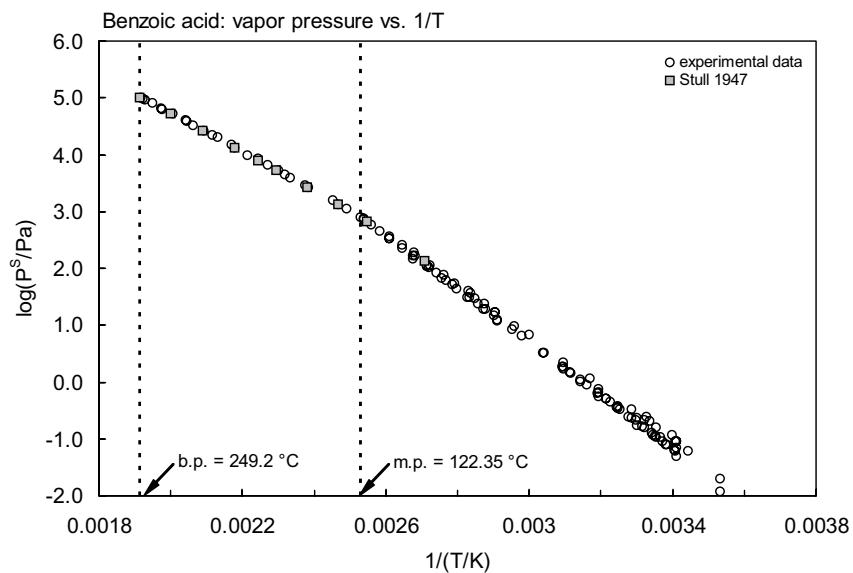
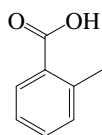


FIGURE 13.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for benzoic acid.

13.1.2.2 2-Methyl benzoic acid (*o*-Toluic acid)

Common Name: *o*-Toluic acid

Synonym: 2-methyl benzoic acid

Chemical Name: *o*-toluic acid, 2-methyl benzoic acid

CAS Registry No: 118-90-1

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

103.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

259 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.062 (115 $^{\circ}C$, Weast 1982–83; Verschueren 1983)

Molar Volume (cm^3/mol):

157.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.91 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968)

3.91 (Weast 1982–83)

3.90 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.17 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

53.56 (Tsonopoulos & Prausnitz 1971)

53.5, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.170 (mp at $103.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

22300* (85.1 $^{\circ}C$, shake flask-residue volume, measured range 85.1–102.4 $^{\circ}C$, Sidgwick et al. 1915)

1185 (shake flask, Fühner 1924)

1162* (shake flask-weight titration, measured range 5–65 $^{\circ}C$, Strong et al. 1989)

1074* (shake flask-UV, Sugunan & Thomas 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log(P/mmHg) = -35.8816 - 3.2354 \times 10^3/(T/K) + 21.133 \cdot \log(T/K) - 3.0165 \times 10^{-2} \cdot (T/K) + 1.1587 \times 10^{-5} \cdot (T/K)^2$;
temp range 377–751 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.18 (shake flask-UV, Tomida et al. 1978)

2.81 (Scherrer & Howard 1979)

2.46 (shake flask at pH 1, Hansch & Leo 1987)

2.27 (shake flask-UV at pH 2, Da et al. 1992)

2.46 (recommended, Sangster 1993)

2.46 (recommended, pH 1, Hansch et al. 1995)

1.72 (RP-HPLC-RT correlation on short ODP column, pH 2, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 16 d (Alexander & Lustigman 1966; quoted, Verschueren 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 13.1.2.2.1

Reported aqueous solubilities of 2-methylbenzoic acid (*o*-toluic acid) at various temperatures

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993	
shake flask-residue volume		shake flask-titration		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
85.1	22300	5	568.3	20	825
109.1	36600	15	806.6	25	1074
118.3	50000	25	1162	35	1620
130.4	69900	35	1695	40	1883
143.7	102000	45	2522		
156.5	202300	55	3778		
160.2	314700	65	5775		
161.2	399200				
160.2	486300	$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 28.92$			
154.6	601600	25°C			
147.4	701200				
119.8	846400				
97.2	905300				
93.7	918800				
94.4	938300				
96.0	959500				
102.4	1000000				
critical solution temp 161.2°C					
triple point 93.5°C					
mp 102.4°C					

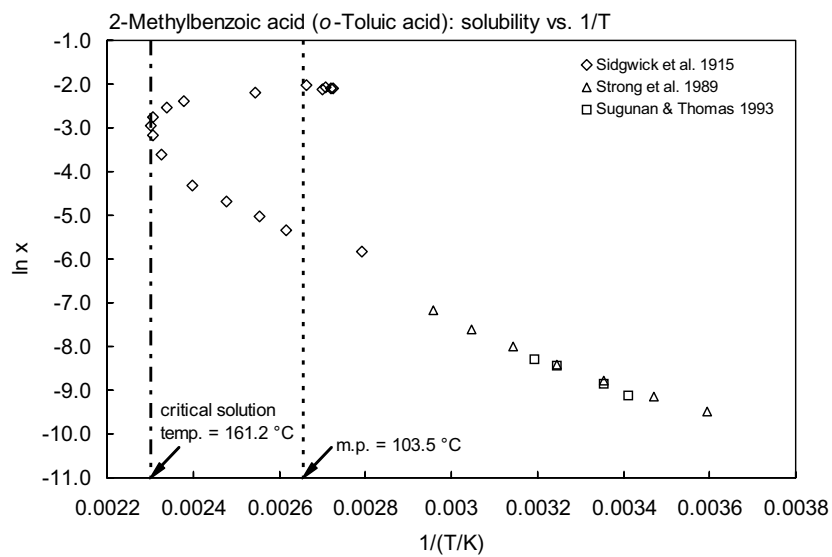
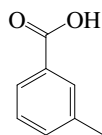


FIGURE 13.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-methylbenzoic acid.

13.1.2.3 3-Methyl benzoic acid (*m*-Toluic acid)

Common Name: *m*-Toluic acid

Synonym: 3-methyl benzoic acid

Chemical Name: *m*-toluic acid, 3-methyl benzoic acid

CAS Registry No: 99-04-7

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

109.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

263.0 (sublimation, Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

1.054 ($112^{\circ}C$, Weast 1982–83; Verschuereen 1983)

Molar Volume (cm^3/mol):

129.2 ($112^{\circ}C$, Stephenson & Malanowski 1987)

157.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.270 (Weast 1982–83)

4.269 (Dean 1985)

4.220 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.73 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

10.96 (Tsonopoulos & Prausnitz 1971)

41.17, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.147 (mp at $109.9^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11600* ($80^{\circ}C$, shake flask-residue volume, measured range 80 – $110.5^{\circ}C$, Sidgwick et al. 1915)

982 (shake flask-residue volume method, Fühner 1924)

1700 (20 – $25^{\circ}C$, shake flask-GC, Urano et al. 1982)

872* (shake flask-weight titration, measured range 5 – $65^{\circ}C$, Strong et al. 1989)

1246* (shake flask-UV, Sugunan & Thomas 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log (P_L/kPa) = 8.1472 - 3280.8/(T/K)$, temp range 473 – $533 K$ (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.37 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)

2.43 (HPLC- k' correlation, Miyake & Terada 1982)

2.41 (shake flask-AS, Miyake et al. 1987)

2.39 (centrifugal partition chromatography CPC, Terada et al. 1987)

2.44; 2.47 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)

2.38 (shake flask-UV at pH 2, Da et al. 1992)

- 2.37 (recommended, Sangster 1993)
 2.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschueren 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.2.3.1

Reported aqueous solubilities of 3-methylbenzoic acid (*m*-toluic acid) at various temperatures

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993	
shake flask-residue volume		shake flask-titration		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
80	11600	5	449.3	20	1070
89.8	15300	15	621	25	1246
118.6	31300	25	872	35	1544
140.5	58800	35	1270	40	1720
153.3	99600	45	1852		
162.2	299400	55	2754		
162.1	401100	65	4115		
160.7	501000	75	6492		
157.7	601500				
145.1	711700	$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 26.15$			
129.6	795700				
121.8	820600				
105.9	866700				
96.4	893200				
94.2	924500				
101.9	969300				
110.5	1000000				
critical solution temp 162.2°C					
triple point		142.0°C			
mp		110.5°C			

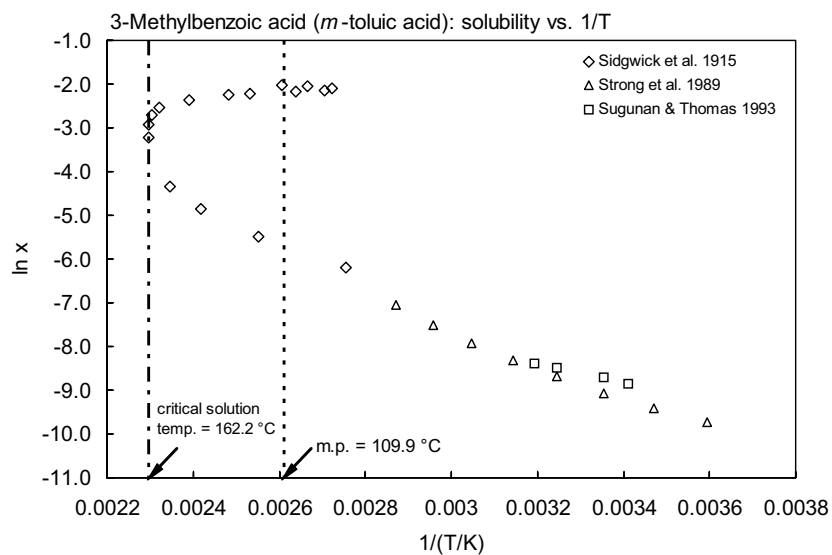
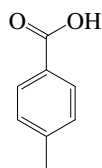


FIGURE 13.1.2.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-methylbenzoic acid (*m*-toluic acid).

13.1.2.4 4-Methyl benzoic acid (*p*-Toluic acid)

Common Name: *p*-Toluic acid

Synonym: 4-methyl benzoic acid

Chemical Name: *p*-toluic acid, 4-methyl benzoic acid

CAS Registry No: 99-94-5

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

179.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

275.0 (sublimation, Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

157.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.37, 4.30 ± 0.09 (quoted, HPLC, Unger et al. 1978)

4.37, 4.41 ± 0.01 (quoted, HPLC, Unger et al. 1978)

4.36 (Weast 1982–83)

4.37, 4.26 (quoted, shake flask-TN, Clarke 1984)

4.362 (Dean 1985)

4.39 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.72 (Tsonopoulos & Prausnitz 1971)

23.81 (differential scanning calorimetry, Li et al. 2001)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

50.21 (Tsonopoulos & Prausnitz 1971)

50.21, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.0304 (mp at $179.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11600* (100, shake flask-residue volume, measured range 100 – $176.8^{\circ}C$, Sidgwick et al. 1915)

383 (selected, Tsonopoulos & Prausnitz 1971)

343* (shake flask-weight titration, measured range 5 – $65^{\circ}C$, Strong et al. 1989)

331* (shake flask-UV, Sugunan & Thomas 1993)

378.5* (shake flask-titration, measured range 278.15 – $343.15\ K$, Apelblat & Manzurola 1999)

$\ln [m/(mol\ kg^{-1})] = -264.605 - 9059.53/(T/K) + 40.069 \cdot \ln (T/K)$; temp range 278 – $343\ K$ (shake flask-titration, Apelblat & Manzurola 1999)

371* (shake flask-laser monitoring observation technique, measured range 288.35 – $370.95\ K$, Li et al. 2001)

393* ($26.4^{\circ}C$, synthetic method-laser technique, measured range 290.25 – $348.45\ K$, Chen & Ma 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

30.93* ($95.20^{\circ}C$, Knudsen effusion, measured range 95.2 – $134.96^{\circ}C$ (Davies & Jones 1954)

$\log (P/mmHg) = 128585 - 4968.7/(T/K)$; temp range 95.2 – $134.96^{\circ}C$ (Knudsen effusion, Davies & Jones 1954)

$\log (P/mmHg) = -67.6587 - 2.2339 \times 10^3/(T/K) + 33.347 \cdot \log (T/K) - 3.7709 \times 10^{-2} \cdot (T/K) + 1.313 \times 10^{-5} \cdot (T/K)^2$; temp range 453 – $773\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.27 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971)
- 2.22 \pm 0.02, 2.26 \pm 0.01 (HPLC-RT correlation, Unger et al. 1978)
- 2.36 (shake flask-UV at pH 2, Ezumi & Kubota 1980)
- 2.43 (calculated-HPLC- k' correlation, Miyake & Terada 1982)
- 2.34 (electrometric titration, Clarke 1984)
- 2.67 (HPLC-RT correlation, Garst 1984)
- 2.66 (centrifugal partition chromatography CPC, Terada et al. 1987)
- 2.38; 2.41 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)
- 2.35 (HPLC-RT correlation, Jenke et al. 1990)
- 2.26 (shake flask-UV at pH 2, Da et al. 1992)
- 2.34 (recommended, Sangster 1994)
- 2.27 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.15, 1.15, 1.30 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 1.77 (soil, quoted exptl., Meylan et al. 1992)
- 1.37 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 8 d (Alexander & Lustigman 1966; quoted, Verschuereen 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.2.4.1

Reported aqueous solubilities of 4-methylbenzoic acid (*p*-toluic) acid at various temperatures

1.

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993		Apelblat & Manzurola 1999	
shake flask-residue volume		shake flask-titration		shake flask-UV		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
100	11600	5	177.8	20	263	5.0	201.5
110	13600	15	243.5	25	331	11.0	249.2
114.4	15100	25	343	35	466	17.0	271.0
133.7	29600	35	486	40	534	21.5	309.1
141.4	49700	45	695			25.0	378.5
150.9	100800	55	1008			25.5	318.6
157.9	202700	65	1485			30.0	469.8
159.1	301400					30.0	488.8
158.5	405700	$\Delta H_{sol}/(kJ\ mol^{-1}) = 26.74$ 25°C				35.0	499.7
158.0	503800					35.0	501.1
152.6	605500					35.0	502.4
145.1	796800					40.0	593.7

TABLE 13.1.2.4.1 (Continued)

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993		Apelblat & Manzurola 1999	
shake flask-residue volume		shake flask-titration		shake flask-UV		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
156.5	925200					40.0	595.0
176.8	1000000					40.0	638.6
						45.0	721.7
Critical solution temp	159.1°C					50.0	887.8
Triple point	142°C					52.0	912.3
mp	176.8°C					55.0	1062
						58.0	1185
						60.0	1283
						61.0	1389
						65.0	1525
						67.0	1702
						70.0	1865
							$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 24.0$
							at 298.15 K
							$\ln S = A + B/T + C \ln T$
							S mol·kg ⁻¹
							A -264.605
							B 9059.53
							C 40.069

2.

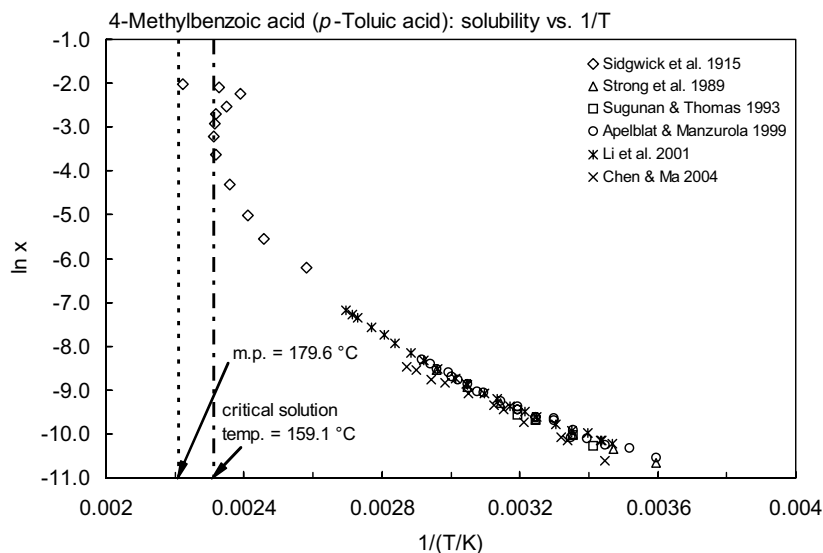
Li et al. 2001		Chen & Ma 2004	
shake flask-laser monitor		synthetic method	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
15.2	272.3	290.25	185.0
17.8	295	299.55	292.7
17.9	295	301.25	315.3
21.3	347.6	311.25	448.6
25.2	370.7	317.25	596.4
29.4	423.6	320.05	657.0
34.7	506.8	327.75	857.8
37.8	567.3	335.35	1109
42.1	650.5	339.85	1190
46.0	756.4	344.95	1465
49.8	869.9	348.35	1570
55.1	1051		
55.3	1074		
58.6	1210		
64.4	1520		
69.1	1838		
73.7	2201		
79.1	2723		
83.3	3260		
87.7	3911		

(Continued)

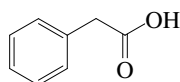
TABLE 13.1.2.4.1 (Continued)

Li et al. 2001		Chen & Ma 2004	
shake flask-laser monitor		synthetic method	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
93.1	4834		
95.5	5204		
97.8	5726		

$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 23.81$

FIGURE 13.1.2.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 4-methylbenzoic acid (*p*-toluic acid).

13.1.2.5 Phenylacetic acid



Common Name: Phenylacetic acid

Synonym: phenylethanoic acid, α -toluic acid, benzenecetic acid

Chemical Name: phenylacetic acid

CAS Registry No: 103-82-2

Molecular Formula: $C_8H_8O_2$, $C_6H_5CH_2COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

76.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

265.5 (Stull 1947; Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.081 (Verschuereen 1983)

Molar Volume (cm^3/mol):

124.8 ($77^{\circ}C$, Stephenson & Malanowski 1987)

157.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.28 ($18^{\circ}C$, Weast 1982–83)

4.31 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.11 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

48.95 (Tsonopoulos & Prausnitz 1971)

41.42, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.312 (mp at $76.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

17700* (thermostatic and synthetic methods, measured range 25 – $86.7^{\circ}C$, Morrison 1944)

16600 ($20^{\circ}C$, Hodgman 1952)

17790 (selected, Tsonopoulos & Prausnitz 1971)

16600 ($20^{\circ}C$, quoted, Verschuereen 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.835 (extrapolated-regression of tabulated data, temp range 97 – $265^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 15568.7/(T/K)] + 9.206178$; temp range 97 – $265.5^{\circ}C$ (Antoine eq., Weast 1972–73)

0.827 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P/kPa) = 8.00148 - 3144.95/(-14.408 + T/K)$; temp range 370 – $539\ K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0056 (calculated- P/C)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.41 (shake flask-AS, Fujita et al. 1964; Leo et al. 1971)

1.41 ± 0.01 (shake flask-UV, Iwasa et al. 1965)

1.51 (shake flask-UV, Yaguzhinskii et al. 1973)

1.94 (RP-LC-RT correlation, Hanai & Hubert 1982)

1.45 (shake flask-UV at pH 3.5, Kuchar et al. 1982)

1.95 ± 0.04 ; 1.51 (exptl.-ALPM, selected best lit. value, Garst 1984)

1.41 (recommended, Sangster 1989, 1993)

1.34 ± 0.14, 1.07 ± 0.49 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k' correlation, Cichna et al. 1995)

1.41 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

1.49, 1.42, 1.45 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)

1.45 (soil, quoted exptl., Meylan et al. 1992)

1.42 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

1.45 (soil, quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 13.1.2.5.1

Reported aqueous solubilities of phenylacetic acid at various temperatures:

Morrison 1944

thermostatic and synthetic

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
25.0	17700
35.0	26005
45.0	39484
41.5	39211
58.4	49695
68.8	59225
76.5	69845
83.0	83188
86.7	93399

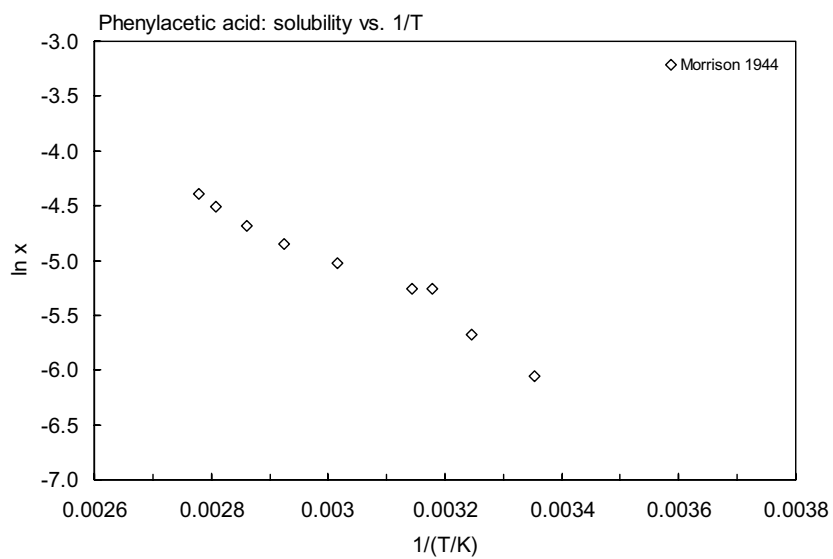
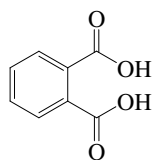


FIGURE 13.1.2.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for phenylacetic acid.

13.1.2.6 Phthalic acid



Common Name: Phthalic acid

Synonym: 1,2-benzene dicarboxylic acid, *o*-phthalic acid

Chemical Name: 1,2-benzene dicarboxylic acid, *o*-phthalic acid

CAS Registry No: 88-99-3

Molecular Formula: $C_8H_6O_4$, $C_6H_4-1,2-(COOH)_2$

Molecular Weight: 166.132

Melting Point ($^{\circ}C$):

230 (dec., Lide 2003)

Boiling Point ($^{\circ}C$):

dec (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.593 (Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

173.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.89, 5.51 (pK_1 , pK_2 , Weast 1982–83)

2.95, 5.408 (pK_1 , pK_2 , Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section)

7014* (shake flask-synthetic method, measured range 25 – $85^{\circ}C$, McMaster et al. 1921):

7160* ($25.8^{\circ}C$, shake flask-synthetic method, measured range 25.8 – $113.8^{\circ}C$, Ward & Cooper 1930)

5400 ($14^{\circ}C$, Verschueren 1983)

6300 (Dean 1985)

7024* (shake flask, measured range 283.65 – 338.15 K, Apelblat & Manzurolo 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log(P/mmHg) = -90.3221 - 3.2214 \times 10^3/(T/K) + 44.109 \cdot \log(T/K) - 5.0056 \times 10^{-2} \cdot (T/K) + 1.6895 \times 10^{-5} \cdot (T/K)^2$;
temp range 464 – 800 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.79 (shake flask-UV, Tomida et al. 1978)

0.15 (electrometric titration, Freese et al. 1979)

0.73 (shake flask at pH 1, Log P Database, Hansch & Leo 1987)

0.71 ($30^{\circ}C$, shake flask-UV at pH 1, Patrunkey & Pflegel 1992)

0.73 (recommended, Sangster 1993)

0.73 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, log K_{OC} :

0.301, 1.49, 0.301	(sediment, Podzol soil, Alfidol soil, von Oepen et al. 1991)
1.07	(soil, quoted exptl., Meylan et al. 1992)
1.87	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.07	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate of biodegradation $78.4 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 2 \text{ d}$ in initial phase, $t_{1/2} = 15 \text{ d}$ in late phase in sludge -amended soil (Roslev et al. 1998)

Biota:

TABLE 13.1.2.6.1**Reported aqueous solubilities of *o*-phthalic acid at various temperatures**

McMaster et al. 1921		Ward & Cooper 1930		Apelblat & Manzurola 1989	
shake flask-synthetic method		shake flask-synthetic method		shake flask-titration	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	T/K	$\text{S/g}\cdot\text{m}^{-3}$
25	7014	25.8	7160	283.65	2617
35	10125	43.7	13210	296.15	6546
45	14460	48.9	16470	298.15	7026
55	21680	58.0	22760	302.65	8633
65	32460	63.7	28970	307.15	9839
75	49260	77.8	53220	309.15	11020
85	78870	85.7	75940	311.15	11638
		94.8	118500	315.15	13936
		101.1	157900	317.15	15146
		113.8	294600	318.15	15164
				319.15	16705
				323.15	18893
				323.15	20554
				327.15	22926
				334.15	29783
				338.15	36955
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 29.0$					

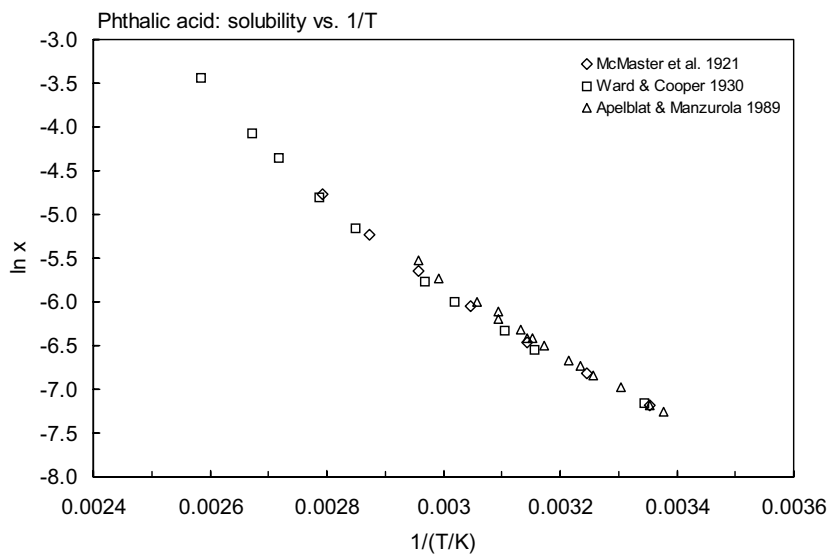
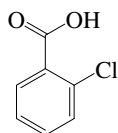


FIGURE 13.1.2.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for phthalic acid.

13.1.2.7 2-Chlorobenzoic acid



Common Name: 2-Chlorobenzoic acid

Synonym: *o*-chlorobenzoic acid

Chemical Name: 2-chlorobenzoic acid, *o*-chlorobenzoic acid

CAS Registry No: 118-91-2

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

140.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Verschuereen 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5440 (Weast 1982–83, Verschuereen 1983)

1.5440 ($25^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

101.4 ($20^{\circ}C$, calculated-density)

155.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.920 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968; Weast 1982–83)

2.877 (Dean 1985)

3.850 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.73 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

62.34 (Tsonopoulos & Prausnitz 1971)

62.26, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0741 (mp at $140.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2130 (Osol & Kilpatrick 1933)

2114 (selected, Tsonopoulos & Prausnitz 1971)

2100 (Verschuereen 1983)

1100 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

$\log (P/mmHg) = -42.9847 - 3.1867 \times 10^3/(T/K) + 23.694 \cdot \log (T/K) - 3.0284 \times 10^{-2} \cdot (T/K) + 1.0828 \times 10^{-5} \cdot (T/K)^2$;
temp range 415–792 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.98 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1979, 1987)

2.63; 2.56 (calculated-fragment const., calculated- π const. Rekker 1977)

2.66 (shake flask-UV, Tomida et al. 1978)

1.99 (centrifugal partition chromatography, Berthod et al. 1988)

2.02 (shake flask-UV at pH 2, Da et al. 1992)

1.99 (recommended, Sangster 1993)

2.05 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by soil microflora: $t_{1/2} > 64$ d, biodegradation by waste water at pH 7.3 and 30°C, $t_{1/2} > 25$ d, and degradation by soil suspension at pH 7.3 and 30°C; $t_{1/2} = 7\text{--}14$ d (Alexander & Lustigman 1966; quoted, Verschueren 1983);
complete degradation of 16 mg/L by soil in 7–14 d (Haller 1978).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

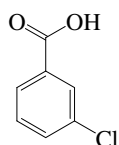
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.8 3-Chlorobenzoic acid



Common Name: 3-Chlorobenzoic acid

Synonym: *m*-chlorobenzoic acid

Chemical Name: 3-chlorobenzoic acid, *m*-chlorobenzoic acid

CAS Registry No: 535-80-8

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

158 (Weast 1982–83; Verschueren 1983; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Verschueren 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4960 ($25^{\circ}C$, Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

104.7 ($25^{\circ}C$, calculated-density)

155.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.82 (Weast 1982–83)

3.83 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.85 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

55.65 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.0496$ (mp at $158^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

385 (Osol & Kilpatrick 1933)

398 (selected, Tsonopoulos & Prausnitz 1971)

400 ($0^{\circ}C$, Verschueren 1983)

400 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.68 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1979)

2.65, 2.52 (calculated-fragment const., calculated- π const, Rekker 1977)

0.89 (HPLC-RT correlation, Veith et al. 1979)

2.57 (HPLC- k' correlation, Miyake & Terada 1982)

2.62 (centrifugal partition chromatography, Terada et al. 1987)

2.51; 2.58 (shake flask at pH 1; HPLC-RT correlation, Wang et al. 1989)

2.72 (shake flask-UV at pH 2, Da et al. 1992)

2.60 (recommended, Sangster 1993)

2.68 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct aqueous photolysis $k = 0.013 \pm 0.001 \text{ min}^{-1}$ with $t_{1/2} = 55 \text{ min}$ (Stegeman et al. 1993).

Oxidation:

Hydrolysis:

Biodegradation: decomposed by soil microflora, $t_{1/2} = 32 \text{ d}$ (Alexander & Lustigman 1966; quoted, Verschueren 1983);

complete degradation of 16 mg/L by soil and by wastewater in 7–14 d (Haller 1978).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

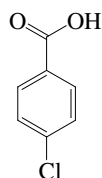
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.9 4-Chlorobenzoic acid



Common Name: 4-Chlorobenzoic acid

Synonym: *p*-chlorobenzoic acid

Chemical Name: 4-chlorobenzoic acid, *p*-chlorobenzoic acid

CAS Registry No: 74-11-3

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

243.0 (Weast 1982–83; Verschueren 1983; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Verschueren 1983)

Density (g/cm^3 at $20^{\circ}C$):

1.541 ($24^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

155.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.98 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968)

3.98 (Weast 1982–83)

3.98, 3.85 (quoted, shake flask-TN, Clarke 1984)

3.986 (Dean 1985)

3.850 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

32.26 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

62.76 (Tsonopoulos & Prausnitz 1971)

62.9, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.00726$ (mp at $243^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

68.0 (Osol & Kilpatrick 1933)

72.6 (selected, Tsonopoulos & Prausnitz 1971)

77.0 (Verschueren 1983)

200 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.65 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)

2.65; 2.52 (calculated-fragment const., calculated- π const., Rekker 1977)

2.53; 2.65 (HPLC- k' correlation, Miyake & Terada 1982)

2.66 (electrometric titration, Clarke 1984)

2.72 (shake flask-OECD 1981 Guidelines., Geyer et al. 1984)

2.65 (centrifugal partition chromatography, Terada et al. 1987)

2.60; 2.67 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)

2.67 (HPLC-RT correlation, Wang et al. 1989)

- 2.65 (HPLC-RT correlation, Hayward et al. 1990)
- 2.71 (countercurrent chromatography, average value, Vallat et al. 1990)
- 2.66 (centrifugal partition chromatography; El Tayar et al. 1991)
- 2.62 (shake flask-UV at pH 2, Da et al. 1992)
- 2.65 (recommended, Sangster 1994)
- 2.65 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- < 1.0, 1.80, 2.23 (golden orfe, algae, activated sludge, Freitag et al. 1982)
- 1.80, 1.99 (alga *chlorella fusca*, wet wt. basis, calculated- K_{OW} , Geyer et al. 1984)
- < 1.0, 1.78, 2.23 (golden ide, algae, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

$k(aq.) \leq 0.15 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2–6 and $22 \pm 1^\circ\text{C}$, with $t_{1/2} \geq 3 \text{ d}$ at pH 7 (Yao & Haag 1991).

Hydrolysis:

Biodegradation: decomposition by a soil microflora, $t_{1/2} = 64 \text{ d}$; degradation by waste water or soil suspension at pH 7.3 and 30°C , $t_{1/2} > 25 \text{ d}$ (quoted, Verschueren 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} \geq 3 \text{ d}$ at pH 7 based on reaction rate with ozone in water (Yao & Haag 1991)

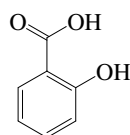
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.10 Salicylic acid



Common Name: Salicylic acid

Synonym: 2-hydroxybenzoic acid, *o*-hydroxybenzoic acid

Chemical Name: salicylic acid, 2-hydroxybenzoic acid

CAS Registry No: 69-72-7

Molecular Formula: $C_7H_6O_3$, HOC_6H_4COOH

Molecular Weight: 138.121

Melting Point ($^{\circ}C$):

159.0 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

256 (Verschueren 1983)

Density (g/cm^3 at $20^{\circ}C$):

1.443 (Weast 1982–83; Verschueren 1983)

Molar Volume (cm^3/mol):

95.7 ($20^{\circ}C$, calculated-density)

147.4 ($158.6^{\circ}C$, Stephenson & Malanowski 1987)

142.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.009 (Korman & La Mer 1936)

3.52 ± 0.03 (HPLC, Unger et al. 1978)

3.29 ± 0.03 (HPLC, Unger et al. 1978)

2.96 (equilibrium titration, Clarke & Cahoon 1987)

2.97 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0484 (mp at $159^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5570* ($50^{\circ}C$, synthetic method, measured range 50 – $159^{\circ}C$, critical solution temp. $89.5^{\circ}C$, Sidgwick & Ewbank 1921)

1840* ($20^{\circ}C$, synthetic method, measured, range 10 – $87^{\circ}C$, Bailey 1925)

1800 ($20^{\circ}C$, Hodgman 1952; Verschueren 1983)

1550 (shake flask-UV, Yalkowsky et al. 1983)

2555* (shake flask-TN, measured range 283.15 – $339.15 K$, Apelblat & Manzurola 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($113.7^{\circ}C$, summary of literature data, temp range 113.7 – $159^{\circ}C$, Stull 1947)

30.93* ($95.20^{\circ}C$, transpiration method, measured range 95.2 – $134.96^{\circ}C$, Davies & Jones 1954)

$\log(P/mmHg) = 12.8585 - 4968.7/(T/K)$, temp range 70.48 – $114.11^{\circ}C$ (transpiration, Davies & Jones 1954)

$\log(P/mmHg) = [-0.2185 \times 18920.7/(T/K)] + 10.822961$; temp range 113.7 – $256.0^{\circ}C$ (Antoine eq., Weast 1972–73)

2.85 ($70.5^{\circ}C$, effusion method, DePablo 1976)

0.0208 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.9834 - 4968.7/(T/K)$; temp range 368 – $408 K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.53812 - 1049.95/(-228.144 + T/K)$; temp range 445 – $504 K$ (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 177.3858 - 1.2871 \times 10^4/(T/K) - 56.301 \cdot \log (T/K) - 1.6667 \times 10^{-7} \cdot (T/K) + 1.1353 \times 10^{-5} \cdot (T/K)^2;$$

temp range 432–739 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.00144 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.26 (shake flask-GC, Hansch & Anderson 1967; quoted, Leo et al. 1971)
- 2.21 (shake flask, unpublished result, Leo et al. 1971)
- 2.24 (shake flask, pH 2, Korenman 1975)
- 2.38 (shake flask-UV, Tomida et al. 1978)
- 2.00 ± 0.01 , 2.18 ± 0.01 (HPLC-RT correlation, Unger et al. 1978)
- 2.26, 2.21, 2.24, 2.25, 0.95 (quoted lit. values; Hansch & Leo 1979)
- 1.90 (HPLC-RT correlation, Butte et al. 1981)
- 2.25 ± 0.03 (exptl.-ALPM, Garst & Wilson 1984)
- 1.13, 1.92 (HPLC- k' correlation, Haky & Young 1984)
- 2.21 (shake flask-HPLC at pH 2, Bundgaard et al. 1986; Bundgaard & Nielsen 1988)
- 2.34 (electrometric titration, Clarke & Cahoon 1987)
- 2.24 (shake flask-radiochemical method, at pH 0.5, Laznicek et al. 1987)
- 1.08 (RP-TLC retention time correlation, Jack et al. 1988)
- 0.78 (shake flask-UV, Kuban 1991)
- 2.64 (centrifugal partition chromatography, Ilchmann et al. 1993)
- 2.26 (recommended, Sangster 1993)
- 2.11 (recommended, pH 7.4, Hansch et al. 1995)
- 1.70 (pH 7.0), -0.90 (pH 7.4); 2.26 (literature values; Hansch et al. 1995)
- 2.02 (shake flask-micro-volume liquid-liquid flow extraction system, Carlsson & Karlberg 2000)
- 1.44 (shake flask, buffered with 20 mM phosphate buffer pH 7.4, Carlsson & Karlberg 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constants $k < 600 \text{ M}^{-1} \text{ s}^{-1}$ at pH 1.3–3, $k = (30 \pm 10) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ at pH 4–7 using 4 mM *t*-BuOH as scavenger for the reaction with ozone in water and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983a);

rate constants $k < 500 \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, $k = (2.8 \pm 3) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water using 4 mM *t*-BuOH as scavenger at pH 1.5–7 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983b).

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschuereen 1983);

average rate of biodegradation $95.0 \text{ mg COD g}^{-1} \cdot \text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:
Biota:

TABLE 13.1.2.10.1
Reported aqueous solubilities of salicylic acid at various temperatures

Sidgwick & Ewbank 1921		Bailey 1925		Apelblat & Manzurola 1989	
synthetic method		synthetic method		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
50.0	5570	10	1310	283.15	1533
56.0	7170	20	1840	298.15	2555
80.0	20260	30	2610	307.15	3385
97.9	52700	40	3950	317.15	4393
101.4	80200	50	5920	318.15	5196
105.6	168200	60	8640	320.15	5156
106.7	340200			323.15	5697
107.2	488180			324.15	6027
109.5	65400			325.15	6502
119.5	80000			327.15	7166
131.8	89750			328.15	7401
159.0	100000			330.65	8502
				334.65	10021
				339.15	11433
critical solution temp 89.5°C				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 24.0$ for temp range 288–313 K	

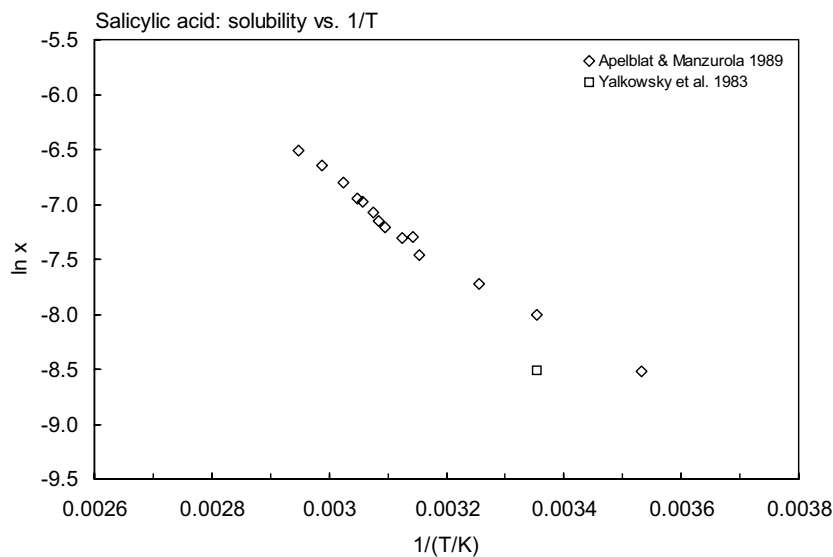


FIGURE 13.1.2.10.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for salicylic acid.

TABLE 13.1.2.10.2

Reported vapor pressures of salicylic acid at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Davies & Jones 1954	
summary of literature data		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
113.7	133.3	95.20	30.93
136.0	666.6	100.49	48.66
146.2	1333	105.18	70.79
156.8	2666	109.96	103.7
172.2	5333	115.01	153.3
182.0	7999	119.98	220.4
193.4	13332	125.13	322.9
210.0	26664	134.96	649.3
230.5	53329		
256.0	101325	mp/°C	158.0–158.6
mp/°C	159	eq. 1	P/mmHg
		A	12.8585
		B	4968.7
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.144$			

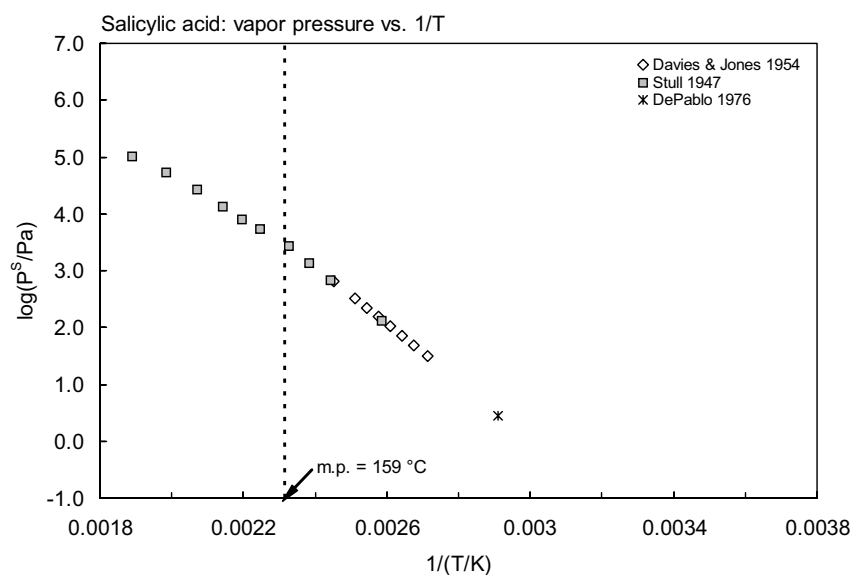
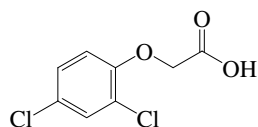


FIGURE 13.1.2.10.2 Logarithm of vapor pressure versus reciprocal temperature for salicylic acid.

13.1.2.11 2,4-Dichlorophenoxyacetic acid (2,4-D) (See also [Chapter 17](#), Herbicides)

Common Name: 2,4-Dichlorophenoxyacetic acid

Synonym: 2,4-D

Chemical Name: 2,4-dichlorophenoxyacetic acid

CAS Registry No: 94-75-7

Molecular Formula: $C_8H_6Cl_2O_3$, $Cl_2C_6H_3OCH_2COOH$

Molecular Weight: 221.038

Melting Point ($^{\circ}C$):

140.5 (Hartley & Kidd 1987; Howard 1991; Lide 2003)

Boiling Point ($^{\circ}C$):

160 (at 0.4 mmHg, Dean 1985; Howard 1991)

215 (Neely & Blau 1985)

Density (g/cm^3 at $30^{\circ}C$):

1.565 (Neely & Blau 1985)

Molar Volume (cm^3/mol):

206.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.77 (potentiometric, Nelson & Faust 1969)

2.87 (spectrophotometric, Cessna & Grover 1978)

2.80 (Reinert & Rogers 1984)

2.64–3.31 (Howard 1991)

2.80 (selected, Wauchope et al. 1992)

2.97 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0736 (mp at $140.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

522 (shake flask-UV, Leopold et al. 1960)

725 (Bailey & White et al. 1965)

725, 400, 900, 550 (review, Günther et al. 1968)

890 (Hamaker 1975)

900 (Kenaga 1980a,b; Kenaga & Goring 1980)

600 ($20^{\circ}C$, Khan 1980)

470 (20 – $25^{\circ}C$, pH 5.6, Geyer et al. 1981)

633, 812 (15, $25^{\circ}C$, shake flask method, average values of 5 laboratories, OECD 1981)

620 ($20^{\circ}C$, Kidd & Hartley 1987; Worthing 1983)

609 (Gerstl & Helling 1987)

682 (Yalkowsky et al. 1987; quoted, Howard 1991)

703 (Gustafson 1989)

900, 600, 890, 703, 1072 (quoted, Wauchope et al. 1992)

890 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

8.0×10^{-5} (Hamaker 1975)

0.180–1.69 (transpiration method, Spencer 1976)

53.0 ($160^{\circ}C$, Kidd & Hartley 1983, 1987)

8.0×10^{-5} (recommended, Neely & Blau 1985; Lyman 1985)

1.00 ($20^{\circ}C$, selected, Suntio et al. 1988)

- 0.0032 (estimated from Henry's law constant, Howard 1991)
 5.6×10^{-5} (selected, Mackay & Stiver 1991)
 1.3×10^{-5} , 8.0×10^{-5} , 1.07×10^{-3} (quoted, Wauchope et al. 1992)
0.00107 (20–25°C, selected, Wauchope et al. 1992)

Henry's Law Constant (Pa·m³/mol):

- 0.55 (calculated-P/C, Suntio et al. 1988)
 1.03×10^{-3} (calculated-bond contribution, Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

- 2.81 (shake flask-AS, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
2.59 (electrometric titration, Freese et al. 1979)
1.57 (Kenaga & Goring 1980, Kenaga 1980b)
1.57, 4.88 (shake flask-OECD 1981 Guidelines, Geyer et al. 1984)
−1.36 (Gerstl & Helling 1987)
2.65 (shake flask, Hansch & Leo 1987)
2.65 (centrifugal chromatography, Ilchmann et al. 1993)
2.81 (recommended, Sangster 1993)
2.81 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 1.11, −0.097 (calculated-S, K_{OW}, Kenaga 1980a)
−2.46, 1.30 (beef fat, fish, Kenaga 1980b)
0.778, 1.94 (alga *Chlorella fusca*: exptl. 24 h exposure, calculated-S, Geyer et al. 1981)
0.778, < 1.0, 1.23 (algae, golden orfe, activated sludge, Freitag et al. 1982)
0.00 (fish, microcosm conditions, Garten & Trabalka 1983)
0.778, 1.23 (algae, calculated-K_{OW}, Geyer et al. 1984)
1.11 (calculated, Isensee 1991)
−5.0 (bluegill sunfish and channel catfish, Howard 1991)
−2.70 (frog tadpoles, Howard 1991)
−3.0, −2.52 (pH 7.8, seaweeds, Howard 1991)
0.778, 0.85 (quoted: alga, fish, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

- 1.30, 2.0 (quoted, calculated, Kenaga 1980a)
1.30, 2.11 (quoted, Kenaga & Goring 1980)
1.68, 1.86, 1.68; 1.76 (commerce soil, Tracy soil, Catlin soil; average value of 3 soils, McCall et al. 1981)
2.25, 2.04, 2.35 (soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
1.29 (soil, Neely & Blau 1985)
1.61 (soil, quoted, Sabljic 1987)
1.75, 2.00 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
1.29–2.13 (soil, quoted values, Howard 1991)
1.30 (selected, Mackay & Stiver 1991)
1.00, 1.23, 2.29 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
1.30, 1.78, 1.51, 1.26, 1.72, 1.75, 1.76 (soil, quoted, Wauchope et al. 1992)
1.30 (soil, selected, Wauchope et al. 1992)
0.68 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

- Volatilization: volatilization from water is negligible, calculated volatilization t_{1/2} = 660 d from soil of 1 cm deep and t_{1/2} = 7.1 yr from 10 cm deep (Howard 1991).
Photolysis: aqueous photolysis t_{1/2} = 2–4 d when irradiated at 356 nm, t_{1/2} = 50 min in water when irradiated at 254 nm, and t_{1/2} = 29–43 d when exposed to September sunlight (Howard 1991).

Oxidation: photooxidation $t_{1/2} = 1.8\text{--}18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991).

Hydrolysis: no hydrolyzable groups and rate constant at neutral pH is zero (Kollig et al. 1987; selected, Howard et al. 1991); generally resistant to hydrolysis, may become important at $\text{pH} > 8$ (Howard 1991).

Biodegradation: degradation kinetics not first-order, time for 50% decomposition in six soils: $t_{1/2} = 5$ d in Commerce soil, $t_{1/2} = 1.5$ d in Catlin soil, $t_{1/2} = 3.9$ d in Keith soil, $t_{1/2} = 3.0$ d in Cecil soil, $t_{1/2} = 2.5$ d in Walla-Walla soil and $t_{1/2} = 8.5$ d in Fargo soil, with an average time of 4 d (McCall et al. 1981);

easily degraded under aerobic conditions with $t_{1/2} = 1.8$ and 3.1 d for cometabolism and metabolism respectively, under anaerobic conditions the degradation rate decreases and the $t_{1/2} = 69$ and 135 d (Liu et al. 1981; quoted, Muir 1991);

second-order $k = (3.6\text{--}28.8) \times 10^{-6}$ $\text{mL cell}^{-1} \text{d}^{-1}$ in natural water (Paris et al. 1981; quoted, Klečka 1985);

first-order $k < 0.14\text{--}0.07$ d^{-1} in river water at 25°C (Nesbitt & Watson 1980; quoted, Klečka 1985);

$k = 0.058 \pm 0.006$ d^{-1} in lake water at 29°C (Subba-Rao et al. 1982; quoted, Klečka 1985; quoted, Muir 1991);

$k = 0.08\text{--}0.46$ d^{-1} in soil at 25°C (McCall et al. 1981; quoted, Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 240\text{--}1200$ h, based on unacclimated aerobic river die-away test data (Nesbitt & Watson 1980a, b; quoted, Howard et al. 1991; Muir 1991);

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}4320$ h, based on unacclimated aqueous screening test data (Liu et al. 1981; selected, Howard et al. 1991);

first-order $k = 0.035$ d^{-1} in die-away test, $k = 0.029$ d^{-1} in CO_2 evolution test in soil and $k = 6.9 \times 10^{-1}$ $\text{mL} \cdot (\text{g bacteria})^{-1} \cdot \text{d}^{-1}$ by activated sludge cultures (Scow 1982);

biodegradation $t_{1/2} = 18$ to > 50 d in clear river water and $t_{1/2} = 10$ to 25 d in muddy water with lag times of 6 to 12 d; degradation with a mixture of microorganisms from activated sludge, soil, and sediments lead to $t_{1/2} = 1.8\text{--}3.1$ d under aerobic conditions and $t_{1/2} = 69\text{--}135$ d under anaerobic conditions (Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 1.8\text{--}18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991);

photooxidation $t_{1/2} = 23.9$ h for reactions with hydroxyl radicals in air (Howard 1991).

Surface water: $t_{1/2} = 48\text{--}96$ h, based on reported photolysis half-lives for aqueous solution irradiated at UV wavelength of 356 nm (Howard et al. 1991);

degradation $t_{1/2} = 14$ d in sensitized, filtered and sterilized river water, based on sunlight photolysis test of $1 \mu\text{g mL}^{-1}$ in distilled water (Zepp et al. 1975; quoted, Cessna & Muir 1991);

typical biodegradation $t_{1/2} = 10$ to < 50 d with longer expected in oligotrophic waters, photolysis $t_{1/2} = 29\text{--}43$ d for water solutions irradiated at sunlight (Howard 1991).

Groundwater: $t_{1/2} = 480\text{--}4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{1/2} < 1$ d for degradation in sediments and lake muds (Howard 1991).

Soil: $t_{1/2} = 240\text{--}1200$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

biodegradation $t_{1/2} < 1$ d to several weeks, $t_{1/2} = 3.9$ and 11.5 d in 2 moist soils and $t_{1/2} = 9.4$ to 254 d in the same soils under dry conditions (Howard 1991);

field $t_{1/2} = 2\text{--}16$ d, with a selected value of 10 d (Wauchope et al. 1992).

Biota: depuration $t_{1/2} = 13.8$ h in daphnids, $t_{1/2} = 1.32$ d in catfish (Ellgehausen et al. 1980).

13.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 13.2.1

Summary of physical properties of carboxylic acids

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol		pK _a
							MW/ρ at 20°C	Le Bas	
Aliphatics:									
Formic acid	64-18-6	HCOOH	46.026	8.3	101	1	37.91	46.2	3.75
Acetic acid	64-19-7	CH ₃ COOH	60.052	16.64	117.9	1	57.24	68.4	4.75
Propionic acid	79-09-4	C ₂ H ₅ COOH	74.079	−20.5	141.15	1	74.60	90.6	4.87
Butyric acid	107-92-6	C ₃ H ₇ COOH	88.106	−5.1	163.75	1	92.00	112.8	4.82
Isobutyric acid	79-31-2	(CH ₃) ₂ CHCOOH	88.106	−46	154.45	1	91.00	112.8	4.86
<i>n</i> -Valeric acid	109-52-4	C ₄ H ₉ COOH	102.132	−33.6	186.1	1	108.77	135.0	4.83
3-Methylbutanoic acid	503-74-2	C ₅ H ₁₀ O ₂	102.132	−29.3	176.5	1	109.70	135.0	4.777
Trimethylacetic acid	75-98-9	(CH ₃) ₃ CCOOH	102.132	35	164	0.798		135.0	4.81
Hexanoic acid (Caproic acid)	142-62-1	C ₅ H ₁₁ COOH	116.158	−3	205.2	1	125.79	157.2	4.87
Octanoic acid	124-07-2	C ₇ H ₁₅ COOH	144.212	16.5	239	1		201.6	4.85
Stearic acid	57-11-4	C ₁₇ H ₃₅ COOH	284.478	69.3	350 dec	0.368	302.38	423.6	4.5
Oleic acid	112-80-1	C ₁₈ H ₃₄ O ₂	282.462	13.4	360	1	316.13	416.2	
Acrylic acid (2-Propenoic acid)	79-10-7	CH ₂ =CHCOOH	72.063	12.5	141	1	68.56	83.2	4.255
2-Butenoic (<i>cis</i> -)	503-64-0	CH ₃ CH=CHCOOH	86.090	15	169	1	83.85	105.4	4.5
2-Butenoic (<i>trans</i> -)	107-93-7	CH ₃ CH=CHCOOH	86.090	71.5	184.7	0.350		105.4	
Vinylacetic acid	625-38-7	CH ₂ =CHCH ₂ COOH	86.090	−35	169	1	85.31	105.4	4.35
2-Methylpropenoic acid	79-41-4	C ₄ H ₆ O ₂	86.090	16	162.5	1	84.79	105.4	4.66
Chloroacetic acid	79-11-8	ClCH ₂ COOH	94.497	63	189.3	0.424	67.29	89.3	2.85
Dichloroacetic acid	79-43-6	Cl ₂ CHCOOH	128.942	13.5	194	1	82.48	110.2	1.26
Trichloroacetic acid	76-03-9	Cl ₃ CCOOH	163.387	59.2	196.5	0.462	100.86	131.1	0.7
Aromatics:									
Benzoic acid	65-85-0	C ₆ H ₅ COOH	122.122	122.35	249.2	0.111		134.8	4.19
2-Methylbenzoic acid	118-90-1	CH ₃ C ₆ H ₄ COOH	136.149	103.5	259	0.170		157.0	3.91
3-Methylbenzoic acid	99-04-7	CH ₃ C ₆ H ₄ COOH	136.149	109.9	263	0.147		157.0	4.27
4-Methylbenzoic acid	99-94-5	CH ₃ C ₆ H ₄ COOH	136.149	179.6	275	0.0304		157.0	4.39
Phenylacetic acid	103-82-2	C ₆ H ₅ CH ₂ COOH	136.149	76.5	265.5	0.312	125.95	157.0	4.31
Phthalic acid	88-99-3	C ₆ H ₄ -1,2-(COOH) ₂	166.132	230 dec	dec	0.00974	104.29	173.6	
2-Chlorobenzoic acid	118-91-2	ClC ₆ H ₄ COOH	156.567	140.2	sublim	0.0741	101.4	155.7	

3-Chlorobenzoic acid	535-80-8	$\text{ClC}_6\text{H}_4\text{COOH}$	156.567	158	sublim	0.0496		155.7	3.82
4-Chlorobenzoic acid	74-11-3	$\text{ClC}_6\text{H}_4\text{COOH}$	156.567	243		0.00726		155.7	3.85
Salicylic acid	69-72-7	$\text{HOC}_6\text{H}_4\text{COOH}$	138.121	159		0.0484	95.72	142.2	2.97
Phenoxyacetic acid	122-59-8	$\text{C}_6\text{H}_5\text{OCH}_2\text{COOH}$	152.148	98.5	285 dec	0.190		164.4	
2,4-Dichlorophenoxyacetic acid	94-75-7	$\text{Cl}_2\text{C}_6\text{H}_3\text{OCH}_2\text{COOH}$	221.038	140.5	215	0.0736		206.2	
2,4,5-Trichlorophenoxyacetic acid	93-76-5	$\text{Cl}_3\text{C}_6\text{H}_2\text{OCH}_2\text{COOH}$	255.483	153	dec	0.0555		227.1	

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

TABLE 13.2.2
Summary of selected physical-chemical properties of carboxylic acids at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol)		
	Solubility			Vapor pressure		log K _{ow}	calcd P/C	exptl ^a	calcd ^b
	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)	P ^S /Pa	P _L /Pa				
Aliphatics:									
Formic acid	miscible			5750	5750	−0.54		0.01832	
Acetic acid	miscible			2079	2079	−0.31		0.01825	0.0285
Propionic acid	miscible			435	435	0.26		0.018	0.0431
Butyric acid	miscible			84	84	0.79		0.0222	0.0650
Isobutyric acid	22800	258.8	258.8	185	185	0.79	0.715	0.0897	
<i>n</i> -Valeric acid	24000	235.0	235.0	19	19	1.39	0.081	0.0478	0.099
3-Methylbutanoic acid	4100	40.14	40.14	25	25		0.623	0.0844	
Hexanoic acid	9580	82.47	82.47	5	5	1.92	0.0606	0.0768	0.149
Octanoic acid	79.8	0.553	0.553	3.72	3.72		6.723		0.338
Stearic acid	340	1.195	3.248		1.69 × 10 ^{−6}	8.23			
Oleic acid				0.00113	0.00113	7.64			
Acrylic acid	miscible			550	550	0.43			
2-Methylpropenoic acid	8900	103.4	103.4	100	100	0.93	0.9673		
Chloroacetic acid	miscible				18.5	0.22			
Dichloroacetic acid	miscible			35	35	0.92			
Trichloroacetic acid					11	1.33			
Aromatics:									
Benzoic acid	3400	27.84	250.8	0.11	0.991	1.89	3.95 × 10 ^{−3}		
2-Methylbenzoic acid	1074	7.888	46.40			2.46			
3-Methyl benzoic acid	1246	9.152	62.26	1.39	9.456	2.37	0.1512		
4-Methylbenzoic acid	331	2.431	79.97			2.34			
Phenylacetic acid	16600	121.9	390.8	0.83	2.660	1.41	6.81 × 10 ^{−3}		
Phthalic acid	7000	42.14	4326			0.73			
2-Chlorobenzoic acid	2100	13.41	181.0			1.99			
3-Chlorobenzoic acid	400	2.555	51.51			2.60			
4-Chlorobenzoic acid	70	0.4471	61.58			2.65			
Salicylic acid	2300	16.65	344.0	0.0208	0.440	2.20	1.25 × 10 ^{−3}		
Phenoxyacetic acid	12000	78.87	415.1			2.81			
2,4-D	890	4.026	54.71	8.0 × 10 ^{−5}	0.001	2.65	1.99 × 10 ^{−5}		
2,4,5-T	278	1.088	19.61						

^a Brimblecombe et al. 1992; ^b Hine & Mookerjee 1975.

TABLE 13.2.3

Suggested half-life classes for carboxylic acids in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aliphatics:				
Formic acid	4	3	4	5
Acetic acid	3	3	4	5
Butyric acid	3	3	4	5
Hexanoic acid (Caproic acid)	3	3	4	5
Stearic acid (Octadecanoic acid)	3	3	4	5
Acrylic acid (2-Propenoic acid)	2	3	4	5
Vinylacetic acid	2	3	4	5
Chloroacetic acid	5	4	5	6
Aromatics:				
Benzoic acid	3	3	4	5
2-Methylbenzoic acid (<i>o</i> -Toluic acid)	3	3	4	5
Phenylacetic acid	3	3	4	5
Phthalic acid	3	3	4	5
2-Chlorobenzoic acid	4	5	6	7
Salicylic acid	3	3	4	5
2,4-Dichlorophenoxyacetic acid (2,4-D)	2	3	5	6
2,4,5-Trichlorophenoxyacetic acid (2,4,5-T)	3	4	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	<10
2	17 (~1 d)	10–30
3	55 (~2 d)	30–100
4	170 (~1 week)	100–300
5	550 (~3 weeks)	300–1,000
6	1,700 (~2 months)	1,000–3,000
7	5,500 (~8 months)	3,000–10,000
8	17,000 (~2 y)	10,000–30,000
9	~5 y	>30,000

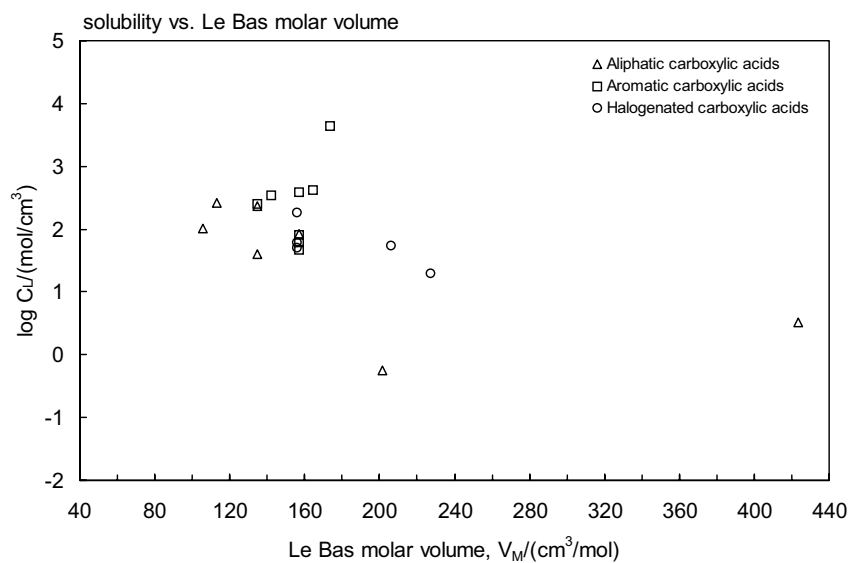


FIGURE 13.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for carboxylic acids.

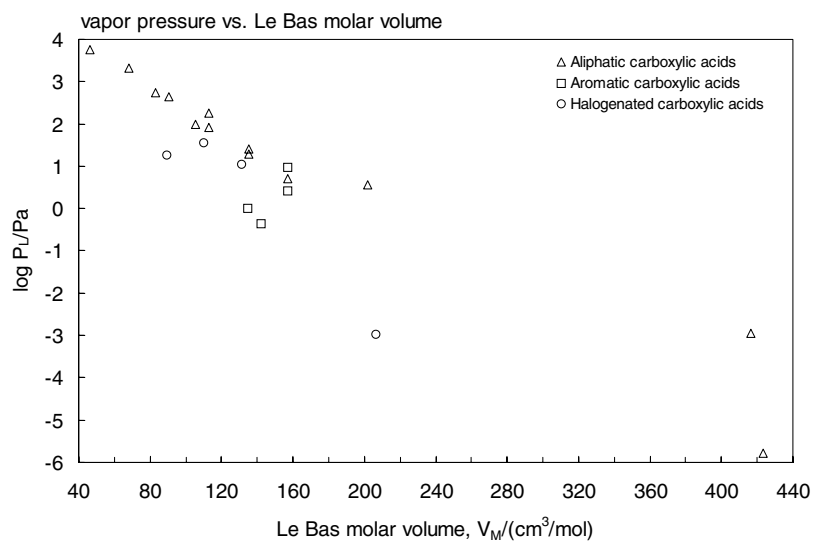


FIGURE 13.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for carboxylic acids.

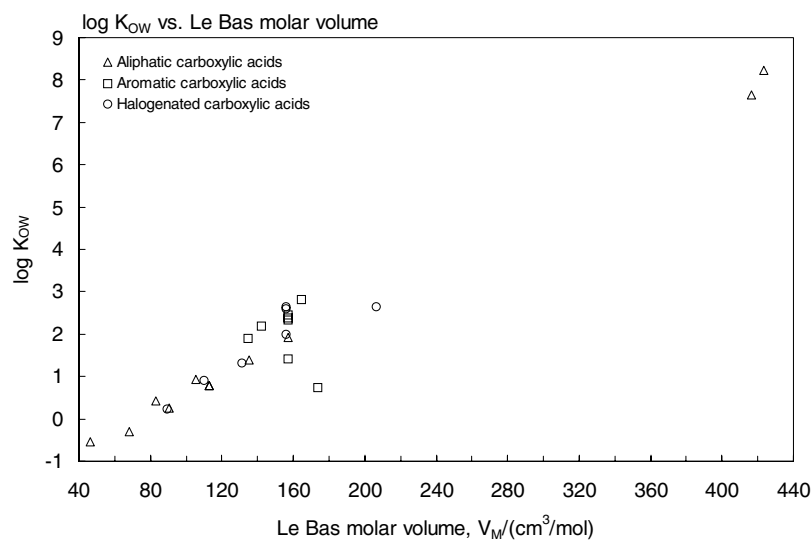


FIGURE 13.2.3 Octanol-water partition coefficient versus Le Bas molar volume for carboxylic acids.

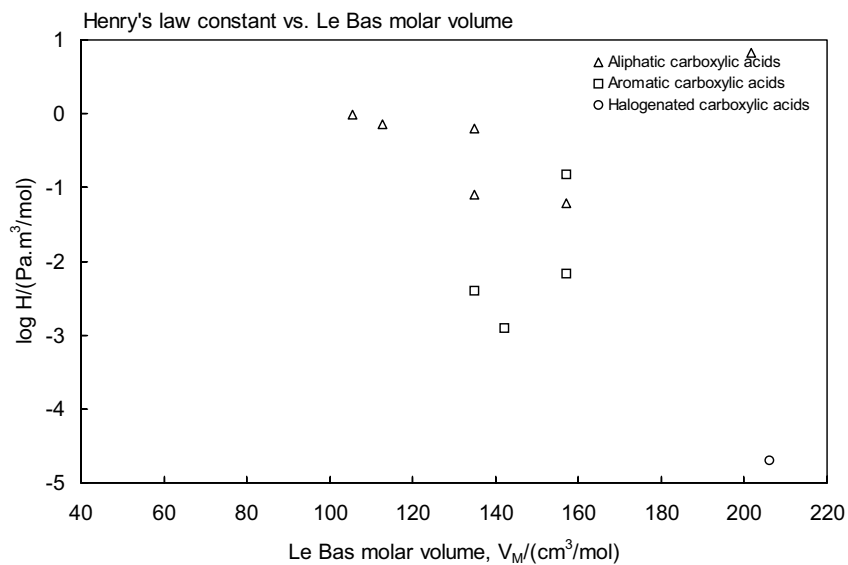


FIGURE 13.2.4 Henry's law constant versus Le Bas molar volume for carboxylic acids.

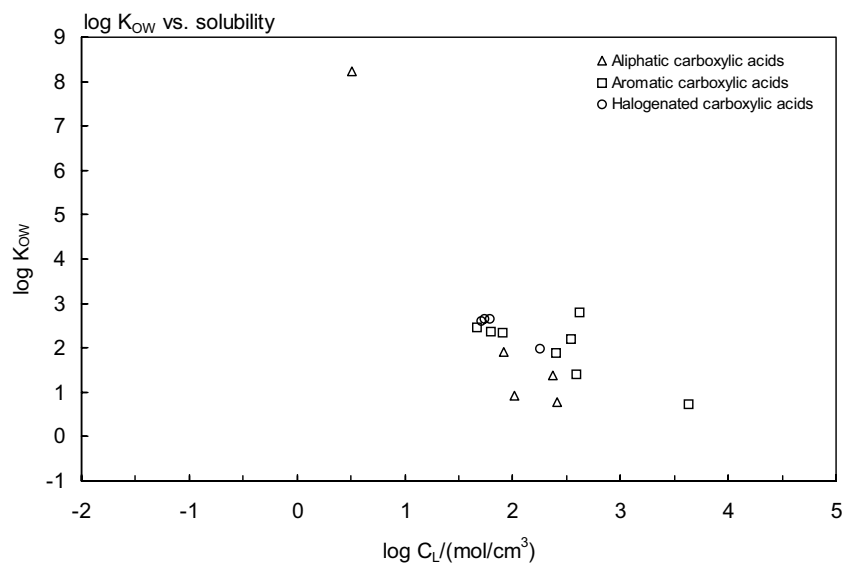


FIGURE 13.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for carboxylic acids.

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14 Phenolic Compounds

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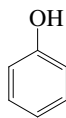
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14.1 LIST OF CHEMICALS AND DATA COMPILATIONS

14.1.1 ALKYLPHENOLS AND OTHER SUBSTITUTED PHENOLS

14.1.1.1 Phenol



Common Name: Phenol

Synonym: carbolic acid, phenic acid, phenylic acid, phenyl hydrate, phenyl hydroxide, hydroxybenzene, oxybenzene

Chemical Name: phenol

CAS Registry No: 108-95-2

Molecular Formula: C_6H_5OH

Molecular Weight: 94.111

Melting Point ($^{\circ}C$):

40.89 (Lide 2003)

Boiling Point ($^{\circ}C$):

181.87 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5479 (supercooled liq., Ericksen & Dobbert 1955)

1.0576 (Weast 1982)

Acid Dissociation Constant, pK_a :

9.90 (Blackman et al. 1955, McLeese et al. 1979)

10.02 (Herington & Kynaston 1957; Callahan et al. 1979)

9.82 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)

10.0 (Serjeant & Dempsey 1979; Paris et al. 1982; Miyake et al. 1987; Tratnyek & Hoigné 1991)

9.92 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Varhaníčková et al. 1995)

10.05 (Saarikoski 1982; Saarikoski & Viluksela 1982)

9.90 (UV absorption, Hoigné & Bader 1983; Scully & Hoigné 1987)

9.99 (Dean 1985; Schultz & Cajina-Quezada 1987; Hersey et al. 1989)

10.93 (Miyake et al. 1987)

10.12 (UV spectrophotometry, Nendza & Seydel 1988)

Molar Volume (cm^3/mol):

89.0 ($20^{\circ}C$, calculated-density)

103.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.13, 45.83 ($25^{\circ}C$, bp, Dreisbach 1955)

47.30 (at normal bp, Biddiscombe & Martin 1958)

45.689 (at normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

68.66 (at $25^{\circ}C$, Biddiscombe & Martin 1958; Andon et al. 1960)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.514 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

36.63 (Tsonopoulos & Prausnitz 1971)

36.0, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.698 (mp at $40.89^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

86600* (synthetic method, measured range $20-65.86^{\circ}C$, Hill & Malisoff 1926)

83000 ($20^{\circ}C$, synthetic method, Jones 1929)

89300* ($22.7^{\circ}C$, thermostatic and synthetic methods, measured range $22.7-60.9^{\circ}C$, Morrison 1944)

- 88360 (shake flask-UV at pH 5.1, Blackman et al. 1955)
 79000* (20°C, synthetic method/shake flask-optical, measured range 0–68.3°C, Ericksen & Dobbert 1955)
 80000 (20°C, Mulley & Metcalf 1966)
 78000 (shake flask-spectrophotometry, Roberts et al. 1977)
 79750 (shake flask-GC, Kraij & Sincic 1980)
 76514 (generator column-HPLC, Wasik et al. 1981)
 150580 (20°C, shake flask-UV, Hashimoto et al. 1984)
 87000 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
 84045* (shake flask-conductimetry, measured range 15.1–35°C, Achard et al. 1996)
 94100* (25.35°C, shake flask-optical method, measured range 298.5–336.7 K, Jaoui et al. 1999)
 83119* (23.15°C, shake flask-optical method, measured range 292.5–333.6 K, Jaoui et al. 2002)
 $\ln [S/(\text{mol kg}^{-1})] = 7.3013 - 853.62/(T/K)$; temp range 288–313 K (eq.-I derived using reported exptl. data, Jaoui et al. 2002)
 $\ln [S/(\text{mol kg}^{-1})] = 10.731 - 1931.7/(T/K)$; temp range 313–332 K (eq.-II derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 133.3* (44.8 °C, static method-manometer, measured range 44.8–181.4 °C, Kahlbaum 1898)
 28531* (141.1 °C, mercury manometer, measured range 141.1–181.1 °C, Goldblum et al. 1947)
 $\log (P/\text{mmHg}) = -2510/(T/K) + 8.395$; temp range: 141.1–181.1°C (Hg manometer, Goldblum et al. 1947)
 55.54* (extrapolated-regression of tabulated data, temp range 40.1–181.9°C, Stull 1947)
 7605* (107.15 °C, ebulliometry, measured range 107.15–181.75 °C, Dreisbach & Shrader 1949)
 1333* (70.50 °C, ebulliometry, measured range 70.50–181.7 °C, Vonterres et al. 1955)
 70.75 (calculated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 7.57893 - 1817.0/(205.0 + t/^{\circ}\text{C})$, temp range: 93–240°C, (Antoine eq. for liquid state, Dreisbach 1955)
 44.26* (24.85°C, gas saturation and diaphragm manometer measurements, measured range 0–37.5°C, Biddiscombe & Martin 1958)
 45.71 (gas saturation and diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
 $\log (P/\text{mmHg}) = 11.5638 - 3586.36/(t/^{\circ}\text{C} + 273)$; temp range 9–40°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 $\log (P_L/\text{mmHg}) = 7.13457 - 1615.072/(t/^{\circ}\text{C} + 174.569)$; temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 45.07 (interpolated- Antoine eq., Andon et al. 1960)
 70.70 (20°C, supercooled liq., Andon et al. 1960)
 83.95 (extrapolated supercooled liquid value, Antoine eq., Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 11891.5/(T/K)] + 8.513843$; temp range 40.1–418.7°C (Antoine eq., Weast 1972–73)
 47.01 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.13301 - 1516.79/(174.954 + t/^{\circ}\text{C})$; temp range 107–182°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
 26.66, 133.3 (20°C, 40°C, Verschuereen 1977, 1983)
 16.27 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 454.610/(T/K)] \times 10^{\{1.00375 - 8.88757 \times 10^{-4} \cdot (T/K) + 6.83750 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 323.205–694.25 K, (Cox eq., Chao et al. 1983)
 46.91, 54.74 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.25543 - 1515.182/(174.182 + t/^{\circ}\text{C})$; temp range 107–181.75°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.70346 - 1793.899/(200.218 + t/^{\circ}\text{C})$; temp range 70.5–181.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 47.00 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.1330 - 1516.79/(174.95 + t/^{\circ}\text{C})$; temp range 107–182°C (Antoine eq., Dean 1985, 1992)
 55.00 (selected, Riddick et al. 1986)
 45.7, 45.32 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_S/\text{kPa}) = 10.6887 - 3586.36/(T/\text{K})$; temp range 282–313 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_S/\text{kPa}) = 10.71099 - 3594.703/(T/\text{K})$; temp range 273–313 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.25947 - 1516.072/(-98.581 + T/\text{K})$; temp range 383–473 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.34757 - 1482.82/(-113.862 + T/\text{K})$; temp range 455–655 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.57957 - 1710.287/(-80.273 + T/\text{K})$; temp range 314–395 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.26694 - 1522.07/(-97.834 + T/\text{K})$; temp range 387–456 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.30177 - 1548.368/(-94.612 + T/\text{K})$; temp range 449–526 K (Antoine eq.-VII, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.92874 - 2146.053/(-17.025 + T/\text{K})$; temp range 520–625 K (Antoine eq.-VIII, liquid, Stephenson & Malanowski 1987)

61.16 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)

$\log (P/\text{Pa}) = 37.91650 - 4155.615/(T/\text{K}) - 9.02308 \cdot \log (T/\text{K}) + 0.04526 \times 10^{-2} \cdot (T/\text{K})$; temp range: 394–455 K (four-parameter vapor pressure eq. using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)

$\log (P/\text{Pa}) = 127.08645 - 7292.585/(T/\text{K}) - 42.92601 \cdot \log (T/\text{K}) + 1.76834 \times 10^{-2} \cdot (T/\text{K})$; temp interval of investigation 380–455 K (four-parameter vapor pressure eq. derived using data of Dreisbach & Shrader 1949, Nesterova et al. 1990)

$\log (P/\text{mmHg}) = 23.5332 - 3.4961 \times 10^3/(T/\text{K}) - 4.899 \cdot \log (T/\text{K}) + 1.216 \times 10^{-4} \cdot (T/\text{K}) + 9.6537 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 314–694 K (vapor pressure eq., Yaws 1994)

173* (40.09°C, ebulliometry, measured range 40–90°C, Tabai et al. 1997)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0402 (exptl., Hine & Mookerjee 1975; Howard 1989)

0.065, 1.082 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.0718* (27.0°C, gas stripping-GC, measured range –2.0 to 27.0°C Abd-El-Bary et al. 1986)

$k_H/\text{kPa} = 2.69 \times 10^9 \exp[-6120/(T/\text{K})]$, temp range –2 to 90°C (gas stripping-GC measurements plus reported data at higher temp., Abd-El-Bary et al. 1986)

1.245, 2.193, 3.322 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

0.0607* (extrapolated from temp dependence eq., Dohnal & Fenclová 1995)

$\ln K_{AW} = 8.701 - 5760/(T/\text{K})$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional literature data, Dohnal & Fenclová 1995)

0.0342* (313.24 K, derived from measured P, temp range 313.240–363.14 K, Tabai et al. 1997)

$k_H/\text{kPa} = 670.117 - 39274.5/(T/\text{K}) - 94.6679$; temp range 313–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

< 0.240 (gas stripping-GC, Altschuh et al. 1999)

0.0536 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

0.0320* (gas stripping-UV, measured range 284–302 K, Harrison et al. 2002)

$\ln [H/(M \text{ atm}^{-1})] = 5850/(T/\text{K}) - 11.6$; temp range 284–302 K, Harrison et al. 2002)

0.157* (dynamic equilibrium/gas stripping-GC/MS, measured range 5–25°C, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$. Additional data at other temperatures designated * are compiled at the end of this section:

1.46 (shake flask-UV, Fujita et al. 1964)

1.46 ± 0.01 (shake flask-UV, Iwasa et al. 1965)

1.42 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)

1.60 (shake flask, Kiezyk & Mackay 1971)

1.47 (Leo et al. 1971)

1.51 (shake flask-UV at pH 7.45, Umeyama et al. 1971)

1.49 (shake flask, Korenman 1972)

- 1.510* (20 °C, shake flask-concn ratio, measured range 10–60 °C, Korenman & Udalova 1974)
 1.46, 1.61 (LC- k' correlation, calculated- π const., Carlson et al. 1975)
 1.54 (shake flask-UV, Davis et al. 1976)
 1.45 (HPLC-RT correlation, Mirreles et al. 1976)
 1.48 \pm 0.02 (shake flask at pH 7, Unger et al. 1978)
 1.48, 1.46, 1.49, 1.51, 0.62, 2.20 (literature values, Hansch & Leo 1979)
 1.46 (HPLC- k' correlation, Butte et al. 1981; Butte et al. 1987)
 1.45 (generator column-HPLC/UV, Wasik et al. 1981)
 1.54 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 1.28, 1.54 (RP-LC- k' correlation, calculated-fragment const. as per Rekker 1977, Hanai & Hubert 1982)
 1.54 (HPLC- k' correlation, Miyake & Terada 1982; Miyake et al. 1987)
 1.62 (inter-laboratory, shake flask average, Eadsforth & Moser 1983)
 1.16 (inter-laboratory, HPLC average, Eadsforth & Moser 1983)
 1.49, 1.53 \pm 0.09 (selected best lit. value, exptl.-ALPM, Garst 1984)
 1.46, 1.55 \pm 0.07 (selected best lit. value, exptl.-ALPM, Garst & Wilson 1984)
 1.08 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
 1.46 (RP-HPLC-RT correlation, Chin et al. 1986)
 1.00, 1.42 (HPLC- k' correlation, Eadsforth 1986)
 1.46 (shake flask-CPC centrifugal partition chromatography, Berthod et al. 1988)
 1.46 (RP-HPLC-capacity ratio correlation, Minick et al. 1988)
 1.46 (HPLC-RT correlation, Shigeota et al. 1988)
 1.52 \pm 0.01 (filter chamber-UV, Hersey et al. 1989)
 1.50 (recommended, Sangster 1989, 1993)
 1.52, 1.58, 1.69 (CPC-RV correlation, Gluck & Martin 1990)
 1.47 (shake flask-UV, Kramer & Henze 1990)
 1.37 \pm 0.06 (liquid-liquid extraction-flow injection-UV, Kubá 1991)
 1.57 (shake flask-GC, Kishino & Kobayashi 1994)
 1.46 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 4.16 (total ^{14}C in fathead minnow, mean exposure level 0.0025 $\mu\text{g}\cdot\text{mg}^{-1}$, Call et al. 1980)
 4.23 (total ^{14}C in fathead minnow, mean exposure level 0.0327 $\mu\text{g}\cdot\text{mg}^{-1}$, Call et al. 1980)
 4.20 (total ^{14}C in fathead minnow, mean value, Call et al. 1980)
 2.20 (goldfish, rate constant ratio k_1/k_2 , Nagel & Ulrich 1980)
 0.97 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 1.30, 2.30, 3.34 (golden ide, algae, activated sludge, Freitag et al. 1985)
 2.30 (*chlorella fusca*, Freitag et al. 1985; quoted, Howard 1989)
 1.20 (algae, maximum apparent BCF, Hardy et al. 1985)
 0.544 (algae, real BCF with biotransformation, Hardy et al. 1985)
 3.14 (*daphnia magna*, estimated- ^{14}C activity and on dry wt. basis, Dauble et al. 1986)
 2.44 (*daphnia magna*, based on elimination phase, Dauble et al. 1986)
 1.28 (*daphnia magna*, Dauble et al. 1986; quoted, Geyer et al. 1991)
 1.24 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, log K_{OC} :

- 1.43 (soil, Kenaga & Goring 1980)
 1.48 (20°C, sorption isotherm, converted form K_{OM} organic carbon in soils, Briggs 1981)
 1.15 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 1.57, 1.96 (silt loams, Scott et al. 1983, quoted, Howard 1989)
 3.46 (untreated fine sediment, Isaacson & Frink 1984)
 3.49 (untreated coarse sediment, Isaacson & Frink 1984)
 1.35 (HPLC- k' correlation, mobile phase buffered to pH 3, Hodson & Williams 1988)
 2.17 (soil, calculated- K_{OW} , Howard 1989)
 2.4, 2.43 (soil: quoted, calculated-MCI χ , Meylan et al. 1992)

- 2.68, 2.38 (natural zeolite modified with a cation surfactant HDTMA with surface coverage of 100, 200 mmol/kg at pH 7, shake flask-sorption isotherm, Li et al. 2000)
- 1.43 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.42, 1.00. 1.24 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
- 1.59, 1.67 (HP:LC- k' correlation, C_{18} column, Hong et al. 1996)
- 1.32; 2.43 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
- 1.56, 1.556, 1.255, 1.307, 1.52 (soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 1.310, 1.750, 1.281, 1.601, 1.544 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 1.310, 1.750, 1.281, 1.601, 1.544 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
- 1.37, 1.34 (soils: organic carbon $OC \geq 0.1\%$ and pH 3.2–7.4, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 3.2$ months for evaporation from water (Howard 1989);

$t_{1/2} = 88$ d, calculated for evaporation from a model river of 1 m deep with a current of 3 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: phototransformation rate $k = 0.015 \text{ h}^{-1}$ with $t_{1/2} = 46$ h in the summer (mean temp 24°C) and $k = 0.0040 \text{ h}^{-1}$ with $t_{1/2} = 173$ h in the winter (mean temp 10°C) in distilled water; $k = 0.018 \text{ h}^{-1}$ with $t_{1/2} = 39$ h in the summer and $k = 0.0074 \text{ h}^{-1}$ with $t_{1/2} = 94$ h in the winter in estuarine water when exposed to full sunlight and microbes (Hwang et al. 1986);

photomineralization rate $k = 0.04 \text{ h}^{-1}$ with $t_{1/2} = 16$ d in the summer and $k = 0.0041 \text{ h}^{-1}$ with $t_{1/2} = 169$ d in the winter in distilled water; $k = 0.095 \text{ h}^{-1}$ with $t_{1/2} = 7$ d in the summer and $k = 0.010 \text{ h}^{-1}$ with $t_{1/2} = 73$ d in winter in estuarine water when exposed to full sunlight and microbes (Hwang et al. 1986);

atmospheric $t_{1/2} = 46$ to 173 h, based on reported half-life for photolysis under sunlight for phenol in distilled water in the summer and winter; aquatic photolysis $t_{1/2} = 46$ to 173 h, based on reported half-life for photolysis under sunlight for phenol in distilled water in the summer and winter (Howard et al. 1991)

Apparent first-order rate constant phototransformation at $\lambda > 285 \text{ nm}$, $k = (3.10 \pm 0.10) \times 10^{-2} \text{ h}^{-1}$ in purified water (Zamy et al. 2004)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen at 25°C with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{NO}_3} = (2.0 \pm 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(300 \pm 1) \text{ K}$ (Carter et al. 1981)

$k = 6.5 \times 10^3 \text{ s}^{-1}$, dye-sensitized photooxidation first-order rate constant, second order $k = (1.3 \pm 0.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM PrOH as scavenger at pH 1.7–2.0 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983a)

$k_{\text{NO}_3} = (2.10 \pm 0.50) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson et al. 1984)

$k_{\text{NO}_3} = (3.64 \pm 0.14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K with reference to reaction for NO_3 radical with 2-methyl-2-butene (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{OH}}(\text{exptl}) = 28.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 45.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1985)

$k_{\text{OH}}(\text{calc}) = 36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{obs}) = 28.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k = (2 \text{ to } 3) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, $1.9 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 9, $4.6 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 9.5, $9.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 10 and $1.8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ at pH 11.5 for the reaction with singlet oxygen at $(19 \pm 2)^\circ\text{C}$ in water (Scully & Hoigné 1987)

$k_{\text{NO}_3} = 3.63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 26.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{NO}_3} = (2.59 \pm 0.52) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ with reference to reaction for NO_3 radicals with *cis*-2-butene (Atkinson 1991)

$k = (2.6 \pm 4) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $(27 \pm 1)^\circ\text{C}$ (Tratnyek & Hoigné 1991)

$k_{\text{OH}} = 10.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 11.44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Müller & Klein 1991)

$k_{\text{NO}_3} = (3.92 \pm 0.25) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ with reference to reaction for NO_3 radical with 2-methyl-2-butene; $k_{\text{OH}} = 26.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1992)

$k_{\text{OH}}(\text{calc}) = 12 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital estimation method, Klamt 1993)

$k_{\text{OH}} = 2.6 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{aq.}) = 6.7 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, the calculated atmospheric lifetime $\tau = 0.45 \text{ d}$ under clear sky; $\tau = 0.38 \text{ d}$ under cloudy conditions at 298 K , reduced to 0.26 d due the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis: no hydrolyzable function group (Howard et al. 1991).

Biodegradation: $t_{1/2} = 1\text{--}2 \text{ d}$ for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964)

decomposition by soil microflora within 1 d (Alexander & Lustigman 1966; quoted, Verschueren 1983)

complete disappearance in soil suspensions in 2 d (Woodcock 1971; quoted, Verschueren 1983)

$k_{\text{B}} = 80.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

$k_{\text{B}} = (0.094 \pm 0.003) \text{ h}^{-1}$ at feed concentration of 180 mg/L at 20°C and $k = (0.095 \pm 0.007) \text{ h}^{-1}$ at feed concentration of 360 mg/L at 20°C in a continuous stirred reactor (Beltrame et al. 1984)

$k_{\text{B}} = 0.035 \text{ d}^{-1}$ with $t_{1/2} = 20 \text{ d}$ in ground water; $k_{\text{B}} = 0.065 \text{ d}^{-1}$ with $t_{1/2} = 11 \text{ d}$ in Lester River water;

$k_{\text{B}} = 0.247 \text{ d}^{-1}$ with $t_{1/2} = 3 \text{ d}$ in Superior harbor waters (Vaishnav & Babeu 1987)

$k_{\text{B}} = 0.03 \text{ h}^{-1}$ and $t_{1/2} = 28 \text{ h}$ for estuarine water in summer (mean temp 24°C) and $k_{\text{B}} = 0.011 \text{ h}^{-1}$ with $t_{1/2} = 62 \text{ h}$ in winter (mean temp. 10°C); $k_{\text{B}} = 0.4 \text{ h}^{-1}$ with $t_{1/2} = 2 \text{ d}$ in summer and $k_{\text{B}} = 0.0051 \text{ h}^{-1}$ with $t_{1/2} = 146 \text{ d}$ in winter in darkness with microbes (Hwang et al. 1986)

$k_{\text{B}} = 0.041\text{--}0.028 \text{ h}^{-1}$ in $10\text{--}100 \text{ mg/L}$ sludge (Urano & Kato 1986)

complete degradation within 1 d in water from 3 lakes, and degradation is somewhat slower in salt water with $t_{1/2} = 9 \text{ d}$ in estuary river (Howard 1989)

$k_{\text{B}}(\text{exptl., average}) = 0.0498 \text{ h}^{-1}$; $k_{\text{B}}(\text{calc}) = 0.0545 \text{ h}^{-1}$ (nonlinear) and $k_{\text{B}}(\text{calc}) = 0.0503 \text{ h}^{-1}$ (linear) (group contribution method, Tabak & Govind 1993)

$t_{1/2}(\text{aerobic}) = 0.25 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 8.0 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: microbial transformation $k = (7.1 \pm 1.3) \times 10^{-12} \text{ L.organism}^{-1} \text{ h}^{-1}$ (Paris et al. 1982);

estimated bacterial transformation $k = 3 \times 10^{-6} \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982);

microbial transformation rate constants in pond and river samples $k = (2.0 \pm 1.5) \times 10^{-10}$ to $(4.8 \pm 3.1) \times 10^{-10} \text{ L organism}^{-1} \text{ h}^{-1}$ at five different sites (Paris et al. 1983; quoted, Steen 1991);

degradation rate constants $k = 1.08 \times 10^{-16} \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies and $k = 0.90 \times 10^{-12}$ to $3.00 \times 10^{-12} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 3.15 \text{ h}^{-1}$; $k_2 = 0.02 \text{ h}^{-1}$ (goldfish, Nagel & Urich 1980)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.61 \text{ d}$ by reaction with OH radicals in air (Howard 1989);

$t_{1/2} = 2.28$ to 22.8 h , based on reaction with OH radical (Howard et al. 1991)

degradation $k = 0.0462 \text{ d}^{-1}$ corresponding to $t_{1/2} = 360 \text{ h}$ in air (Guinee & Heijungs 1993);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994);

calculated lifetimes of 5.3 h and 9.0 min for reactions with OH, NO_3 radical, respectively (Atkinson 2000).

atmospheric lifetime $\tau = 0.45 \text{ d}$ under clear sky and $\tau = 0.38 \text{ d}$ under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K , reduced to $\tau = 0.26 \text{ d}$ due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: rate constant $k = (1.3 \pm 0.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 2.0–6.0 (Hoigné & Bader 1983);

$t_{1/2} = 46 \text{ h}$ in summer, $t_{1/2} = 173 \text{ h}$ in winter in distilled water and $t_{1/2} = 39 \text{ h}$ in summer, $t_{1/2} = 94 \text{ h}$ in winter in estuarine water, based on phototransformation rate when exposed to full sunlight and microbes (Hwang et al. 1986)

$t_{1/2} = 43 \text{ h}$ in summer, $t_{1/2} = 118 \text{ h}$ in winter in poisoned estuarine water, based on photo-transformation rate and $t_{1/2} = 384 \text{ h}$ or 16 d in summer, $t_{1/2} = 2640 \text{ h}$ or 110 d in winter in poisoned estuarine water, based on photomineralization rate (Hwang et al. 1986);

$t_{1/2}$ = 384 h or 16 d in summer, $t_{1/2}$ = 4056 h or 169 d in winter in distilled water; and $t_{1/2}$ = 168 h or 7 d in summer, $t_{1/2}$ = 1752 h or 73 d in winter in estuarine water, based on photo-mineralization rate when exposed to full sunlight and microbes (Hwang et al. 1986);

$t_{1/2}$ = 2000 h in water at pH 8 and $19 \pm 2^\circ\text{C}$ for the reaction with singlet oxygen (Scully & Hoigné 1987); biodegradation $t_{1/2}$ = 11 d in river waters and $t_{1/2}$ = 3 d in Superior harbor waters (Vaishnav & Babeu 1987); complete degradation within 1 d in water from 3 lakes, and degradation is somewhat slower in salt water with $t_{1/2}$ = 9 d in estuary river (Howard 1989);

$t_{1/2}$ = 77 to 3840 h in water, based on reported reaction rate constant for RO_2 radical with the phenols class, $t_{1/2}$ = 5.3 to 56.5 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); degradation rate constant $k = 0.0217 \text{ d}^{-1}$ corresponding to a $t_{1/2}$ = 766 h in water (quoted from Howard 1989, Guinee & Heijungs 1993)

$t_{1/2}(\text{aerobic}) = 0.25 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 8 \text{ d}$ in natural waters (Capel & Larson 1995)

Groundwater: biodegradation $t_{1/2}$ = 20 d (Vashnav & Babeu 1987);

$t_{1/2}$ = 12 to 168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 2 d in Dunkirk silt loam, 1 d in Mardin silt loam (Alexander & Aleem 1961)

degradation in soil completed in 2–5 d even in subsurface soils and $t_{1/2}$ = 2.70 and 3.51 h of low concentration of phenol in 2 silt loam soils (Howard 1989);

$t_{1/2}$ = 24 to 240 h, based on aerobic soil die-away data (Howard et al. 1991);

$t_{1/2}$ = 4.1 d in a slightly basic sandy loam soil containing 3.25% organic matter and $t_{1/2}$ = 23 d in acidic clay soil with < 1.0% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992)

degradation rate constant $k = 0.227 \text{ d}^{-1}$ corresponding to a $t_{1/2}$ = 73.3 h in soil (quoted from Howard 1989, Guinee & Heijungs 1993).

Biota: elimination from goldfish within 4 h (Nagel & Ulrich 1980);

depuration $t_{1/2}(\text{obs}) = 336 \text{ h}$, $t_{1/2}(\text{calc}) = 385 \text{ h}$ for exposure level of $0.0025 \mu\text{g mL}^{-1}$ and $t_{1/2}(\text{obs.}) = 438 \text{ h}$, $t_{1/2}(\text{calc}) = 497 \text{ h}$ for exposure level of $0.0375 \mu\text{g mL}^{-1}$ (Call et al. 1980);

depuration $t_{1/2}(\text{calc}) = 8$ to 44 min in algae (Hardy et al. 1985);

half-lives in fish $t_{1/2} < 1 \text{ d}$ for goldfish, $t_{1/2} = 14$ –18 d for minnow (Niimi 1987)

TABLE 14.1.1.1.1

Reported aqueous solubilities of phenol at various temperatures

1.

Hill & Malisoff 1926		Morrison 1944		Erichsen & Dobbert 1955		Achard et al. 1996	
volumetric method		thermostatic and synthetic		shake flask-optical method		shake flask-conductivity	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20.0	83600	22.7	89300	0	73000.	15.1	76044
25.0	86600	26.9	93159	10	75000	25.0	84045
30.0	92200	32.3	98617	20	79000	35.0	93098
35.0	99100	36.0	104169	30	86000		
57.30	148700	43.7	108968	40	97000		
62.74	193500	47.7	128823	50	115000		
65.79	277700	50.5	138892	60	153000		
66.01	291300	53.5	149807	62	166000		
65.79	202100	55.8	162323	64	183000		
65.84	313500	57.8	174650	66	215000		
65.86	322300	60.9	203538	67	252000		
65.84	327900			68	316000		
				68.3	365000		

(Continued)

TABLE 14.1.1.1.1 (Continued)

2.

Jaoui et al. 1999		Jaoui et al. 2002	
static visual method		static visual method*	
T/K	S/g·m ⁻³	T/K	S/g·m ⁻³
298.5	94100	292.5	81011
307.5	99328	296.1	82959
313.4	104556	296.3	83119
313.7	143764	300.2	86290
319.8	118149	302.7	88341
324.8	134877	305.8	90901
331.5	151606	308.4	93065
336.7	182970	313.3	97186
		315.4	100169
		322.4	114416
		326.8	124024
		331.3	134394
		333.6	139814

some data from Achard et al.
1996, Jaoui et al. 1999

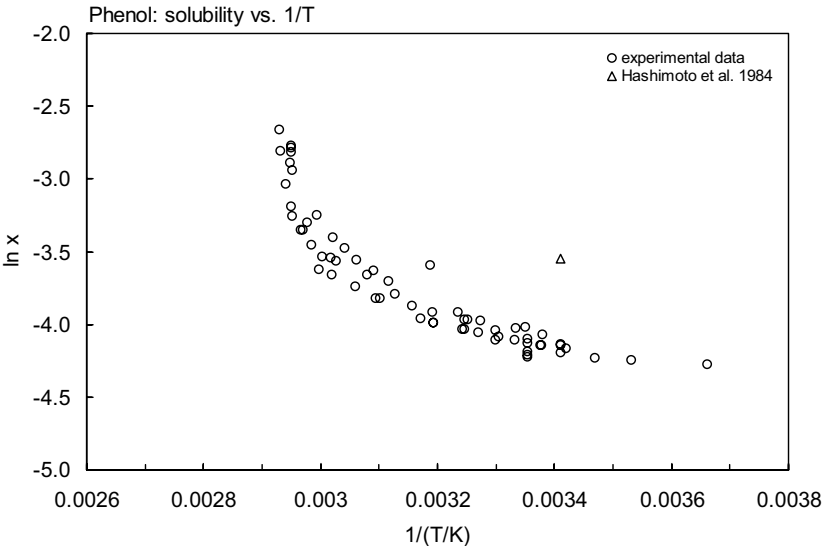


FIGURE 14.1.1.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for phenol.

TABLE 14.1.1.1.2

Reported vapor pressures of phenol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Kahlbaum 1898*		Stull 1947		Goldblum et al. 1947		Dreisbach & Shrader 1949	
static-manometer		summary of literature data		mercury manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
44.8	133.3	40.1	133.3	141.1	28531	107.15	7605
51.5	266.6	62.5	666.6	152.6	42263	113.81	10114
55.8	400.0	73.8	1333	164.4	61061	125.95	16500
59.3	533.3	86.0	2666	168.3	68661	152.37	42066
62.5	666.6	100.1	5333	173.5	80127	167.63	67661
73.5	1333.2	108.4	7999	181.0	98659	181.75	101325
85.8	2666.4	121.4	13332	140.2	27598		
93.8	3999.7	139.0	26664	145.1	32797	bp/°C	181.75
99.8	5533	160.0	53329	171.4	75194		
104.4	6661	181.9	101325	176.6	87060		
113.7	9992			181.1	98525		
120.2	13332	mp/°C	40.6				
139.0	26664			eq. 1	P/mmHg		
151.0	39997			A	8.395		
160.0	53329			B	2510		
167.0	66661						
173.0	79993						
179.0	93326						
181.4	101325						

*complete list see [ref.](#)

2.

Vonterres et al. 1955		Biddiscombe & Martin 1958				Tabai et al. 1997	
ebulliometry		gas saturation/diaphragm manometer				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		solid		liquid			
70.50	1333	0	3.746	121.25	13583	40.09	173
90.20	3333	5.1	6.159	131.183	20005	50.0	345
104.2	6666	9.25	9.413	138.014	25635	60.0	655
113.0	9999	9.85	10.40	140.704	28226	70.03	1187
121.5	13332	10.4	10.47	147.204	35310	79.97	2048
132.5	19998	14.5	16.0	155.343	46139	89.99	3415
140.1	26664	18.25	22.93	156.196	47902		
147.0	33330	18.25	23.20	156.528	53130		
152.0	39997	19.6	26.66	159.799	54843		
153.0	43330	22.0	35.60	160.124	58843		
156.0	46663	24.85	44.26	163.795	60104		
160.0	53329	28.15	63.73	168.945	70154		

(Continued)

TABLE 14.1.1.1.2 (Continued)

Vonterres et al. 1955		Biddiscombe & Martin 1958				Tabai et al. 1997	
ebulliometry		gas saturation/diaphragm manometer				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
164.0	59995	30.5	74.39	169.991	72357		
167.0	73327	32.95	92.93	171.025	74590		
170.5	73327	35.0	108.5	172.635	78154		
173.0	79993	37.45	138.7	173.066	79148		
176.0	86659			175.767	85526		
179.0	93325	bp/°C	181.839	178.196	91590		
181.7	101325			179.878	94918		
		Antoine eq. for temp range:		180.863	98625		
		0–40°C		181.551	100497		
		eq. 1	P/mmHg	182.053	101904		
		A	11.5638				
		B	3586.36	Antoine eq. for temp range:			
		C	273	110–200°C			
				eq. 2	P/mmHg		
		ΔH_v /(kJ mol ⁻¹)		A	7.13457		
		at bp	47.304	B	1516.072		
		at 25°C	68.66	C	174.569		

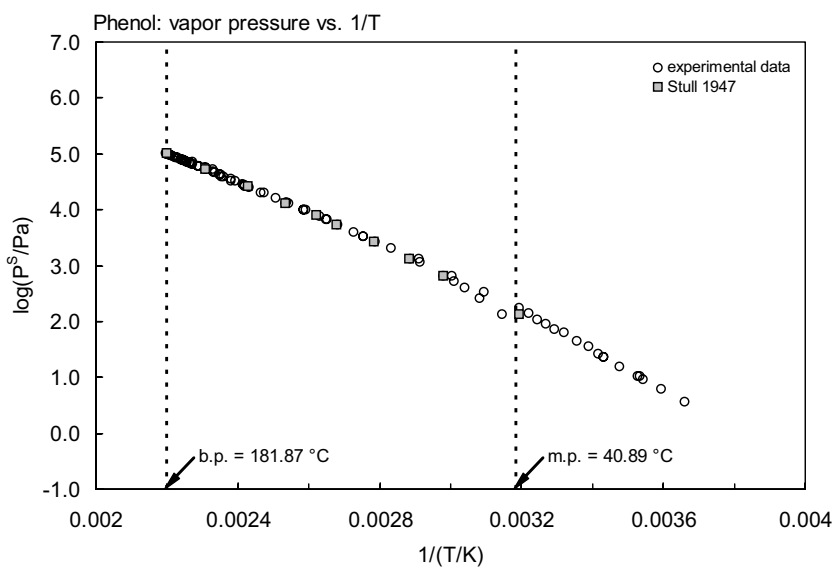


FIGURE 14.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for phenol.

TABLE 14.1.1.1.3

Reported Henry's law constants of phenol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)		
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)		
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)					
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)		
$\ln k_H = A - B/(T/K) - C \cdot \ln (T/K)$		(5)					
Abd-El-Bary et al. 1986		Dohnal & Fenclová 1995		Tabai et al. 1997		Feigenbrugel et al. 2004	
gas stripping-GC/FID		vapor-liquid equilibrium		derived from measured P		gas stripping-GC/MS	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)
−2.0	0.0072	4.0	0.0127*	313.24	0.0342	278.15	0.0222
4.0	0.0127	18.3	0.0373*	323.15	0.090	278.15	0.0299
18.3	0.0373	27.0	0.0721*	333.15	0.202	278.20	0.0280
27.0	0.0718	80.3	1.552*	343.18	0.355	278.25	0.0337
44.4	0.193*	100.0	3.537*	353.12	0.506	283.05	0.0340
56.3	0.437*	75.9	1.245	363.14	0.999	283.15	0.0456
75.0	1.233*	88.7	2.193			283.15	0.0328
90.0	2.376*	98.6	3.322	eq. 5	k _H /kPa	283.25	0.0428
		25.0	0.0607#	A	670.117	283.25	0.0404
*data from literature		25.0	0.0605\$	B	29374.5	288.15	0.0590
			#calculated from eq. 1	C	94.6679	288.15	0.0928
			\$calculated from eq. 3	temp range 313–363 K		288.25	0.0560
			*data from literature			293.15	0.1166
eq. 3	k _H /kPa					293.15	0.169
A	21.7128	eq. 1	K _{AW}	Harrison et al. 2002		293.15	0.1093
B	6120.0	A	8.701	gas stripping-UV		293.15	0.1065
eq. derived included lit. data		B	5760	T/K	H/(Pa m³/mol)	293.25	0.0960
		enthalpy of hydration:				293.25	0.1071
		$\Delta H_K/(\text{kJ mol}^{-1}) = 47.9 \pm 0.5$		284	0.0122	298.15	0.0904
		OR		284.5	0.0110	298.15	0.2022
		eq. 3	k _H /kPa	289.5	0.0199	298.15	0.1375
		A	21.443	293.5	0.0262		
		B	6032	298	0.0320		
		$\Delta H_K/(\text{kJ mol}^{-1}) = 50.2 \pm 0.4$		302	0.0379		
				eq. 4	H/(M atm ^{−1})		
				A	−11.6		
				B	−5850		

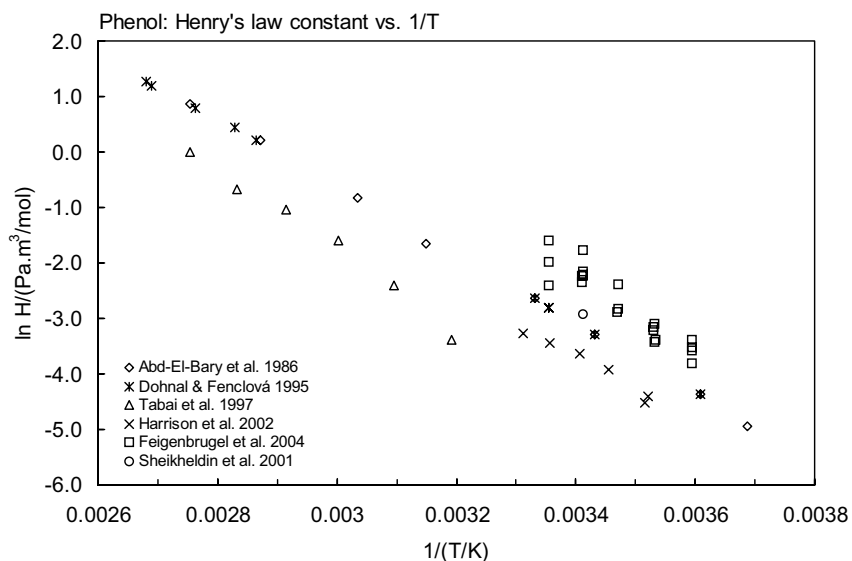


FIGURE 14.1.1.1.3 Logarithm of Henry's law constant versus reciprocal temperature for phenol.

TABLE 14.1.1.1.4

Reported octanol-water partition coefficients of phenol at various temperatures

Korenman & Udalova 1974

shake flask-concn ratio	
t/°C	log K _{OW}
10	1.531
20	1.510
30	1.461
40	1.433
50	1.396
60	1.369
log K _{OW} = A – B/(T/K)	
A	0.4479
B	–305.877

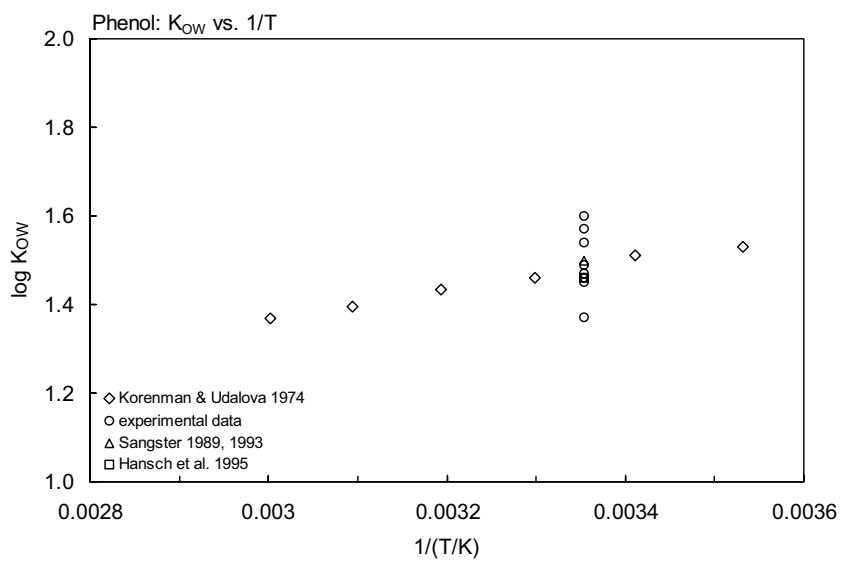
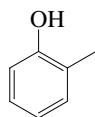


FIGURE 14.1.1.1.4 Logarithm of K_{OW} versus reciprocal temperature for phenol.

14.1.1.2 *o*-Cresol

Common Name: *o*-Cresol

Synonym: 2-hydroxytoluene, 2-methylphenol, *o*-cresylic acid, *o*-hydroxytoluene, 2-cresol, 1,2-cresol

Chemical Name: 2-methylphenol

CAS Registry No: 95-48-7

Molecular Formula: C_7H_8O , $C_6H_4(CH_3)OH$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

31.03 (Lide 2003)

Boiling Point ($^{\circ}C$):

191.04 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0273 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

10.28 (Pearce & Simkins 1968)

10.20 (Hoigné & Bader 1983; Weast 1982–83)

10.26 (Dean 1985)

Molar Volume (cm^3/mol):

104.4 ($30^{\circ}C$, Stephenson & Malanowski 1987)

125.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

46.94 (Biddiscombe & Martin 1958)

45.91 (at normal boiling point, Andon et al. 1960)

42.7 (Dean 1992)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

76.02 (at $25^{\circ}C$, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.8 (Tsonopoulos & Prausnitz 1971; Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

52.01 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.873 (mp at $31.03^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

30100* ($35.3^{\circ}C$, shake flask, measured range 35.3 – $162.8^{\circ}C$, critical solution temp $162.8^{\circ}C$, Sidgwick et al. 1915)

24970 (shake flask-residue volume method, Booth & Everson 1948)

25950 (shake flask-UV at pH 5.1, Blackman et al. 1955)

25000* ($20^{\circ}C$, synthetic method/shake flask-optical, measured range 0 – $166.5^{\circ}C$, Ericksen & Dobbert 1955)

25000 (shake flask-UV spectrophotometry, Roberts et al. 1977)

2725 (generator column-HPLC, Wasik et al. 1981)

31000, 56000 ($40^{\circ}C$, $100^{\circ}C$, Verschueren 1983)

42608, 48061, 52241 (75.9 , 88.7 , $98.5^{\circ}C$, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

26820* (calculated-activity coeff. γ^{∞} data, measured range 25 – $35^{\circ}C$, Dohnal & Fenclová 1995)

26800 (shake flask-HPLC/UV at pH 3.6, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

23065* ($142.3^{\circ}C$, mercury manometer, measured range 142.3 – $190.8^{\circ}C$, Goldblum et al. 1947)

- $\log (P/\text{mmHg}) = -2520/(T/K) + 8.308$; temp range 142.3–177.1°C (Hg manometer, Goldblum et al. 1947)
 58.16* (extrapolated-regression of tabulated data, temp range 38–190.5°C, Stull 1947)
 7605* (113.11°C, ebulliometry, measured range 113.11–190.95°C, Dreisbach & Shrader 1949)
 56.72 (calculated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 7.49476 - 1777.8/(203.0 + t/^{\circ}\text{C})$; temp range 97–250°C (Antoine eq. for liquid state, Dreisbach 1955)
 38.60 (gas saturation and diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
 37.32* (25.25°C, gas saturation -diaphragm manometer, temp range 0–28°C, Biddiscombe & Martin 1958)
 $\log (P/\text{mmHg}) = 12.7778 - 3970.17/(t/^{\circ}\text{C} + 273)$; temp range 0–30°C (Antoine eq. gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 $\log (P/\text{mmHg}) = 7.07055 - 1542.299/(t/^{\circ}\text{C} + 177.110)$; temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 $\log (P/\text{mmHg}) = [-0.2185 \times 12487.3/(T/K)] + 8.79055$; temp range 38.2–190.8°C (Antoine eq., Weast 1972–73)
 30.7 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 6.91172 - 1435.503/(165.158 + t/^{\circ}\text{C})$; temp range 120–191°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
 32.0 (Verschueren 1977, 1983)
 38.32 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 463.986/(T/K)] \times 10^{\{1.01555 - 9.95980 \times 10^{-4} \cdot (T/K) + 7.92834 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 313.20–697.65 K (Cox eq., Chao et al. 1983)
 30.3, 22.5 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.02377 - 1427.165/(164.218 + t/^{\circ}\text{C})$; temp range 120–191°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 5.82809 - 1299.971/(148.886 + t/^{\circ}\text{C})$; temp range 142.3–189.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 30.74 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 6.9117 - 1435.5/(165.16 + t/^{\circ}\text{C})$; temp range 120–191°C (Antoine eq., Dean 1985, 1992)
 37.70 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.68858 - 3909.409/(T/K)$; temp range 273–303 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19545 - 1542.299/(-96.04 + T/K)$; temp range 383–473 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.47616 - 1714.489/(-79.841 + T/K)$; temp range 304–409 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19561 - 1543.097/(-95.902 + T/K)$; temp range 399–470 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.24893 - 1584.403/(-90.794 + T/K)$; temp range 463–526 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.82237 - 2134.352/(-19.536 + T/K)$; temp range 517–630 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)
 40.0 (Riddick et al. 1986)
 39.4 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 99.85294 - 6347.665/(T/K) - 32.60231 \cdot \log (T/K) + 1.24267 \times 10^{-2} \cdot (T/K)$; temp interval of investigation: 412–467 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 89.4591 - 6.0489 \times 10^3/(T/K) - 29.481 \cdot \log (T/K) + 1.0936 \times 10^{-4} \cdot (T/K) + 1.9933 \times 10^{-12} \cdot (T/K)^2$; temp range 304–698 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.124, 0.07, 1.082 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.284, 0.162 (8, 25°C, calculated, Leuenberger et al. 1985)
 0.0852 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.176* (°C, calculated-activity coeff. γ^{∞} data, measured range 25–35°C, Dohnal & Fenclová 1995)

3.352, 5.386, 8.652 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.178 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{AW} = 9.091 - 5556/(T/K)$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 0.159 (gas stripping-GC, Altschuh et al. 1999)
 0.102 (calculated-group contribution, Lee et al. 2000)
 0.217 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)
 0.0965* (gas stripping-UV, measured range 281–302 K, Harrison et al. 2002)
 $\ln [H/(M \text{ atm}^{-1})] = 6680/(T/K) - 15.4$; temp range 281–302 K, Harrison et al. 2002)
 0.146, 0.239* (20, 25°C, dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.04 (shake flask-UV, Korenman & Pereshein 1970)
 1.95 (from Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Leo 1985)
 1.95 (LC- k' correlation, Carlson et al. 1975)
 2.045 (shake flask, Korenman et al. 1980)
 2.17 (HPLC- k' correlation, Butte et al. 1981; Butte et al. 1987)
 1.96 (generator column-HPLC, Wasik et al. 1981)
 1.99 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 1.98 (recommended, Sangster 1989)
 1.97, 1.98 (COMPUTOX data bank, Kaiser 1993)
 1.95 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.26 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)
 1.03 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

1.34 (Brookstone clay loam soil at pH 5.7, Boyd 1982; quoted, Howard 1989)
 1.26 (calculated-S, Boyd 1982; quoted, Howard 1989)
 1.76 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 3.41 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ (relative rate method with reference 2-methyl-2-butene Perry et al. 1977; Atkinson et al. 1979)

$k_{NO_3} = (12 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ (relative rate method with reference to with 2-methyl-2-butene Japar & Niki 1975; Graham & Johnston 1978; Carter et al. 1981)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation with singlet oxygen at 25°C in the aquatic system with half-life > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 20 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 0.3 \text{ d}$ (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{NO_3} = (13.9 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ (relative rate method with reference to the reaction of NO_3 radical with 2-methyl-2-butene, Carter et al. 1981; quoted, Atkinson 1991)

photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reaction rate constants for OH and RO_2 radicals with the phenol class (Güsten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991)

$k_{O_3} = (2.55 \pm 0.39) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$; calculated tropospheric lifetimes of 45 d and 0.3 d due to reaction with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)

$k_{OH} = 2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ with half-life of 0.3 d in the atmosphere (Mill 1982)

$k_{OH} = 2.0 \times 10^{13} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k = (1.2 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.5–2.0 (Hoigné & Bader 1983b)

$k_{\text{OH}} = 4.1 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 1 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = (1.20 \pm 0.34) \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson et al. 1984)

$k_{\text{NO}_3} = (15.6 \pm 1.7) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ with reference to the reaction of NO_3 radical with *m*-cresol at $(298 \pm 1) \text{ K}$ (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{NO}_3} = 22 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ with $2.4 \times 10^8 \text{ NO}_3$ radical/ cm^3 at room temp. and a loss rate of 450 d^{-1} with $t_{1/2} = 1.6\text{--}16 \text{ h}$ (Atkinson et al. 1984, 1985; quoted, Atkinson 1985)

$k_{\text{OH}} = 40 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radical/ cm^3 at room temp. and a loss rate of 1.7 d^{-1} (Atkinson 1985; quoted, Howard et al. 1991)

$k_{\text{OH}}(\text{exptl}) = 37 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{calc}) = 44.8 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}}(\text{exptl}) = 40 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 44 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 4.2 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{NO}_3} = (13.7 \pm 0.9) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at $(296 \pm 2) \text{ K}$, and $k_{\text{OH}} = 42 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ for at room temp. (Atkinson et al. 1992)

$k_{\text{OH}}(\text{calc}) = 30.36 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}} = 4.9 \times 10^{-11} \text{ cm}^3 \cdot \text{mol}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{aq.}) = 1.1 \times 10^{-10} \text{ M}^{-1} \text{ s}^{-1}$, the calculated atmospheric lifetime $\tau = 0.24 \text{ d}$ under clear sky; $\tau = 0.22 \text{ d}$ under cloudy conditions at 298 K, reduced to 0.17 d due the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis:

Biodegradation: 1 to 2 d for bacteria to utilize 95% of 300 ppm in the parent substrate (Tabak et al. 1964)

$t_{1/2} = 2 \text{ d}$ at 20°C and 7 d at 4°C in river water (Ludzack & Ettinger 1960; quoted, Howard 1989)

completely degraded by a soil microflora within one day (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate of biodegradation $k = 54.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168 \text{ h}$, based on unacclimated aerobic screening test data (Takemoto et al. 1981; Urushigawa et al. 1983; quoted, selected, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$k(\text{exptl.}) = 0.0679 \text{ h}^{-1}$ compared to group contribution method predicted $k(\text{calc}) = 0.0728 \text{ h}^{-1}$ (nonlinear) and $k = 0.0567 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993)

$t_{1/2}(\text{aerobic}) = 2 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 15 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: microbial transformation $k = (2.7 \pm 1.3) \times 10^{-10} \text{ L} \cdot \text{organism}^{-1} \cdot \text{h}^{-1}$ (Paris et al. 1983; quoted, Steen 1991).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 1.6\text{--}16 \text{ h}$ in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);

loss rate $k = 10.8 \times 10^{-4} \text{ min}^{-1}$ in outdoor Teflon chambers in the dark (Grosjean 1985);

photodegradation $t_{1/2} \sim 9.6 \text{ h}$ in air, based on measured rate constant for the reaction with photochemically generated hydroxyl radicals (quoted, Howard 1989);

atmospheric transformation lifetime $\tau < 1 \text{ d}$ (estimated, Kelly 1994);

calculated lifetimes of 2.2 h, 2 min and 65 d for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

calculated atmospheric lifetime $\tau = 0.24 \text{ d}$ under clear sky and $\tau = 0.22 \text{ d}$ under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to $\tau = 0.19 \text{ d}$ due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reaction rate constants for OH and RO_2 radicals with the phenol class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991)

rate constant $k = (1.2 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 1.5/2.0 (Hoigné & Bader 1983)

$t_{1/2}(\text{aerobic}) = 2 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 15 \text{ d}$ in natural waters (Capel & Larson 1995)

Ground water: estimated $t_{1/2} \sim 0.01 \text{ yr}$ for cresols at Noordwijk (Zoeteman et al. 1981).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} = 5.1$ d in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 1.6$ d in slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.1.2.1

Reported aqueous solubilities of *o*-cresol at various temperatures

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Dohnal & Fenclová 1995	
shake flask-synthetic method		shake flask-optical method		vapor-liquid equil.-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
35.3	30100	0	22000	25	26820
50.2	32200	20	25000	30	28470
61.7	34700	40	28000	35	30810
70.6	37500	60	32000	75.9	42608
77.7	41000	80	38000	88.7	48061
84.6	45100	100	48000	98.5	52241
130.6	65200	120	67000	100	53640
148.7	104600	130	82000		
158.7	193600	140	102000		
161.7	300600	150	136000		
162.8	408900	160	202000		
160.0	501400	162	228000		
157.7	598000	164	275000		
145.7	693000	166	352000		
129.6	761400	166.5	400000		
87.5	823700				
56.6	845800				
33.6	866000				
25.6	861400				
8.3	875200				
9.1	886800				
10.2	898900				
11.1	908500				
12.9	926200				
15.3	940800				
22.3	974600				
26.9	990100				
29.9	1000000				
critical solution temp 162.8°C					
triple point 8°C					

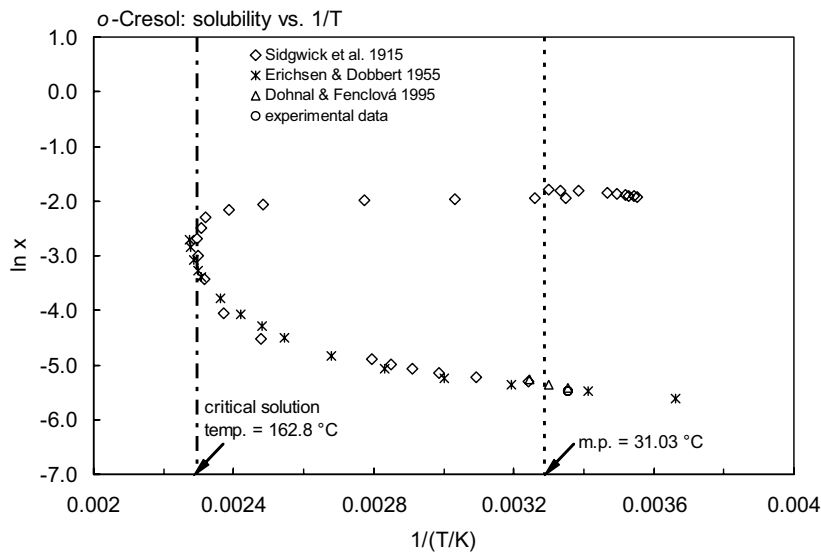


FIGURE 14.1.1.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for o-cresol.

TABLE 14.1.1.2.2
Reported vapor pressures of o-cresol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)				(1)	ln P = A – B/(T/K)				(1a)
log (P/mmHg) = A – B/(C + t/°C)				(2)	ln P = A – B/(C + t/°C)				(2a)
log (P/Pa) = A – B/(C + T/K)				(3)					
log (P/mmHg) = A – B/(T/K) – C·log (T/K)				(4)					
Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						solid		liquid	
38.2	133.3	142.3	23065	113.11	7605	0	2.680	138.575	20410
64.0	666.6	153.3	33731	120.22	10114	2.90	2.093	146.128	26548
76.7	1333	164.5	47729	132.63	16500	5.0	4.213	152.680	33025
90.5	2666	171.2	58529	160.17	42066	5.60	4.680	158.592	39922
105.8	5333	183.5	81993	176.14	67661	9.80	6.933	163.551	46571
115.5	7999	189.8	97859	190.95	101325	10.05	7.773	168.080	53394
127.4	13332	143.7	24265	bp/°C	190.95	14.85	13.20	172.002	59935
146.7	26664	166.8	51329			14.90	12.60	175.642	66563
168.4	53329	172.0	61328			17.40	18.27	179.039	73277
190.8	101325	179.4	73861			19.50	22.0	182.183	79956
mp/°C	30.8	177.1	69194	20.0		22.40	185.185	86782	
				20.35		22.66	187.735	92934	
				24.35		34.66	188.487	94810	
				25.25		37.33	189.013	96149	
		eq. 1	P/mmHg	26.65		45.20	189.455	97276	
		A	8.308	27.25		48.40	189.973	98613	
		B	2520	28.35		66.66	190.371	99650	
							190.486	99953	
							190.545	100125	

(Continued)

TABLE 14.1.1.2.2 (Continued)

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						bp/°C	191.003	191.046	101452
								191.135	101668
						for temp range:		191.511	102686
						0–30°C			
						eq. 2	P/mmHg		
						A	11.5638	for temp range:	
						B	3586.36	110–200°C	
						C	273	eq. 2	P/mmHg
								A	7.13457
						ΔH_v /(kJ mol ⁻¹)		B	1516.072
						at bp	46.94	C	174.569
						at 25°C	76.02		

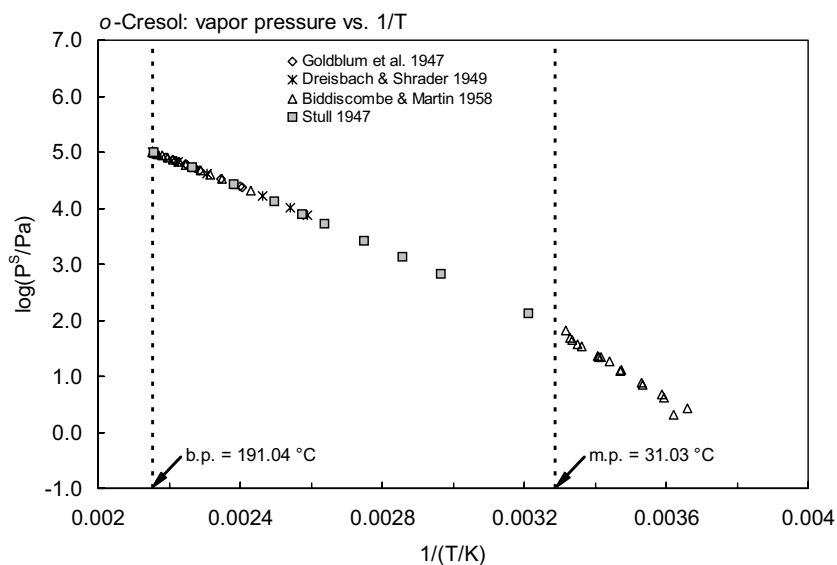


FIGURE 14.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for o-cresol.

TABLE 14.1.1.2.3

Reported Henry's law constants of *o*-cresol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
Dohnal & Fenclová 1995		Harrison et al. 2002		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-UV		gas stripping-GC/MS	
t/°C	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)
25	0.176*	281	0.0224	278.25	0.0348
30	0.245*	284.5	0.0313	278.25	0.0355
35	0.341*	289.5	0.0596	278.35	0.0286
75.9	3.352	293.5	0.0650	283.15	0.0707
88.7	5.386	298	0.0965	283.15	0.0556
98.5	8.652	302	0.1165	283.25	0.0565
100	9.028			288.10	0.0842
25.0	0.1777#	eq. 4	H/(M atm ⁻¹)	288.15	0.1137
25.0	0.1764\$	A	-15.4	288.20	0.0855
		B	-6680	293.10	0.1603
#calculated from eq. 1				293.15	0.1626
\$calculated from eq. 3				293.15	0.1554
*data from literature				293.15	0.1371
				293.15	0.1883
eq. 1	K _{AW}			293.25	0.1537
A	9.091			298.15	0.2356
B	5556			298.15	0.2362
enthalpy of hydration:				293	0.1464
ΔH _K /(kJ mol ⁻¹) = 46.2 ± 0.4				298	0.2390
OR					
eq. 3	k _H /kPa				
A	21.832				
B	5827				
ΔH _K /(kJ mol ⁻¹) = 48.5 ± 0.4					

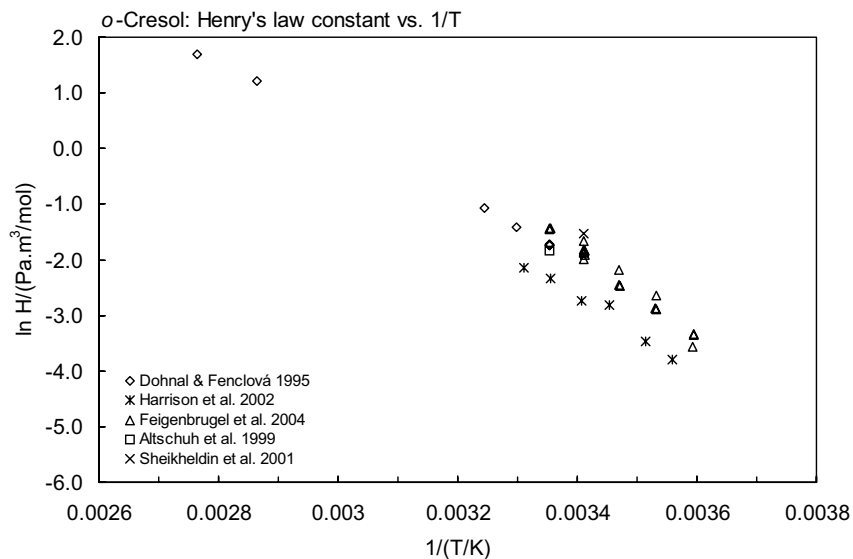
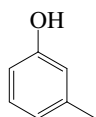


FIGURE 14.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for *o*-cresol.

14.1.1.3 *m*-Cresol

Common Name: *m*-Cresol

Synonym: *m*-cresylic acid, 1-hydroxy-3-methylbenzene, 3-hydroxytoluene, *m*-hydroxytoluene, 3-methylphenol, *m*-methylphenol, 3-cresol

Chemical Name: *m*-cresol, 3-methylphenol

CAS Registry No: 108-39-4

Molecular Formula: C_7H_8O , $C_6H_4(CH_3)OH$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

12.24 (Lide 2003)

Boiling Point ($^{\circ}C$):

202.27 (Lide 2003)

Density (g/cm^3):

1.0336 (Weast 1982–83)

1.0302 (25 $^{\circ}C$, Riddick et al. 1986)

Acid Dissociation Constant, pK_a :

10.09 (Pearce & Simkins 1968; Riddick et al. 1986; Howard 1989)

10.0 (Hoigné & Bader 1983; Dean 1985)

10.01 (Weast 1982–83)

Molar Volume (cm^3/mol):

105.6 (calculated-density, Rohrschneider 1973)

125.6 (calculated-Le Bas-method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.38 (at normal bp, Biddiscombe & Martin 1958)

47.40 (at normal boiling point, Andon et al. 1960)

61.714 (at 25 $^{\circ}C$, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.53 (Tsonopoulos & Prausnitz 1971)

10.70 (Riddick et al. 1986; Dean 1992)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

37.53 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F : 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

23600* (24.7 $^{\circ}C$, shake flask, measured range –2 to 87.58 $^{\circ}C$, critical solution temp 147 $^{\circ}C$, Sidgwick et al. 1915)

22664 (shake flask-residue volume method, Booth & Everson 1948)

22000* (20 $^{\circ}C$, synthetic method/shake flask-optical, measured range 0–148 $^{\circ}C$, Ericksen & Dobbert 1955)

25000 (shake flask-spectrophotometry, Roberts et al. 1977)

2800 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)

23500, 58000 (20 $^{\circ}C$, 100 $^{\circ}C$, Verschueren 1977, 1983)

23790* (20.35 $^{\circ}C$, equilibrium cell-concn ratio-GC, measured range 20.35–139 $^{\circ}C$, Leet et al. 1987)

24125, 23194* (24.7, 25 $^{\circ}C$, calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)

46935, 54615, 58327 (75.9, 88.7, 98.5 $^{\circ}C$, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

19600 (shake flask-HPLC/UV at pH 4.45, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of the section):

- 20265* (149.5°C, mercury manometer, measured range 149.5–201.1°C, Goldblum et al. 1947)
 $\log(P/\text{mmHg}) = -2650/(T/K) + 8.457$; temp range 149.5–201.1°C (Hg manometer, Goldblum et al. 1947)
- 23.95* (extrapolated-regression of tabulated data, temp range 52–202.8°C, Stull 1947)
- 25.83 (calculated-Antoine eq., Dreisbach 1955)
 $\log(P/\text{mmHg}) = 7.53165 - 1875.3/(201.0 + t/^{\circ}\text{C})$, temp range: 110–240°C, (Antoine eq. for liquid state, Dreisbach 1955)
- 1333* (85.5°C, ebulliometry, measured range 85.5–202.1°C, Vonterres et al. 1955)
- 19.0 (gas saturation-diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
- 18.278* (24.90°C, gas saturation-diaphragm manometer, temp range 0–39°C, Biddiscombe & Martin 1958)
 $\log(P/\text{mmHg}) = 9.9653 - 3223.45/(t/^{\circ}\text{C} + 273)$; temp range 11–40°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
- $\log(P/\text{mmHg}) = 7.15904 - 1603.811/(t/^{\circ}\text{C} + 172.646)$; temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; measurements, Andon et al. 1960)
- $\log(P/\text{mmHg}) = [-0.2185 \times 13483.8/(T/K)] + 9.135933$; temp range 52–202.8°C (Antoine eq., Weast 1972–73)
- 22.28 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 7.50798 - 1856.356/(199.065 + t/^{\circ}\text{C})$, temp range 149.5–201°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
- 4120* (114.99°C, diaphragm gauge, measured range 114.99–216.72 °C, Nasir et al. 1980)
- 5.33, 16.0 (20°C, 30°C, Verschuere 1977, 1983)
- 36.43 (calculated-Cox eq., Chao et al. 1983)
 $\log(P/\text{mmHg}) = [1 - 475.222/(T/K)] \times 10^{0.965085 - 6.89845 \times 10^{-4} \cdot (T/K) + 4.47100 \times 10^{-7} \cdot (T/K)^2}$; temp range: 278.05–705.85 K, (Cox eq., Chao et al. 1983)
- 22.1, 11.9 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.62485 - 1850.362/(198.462 + t/^{\circ}\text{C})$; temp range 149.5–201°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log(P/\text{kPa}) = 6.28411 - 1580.594/(167.548 + t/^{\circ}\text{C})$; temp range 88.5–202.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 22.29 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.5080 - 1856.36/(199.07 + t/^{\circ}\text{C})$; temp range 150–201°C (Antoine eq., Dean 1985, 1992)
- 19.10 (Riddick et al. 1986)
- 79960* (466.35 K, vapor-liquid equilibrium, measured range 466.35–588.68 K, Klara et al. 1987)
- 19.08; 18.61 (interpolated-Antoine eq.-III, IV, Stephenson & Malanowski 1987)
 $\log(P_s/\text{kPa}) = 8.0462 - 2930.845/(T/K)$; temp range 273–285 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.28394 - 1603.811/(-100.504 + T/K)$; temp range 383–473 K, (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 9.0902 - 3223.45/(T/K)$; temp range 284–313 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 7.150 - 2123.548/(-59.018 + T/K)$; temp range 285–416 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.28579 - 1605.855/(-100.232 + T/K)$; temp range 410–477 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 5.80987 - 1293.277/(-135.465 + T/K)$; temp range 471–531 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.64135 - 2069.208/(-26.534 + T/K)$, temp range: 523–633 K, (Antoine eq.-VII, liquid, Stephenson & Malanowski 1987)
- 19.70 (extrapolated-Antoine eq., Nesterova et al. 1990)
 $\log(P/\text{Pa}) = 64.02580 - 5272.296/(T/K) - 18.84252 \cdot \log(T/K) + 0.52858 \times 10^{-2} \cdot (T/K)$; temp range: 409–477 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
- $\log(P/\text{mmHg}) = 105.528 - 6.9748 \times 10^3/(T/K) - 35.083 \cdot \log(T/K) + 1.2508 \times 10^{-2} \cdot (T/K) - 2.4317 \times 10^{-12} \cdot (T/K)^2$; temp range 285–706 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.0203, 0.0881 (8, 25°C , calculated, Leuenberger et al. 1985)
 0.0875, 0.0627 (calculated-P/C, estimated-bond contribution, Meylan & Howard 1991)
 0.0718 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.1068 (calculated-P/C, Shiu et al. 1994)
 0.0810, 0.0865* (24.7, 25°C , calculated-activity coeff. γ^∞ data, Dohnal & Fenclová 1995)
 1.683, 2.990, 4.635 (75.9, 88.7, 98.5°C , vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.0848 (extrapolated-vapor liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{\text{AW}} = 8.909 - 5722/(T/\text{K})$, temp range $20\text{--}100^\circ\text{C}$ (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 0.0868 (gas stripping-GC, Altschuh et al. 1999)
 0.0641 (20°C , single equilibrium static technique SEST, Sheikheldin et al. 2001)
 0.0765, 0.127* (20, 25°C , dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.96 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1985)
 2.02 (shake flask, Korenman et al. 1980)
 1.94 (HPLC-RT correlation, Butte et al. 1981)
 1.96 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)
 1.96 (shake flask-UV, Saarikoski & Viluksela 1982)
 1.98 (recommended, Sangster 1989, 1993)
 1.96 (COMPUTOX databank, Kaiser 1993)
 1.96 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.30 (golden ide, after 3 d, Freitag et al. 1985)
 3.69 (algae, after 1 d, Freitag et al. 1985)
 3.04 (activated sludge, after 5 d, Freitag et al. 1985)
 1.03 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.54 (Brookstone clay loam soil, Boyd 1982)
 1.26 (calculated-S, Boyd 1982)
 1.76 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct aqueous photolysis $k = 0.011 \pm 0.001 \text{ min}^{-1}$ with $t_{1/2} = 60.4 \text{ min}$ (Stegeman et al. 1993).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{NO}_3} = (7 \pm 1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to the reaction of NO_3 radical with 2-methyl-2-butene (Japar & Niki 1975; Graham & Johnston 1978; Carter et al. 1981)

$k_{\text{OH}} = 48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to the reaction of OH radical with 2-methyl-2-butene (Atkinson et al. 1979; Carter et al. 1981)

$k_{\text{NO}_3} = (8.10 \pm 1.16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(300 \pm 1) \text{ K}$ with reference to the reaction of NO_3 radical with 2-methyl-2-butene (Carter et al. 1981; quoted, Atkinson 1991)

$k_{\text{O}_3} = (1.94 \pm 0.35) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$; calculated tropospheric lifetimes of 60 d and 0.2 d due to reaction with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)

photooxidation half-life of 66–3480 h in water, based on reported reaction rate constants for OH and RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991)

$k = (1.3 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.5/2.0 (Hoigné & Bader 1983b)

$k_{\text{OH}} = 5.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = 1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)
 $k_{\text{NO}_3} = (9.20 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson et al. 1984)
 $k_{\text{NO}_3} = (15.9 \pm 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 1 \text{ K}$ with reference to the reaction of NO_3 radical with phenol (Atkinson et al. 1984; quoted, Atkinson 1991)
 $k_{\text{OH}}(\text{calc}) = 93.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{\text{OH}}(\text{exptl}) = 57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)
 $k_{\text{OH}} = 6.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (recommended, Atkinson 1989, 1990)
 $k_{\text{NO}_3} = (9.74 \pm 0.74) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to the reaction of NO_3 radical with 2-methyl-2-butene, and $k_{\text{OH}} = 64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1992)
 $k_{\text{OH}}(\text{calc}) = 34.42 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)
 $k_{\text{OH}} = 5.2 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, the calculated atmospheric lifetime $\tau = 0.22 \text{ d}$ under clear sky; $\tau = 0.19 \text{ d}$ under cloudy conditions at 298 K, reduced to 0.13 d due the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis:

Biodegradation: $t_{1/2} = 1\text{--}2 \text{ d}$ for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964) completely degraded by a soil microflora within one day (Alexander & Lustigman 1966; quoted, Verschueren 1983)
 average rate $k = 55.0 \text{ mg COD g}^{-1} \cdot \text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
 $t_{1/2}(\text{aq. aerobic}) = 48\text{--}696 \text{ h}$, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);
 $t_{1/2}(\text{aq. anaerobic}) = 360\text{--}1176 \text{ h}$, based on anaerobic screening test data (Horowitz et al. 1982; Shelton & Tiedje 1981; selected, Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 8.0 \text{ h}$, based on rate constant for the gas phase reaction with OH radical in air (Atkinson et al. 1979; quoted, Howard 1989);
 photooxidation $t_{1/2} = 1.1\text{--}11.3 \text{ h}$ in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);
 atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).
 calculated atmospheric lifetime $\tau = 0.22 \text{ d}$ under clear sky and $\tau = 0.19 \text{ d}$ under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to $\tau = 0.13 \text{ d}$ due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)
 Surface water: $t_{1/2} = 48\text{--}696 \text{ h}$, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);
 $k = (1.3 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 1.5/2.0 (Hoigné & Bader 1983);
 photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reported reaction rate constants for OH and RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991).
 Ground water: estimated half-life for cresols, $t_{1/2} = 0.01 \text{ yr}$ at Noordwijk (Zoeteman et al. 1981);
 $t_{1/2} = 96\text{--}1176 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 48\text{--}696 \text{ h}$, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);
 $t_{1/2} = 11.3 \text{ d}$ in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 0.6 \text{ d}$ in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.1.3.1

Reported aqueous solubilities of *m*-cresol at various temperatures

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Leet et al. 1987		Dohnal & Fenclová 1995	
shake flask-synthetic method		shake flask-optical method		equilibrium cell-conc ratio		vapor-liquid equil.-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
-0.20	22400	0	20000	20.35	23790	24.7	24125
24.7	23600	20	22000	40.05	25390	25	23194
47.0	26600	40	25000	58.45	30190	75.8	46935
61.9	30300	60	31000	77.25	37368	88.7	54615
74.5	35400	80	40000	98.15	49804	98.5	58327
87.5	42400	100	53000	119.75 ^a	78100		
116.9	65900	120	88000	138.95 ^b	143583		
139.4	119900	130	113000				
146.9	324000	140	156000	superscript a, at 204 kPa			
147.0	350700	142	170000	superscript b, at 366 kPa			
146.6	410600	144	189000				
140.5	612700	146	221000				
124.8	703200	147	264000				
109.3	804600	148	380000				
82.8	804600						
67.7	826000						
57.1	837000						
46.5	847900						
34.5	858500						
20.3	870500						
13.2	875800						

critical solution temp 147°C
mp/°C 4.0

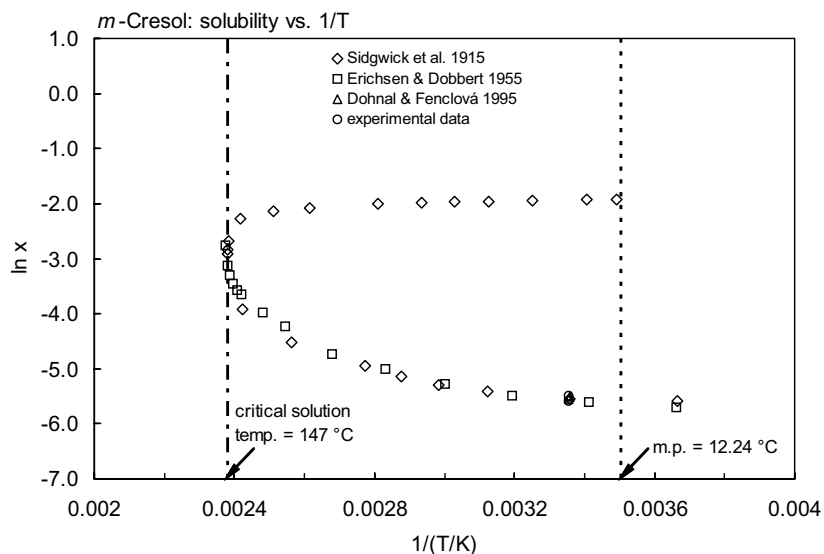
FIGURE 14.1.1.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *m*-cresol.

TABLE 14.1.1.3.2

Reported vapor pressures of *m*-cresol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Stull 1947		Goldblum et al. 1947		Vonterres et al. 1955	
summary of literature data		static method-manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
52.0	133.3	149.5	20265	85.5	1333
76.0	666.6	164.3	33464	105.2	3333
87.8	1333	172.0	42796	121.7	6666
101.4	2666	179.6	53862	131.6	9999
116.0	5333	187.4	67328	139.1	13332
125.8	7999	192.1	76927	150.0	19998
138.0	13332	196.3	86526	158.5	26664
157.3	26664	201.1	98925	163.1	33330
179.0	53329	149.6	20398	170.1	39997
202.8	101325	154.1	23731	173.0	43330
		176.4	48796	175.0	45553
mp/°C	10.8	183.4	60128	179.8	53329
		201.1	98925	183.5	66661
				189.8	73327
		eq. 1	P/mmHg	192.5	79993
		A	8.457	196.0	86659
		B	2650	198.8	93325
				202.1	101325

2.

Biddiscombe & Martin 1958				Nasir et al. 1980		Klara et al. 1987	
gas saturation		ebulliometry		diaphragm gauge		vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
			liquid				
0	2.00*	135.835	12174	114.99	4120	466.35	79960
4.90	2.933*	149.804	20418	121.25	5789	472.95	85540
7.20	4.533*	157.610	26762	127.46	7849	493.75	160600
9.15	4.40*	163.741	32816	133.4	10286	510.86	237900
11.0	5.866	169.814	39930	142.92	15223	531.35	366200
15.0	7.333	174.784	46538	156.29	25337	565.45	695500
17.65	9.866	179.331	53388	167.90	37430	588.68	1028500
19.80	11.47	182.979	59446	187.33	67950		
21.50	14.13	186.818	66415	203.4	106385	eq. 3	P/kPa
24.90	18.27	190.266	73225	216.72	149432	A	15.5337
26.95	27.73	193.424	79951			B	4594.0
29.75	30.80	196.418	86769			C	54.34
30.85	36.80	199.003	93024				

TABLE 14.1.1.3.2 (Continued)

Biddiscombe & Martin 1958				Nasir et al. 1980		Klara et al. 1987	
gas saturation		ebulliometry		diaphragm gauge		vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
33.25	43.20	199.694	94754				
39.10	57.60	200.250	96156				
	*solid	200.658	97201				
		201.216	98639				
bp/°C	202.231	201.557	99550				
		202.156	101118				
Antoine eq. for temp range:		202.737	102665				
11–40°C							
eq. 2	P/mmHg	Antoine eq. for temp range					
A	9.9653	110–200°C					
B	3223.45	eq. 2	P/mmHg				
C	273	A	7.15904				
		B	1603.811				
		C	172.646				
ΔH_v /(kJ mol ⁻¹)							
at bp	49.375						
at 25°C	61.714						

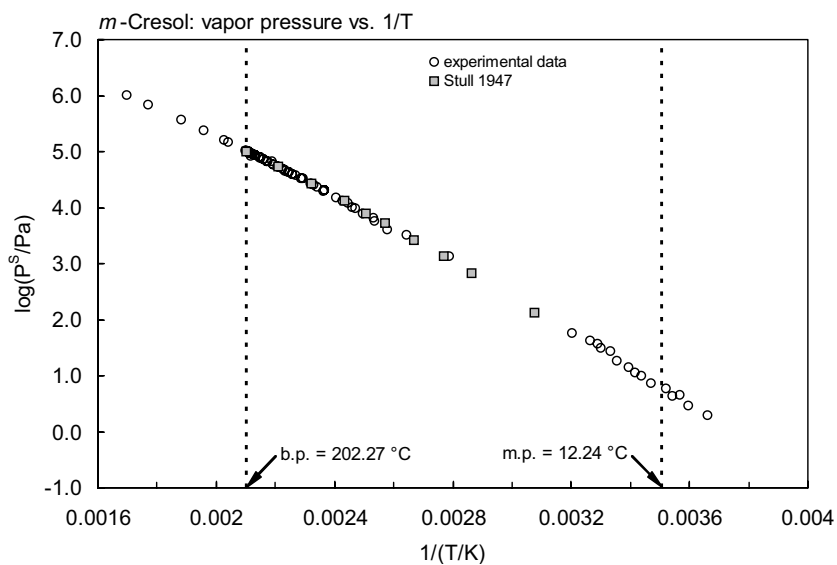
FIGURE 14.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for *m*-cresol.

TABLE 14.1.1.3.3

Reported Henry's law constants of *m*-cresol at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K) \quad (1) \quad \log K_{AW} = A - B/(T/K) \quad (1a)$$

$$\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \quad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)$$

$$\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)$$

$$\ln H = A - B/(T/K) \quad (4) \quad \log H = A - B/(T/K) \quad (4a)$$

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)$$

Dohnal & Fenclová 1995		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-GC/MS	
t/°C	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)
24.7	0.0810*	278.15	0.0148
25.0	0.0865*	278.25	0.0192
75.9	1.683	283.15	0.0283
88.7	2.990	283.25	0.0378
98.5	4.635	283.25	0.0272
25.0	0.0848#	283.25	0.0293
25.0	0.0846\$	288.15	0.0444
		288.25	0.0450
#calculated from eq. 1		293.15	0.0976
\$calculated from eq. 3		293.15	0.0682
*data from literature		293.15	0.0723
		293.15	0.0786
eq. 1	K _{AW}	293.15	0.0771
A	8.909	293.15	0.0976
B	5722	293.25	0.0901
		293.15	0.0810
enthalpy of hydration:		298.15	0.1306
ΔH _K /(kJ mol ⁻¹) = 47.6 ± 0.5		298.15	0.1252
OR		293	0.0765
eq. 3	k _H /kPa	298	0.1270
A	21.650		
B	5994		
ΔH _K /(kJ mol ⁻¹) = 49.8 ± 0.6			

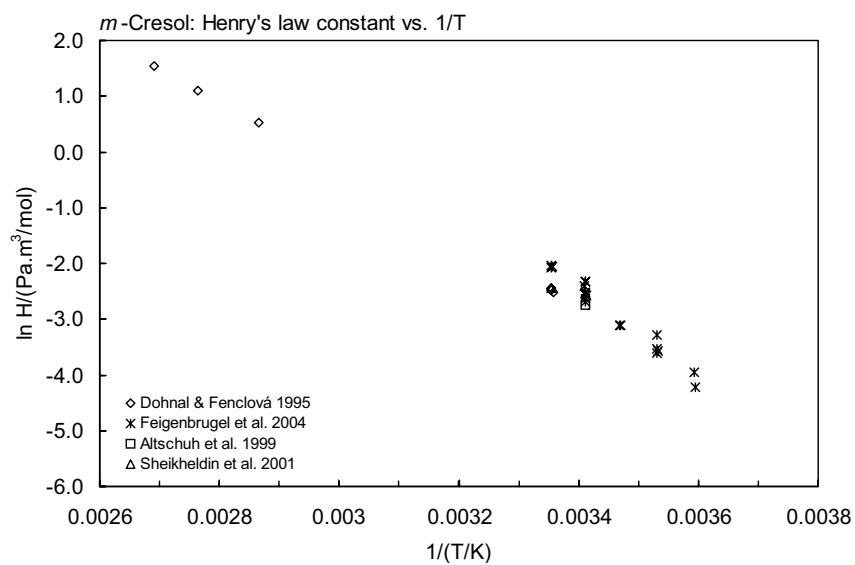
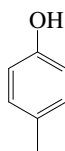


FIGURE 14.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for *m*-cresol.

14.1.1.4 *p*-Cresol

Common Name: *p*-Cresol

Synonym: *p*-cresylic acid, 1-hydroxy-4-methylbenzene, 4-hydroxytoluene, 4-methylphenol, *p*-hydroxytoluene, *p*-methylphenol, 4-cresol

Chemical Name: 4-methylphenol

CAS Registry No: 106-44-5

Molecular Formula: C_7H_8O , $CH_3C_6H_4OH$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

34.77 (Lide 2003)

Boiling Point ($^{\circ}C$):

201.98 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0178 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

10.26 (Pearce & Simkins 1968, Dean 1985, Riddick et al. 1986; Howard 1989)

10.28 (Serjeant & Dempsey 1979; Tratnyek & Hoigné 1991; Haderlein & Schwarzenbach 1993)

10.17 (Weast 1982–83)

Molar Volume (cm^3/mol):

125.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.53 (at normal bp, Biddiscombe & Martin 1958)

47.55 (at normal boiling point, Andon et al. 1960)

43.2 (Dean 1992)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

73.93 (at $25^{\circ}C$, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.72 (Tsonopoulos & Prausnitz 1971; Dean 1992)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

53.22 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.802 (mp at $34.77^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

22400* ($40.2^{\circ}C$, shake flask, measured range 40.2 – $143.5^{\circ}C$, critical solution temp $143.5^{\circ}C$, Sidgwaick et al. 1915)

24230 (shake flask-residue volume method, Booth & Everson 1948)

19000 (shake -flask-UV, Blackman et al. 1955)

17000* ($20^{\circ}C$, synthetic method/shake flask-optical, measured range 0 – $143.7^{\circ}C$, Ericksen & Dobbert 1955)

21000 (shake flask-spectrophotometry, Roberts et al. 1977)

24000, 53000 ($40^{\circ}C$, $100^{\circ}C$, Verschueren 1977, 1983)

21500* (calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)

43534, 50064, 54615 (75.9 , 88.7 , $98.5^{\circ}C$, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

22000 (shake flask-HPLC/UV at pH 3.9, Varhaníčkova et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

17599* ($145.7^{\circ}C$, mercury manometer, measured range 145.7 – $200.8^{\circ}C$, Goldblum et al. 1947)

- $\log (P/\text{mmHg}) = -2680/(T/K) + 8.524$; temp range 145.7–200.9°C (Hg manometer, Goldblum et al. 1947)
 21.89* (extrapolated-regression of tabulated data, temp range 53–201.8°C, Stull 1947)
 7605* (128.65 °C, ebulliometry, measured range 128.65–201.88 °C, Dreisbach & Shrader 1949)
 26.34 (calculated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 7.52971 - 1872.4/(201.0 + t/^{\circ}\text{C})$; temp range 97–250°C (Antoine eq. for liquid state, Dreisbach 1955)
 15.91 (gas saturation-diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
 12.93* (23.35°C, gas saturation-diaphragm manometer, measured range 0–34.15°C, Biddiscombe & Martin 1958)
 $\log (P/\text{mmHg}) = 12.0298 - 3861.98/(t/^{\circ}\text{C} + 273)$; temp range 0–34°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 $\log (P/\text{mmHg}) = 7.11767 - 1566.029/(t/^{\circ}\text{C} + 167.680)$; temp range 110–200°C (Antoine eq. from gas-saturation-diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 133.3 (53°C, Andon et al. 1960; Haque et al. 1980)
 $\log (P/\text{mmHg}) = [-0.2185 \times 13611.7/(T/K)] + 9.190555$; temp range 53–201.8°C (Antoine eq., Weast 1972–73)
 11.8 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.03508 - 1511.08/(161.854 + t/^{\circ}\text{C})$; temp range 128–210.88°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
 13.94 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 475.109/(T/K)] \times 10^{\{1.07944 - 11.6938 \times 10^{-4} \cdot (T/K) + 9.28202 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 323.20–704.65 K, (Cox eq., Chao et al. 1983)
 11.8, 17.5 (calculated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.15637 - 1508.694/(161.594 + t/^{\circ}\text{C})$, temp range 128–201.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.44531 - 1713.242/(183.846 + t/^{\circ}\text{C})$; temp range 15.7–200.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 11.83 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.03508 - 1511.08/(161.85 + t/^{\circ}\text{C})$; temp range 128–202°C (Antoine eq., Dean 1985, 1992)
 17.3 (Riddick et al. 1986)
 15.6 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 12.098 - 3861.98/(T/K)$; temp range 273–307 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.16859 - 3868.314/(T/K)$; temp range 277–307 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.24257 - 1566.029/(-105.47 + T/K)$; temp range 383–473 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.83697 - 1930.688/(-73.422 + T/K)$; temp range 308–393 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.2376 - 1563.08/(-105.776 + T/K)$; temp range 385–477 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19164 - 1533.535/(-108.781 + T/K)$; temp range 463–533 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.99685 - 2310.405/(-10.362 + T/K)$; temp range 523–635 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 16.1 (extrapolated-Antoine eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 93.42570 - 6409.054/(T/K) - 29.82622 \cdot \log (T/K) + 1.03314 \times 10^{-2} \cdot (T/K)$; temp range: 397–476 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 122.8998 - 7.6175 \times 10^3/(T/K) - 41.637 \cdot \log (T/K) + 1.5709 \times 10^{-2} \cdot (T/K) - 8.9199 \times 10^{-13} \cdot (T/K)^2$; temp range 308–705 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.0802; 0.0699; 1.0820 (exptl., calculated-group contribution; calculated-bond contribution Hine & Mookerjee 1975)

0.0223, 0.0973 (8, 25°C, calculated, Leuenberger et al. 1985)
 0.689 (calculated-P/C, Neely & Blau 1985)
 0.0397 (calculated-VLE vapor liquid equilibrium data, Yaws et al. 1991)
 0.0653 (calculated-P/C, Shiu et al. 1994)
 0.0783*, 0.297 (25, 40.2°C, calculated-activity coeff. γ^∞ data, Dohnal & Fenclová 1995)
 1.735, 3.144, 4.774 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.0801 (extrapolated-vapor liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{AW} = 9.328 - 5865/(T/K)$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 < 0.347 (gas stripping-GC, Altschuh et al. 1999)
 0.102 (calculated-group contribution, Lee et al. 2000)
 0.0582, 0.0989* (20, 25°C, dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.94 (shake flask-UV, Fujita et al. 1964)
 1.92, 1.94, 1.95 (quoted literature values, Leo et al. 1971; Hansch & Leo 1979, Hansch & Leo 1985)
 1.99 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
 1.94 (LC- k' correlation, Carlson et al. 1975)
 2.17 (shake flask, Korenman et al. 1980)
 1.97 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 1.92, 1.98 ± 0.07 (selected best lit. value, exptl.-ALPM, Garst & Wilson 1984)
 1.62 (HPLC- k' correlation, Haky & Young 1984)
 1.73 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
 1.91 (HPLC- k' correlation, Miyake et al. 1987)
 1.94 (RP-HPLC-capacity ratio, Minick et al. 1988)
 1.94 (recommended, Hansch et al. 1995)
 1.90; 2.06, 2.12, 1.94 (solid-phase microextraction; calculated- K_{OW} program, calculated-CLOGP, quoted exptl., Dean et al. 1996)
 1.53, 1.53, 1.69, 1.76 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.26 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

2.81 (Coyote Creek sediment, Smith et al. 1978)
 1.69 (Brookstone clayloam soil, Boyd 1982)
 -0.046 (predicted-S, Boyd 1982)
 1.76 (calculated- K_{OW} , Kollig 1993)
 2.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.15, 2.33 (soils: organic carbon $OC \geq 0.1\%$ and pH 2.0–7.4, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 167$ d, estimated from a lake as calculated from equations of Mackay & Wolkoff 1973 (Smith et al. 1978).

Photolysis:

$k = 6.8 \times 10^{-7} \text{ s}^{-1}$ under overcast weather of April at 25°C; $t_{1/2} \sim 4800$ h in river, $t_{1/2} > 10000$ h in both eutrophic lake and pond and $t_{1/2} = 2400$ h in oligotrophic lake, based on an average photolysis rate on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978; quoted, Howard 1989)
 photolytic $t_{1/2} = 5800$ h in aquatics (Haque et al. 1980).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 144\text{--}11325$ h in water, based on measured rate data for reactions with singlet oxygen and hydroxyl radical in aqueous solution (Anbar & Neta 1967; Scully & Hoigne 1987; quoted, Howard et al. 1991)

$k_{\text{NO}_3} = (13 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 ± 1 K (Japar & Niki 1975; Graham & Johnston 1978; quoted, Carter et al. 1981)

$k(\text{aq.}) = 20 \text{ M}^{-1} \text{ s}^{-1}$, averaged over 24-h day (Smith et al. 1978)

$k_{\text{OH}} = 38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 ± 1 K (Atkinson et al. 1979; quoted, Carter et al. 1981)

photooxidation $t_{1/2} = 10$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson et al. 1979; quoted, Howard 1989)

$k_{\text{NO}_3} = (15 \pm 2.4) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 300 ± 1 K in air (relative rate technique with reference to 2-methyl-2-butene, Carter et al. 1981; quoted, Atkinson 1991)

$k_{\text{O}_3} = (4.71 \pm 0.66) \times 10^{-19} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K; calculated tropospheric lifetimes of 25 d and 0.3 d due to reaction with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)

$k = (3.0 \pm 0.6) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.5/2.0 (Hoigné & Bader 1983b)

$k_{\text{OH}} = 4.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = 1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{OH}} = (16.6 \pm 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 1 K (relative technique with reference to *m*-cresol, Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{NO}_3} = (1.27 \pm 0.36) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K in air (Atkinson et al. 1984)

photooxidation $t_{1/2} = 1.5\text{--}15$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991)

$k_{\text{OH}}(\text{exptl}) = 44.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{obs.}) = 41 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 56.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{exptl}) = 42 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1985; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{\text{OH}}(\text{calc}) = 44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{exptl}) = 44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990)

$k = 1.1 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8.3, $2.4 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8.8, $1.6 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ at pH 10, $3.5 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ at pH 11.5 for the reaction with singlet oxygen in water at $(19 \pm 2)^\circ\text{C}$ (Scully & Hoigné 1987)

$k_{\text{NO}_3} = 21.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 4.7 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k = (9.6 \pm 2.8) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $(27 \pm 1)^\circ\text{C}$ (Tratnyek & Hoigné 1991)

$k_{\text{NO}_3} = (10.7 \pm 1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K, $k_{\text{OH}} = 47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1992)

$k_{\text{OH}}(\text{calc}) = 30.83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}} = 5.2 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{aq.}) = 1.2 \times 10^{-10} \text{ M}^{-1} \text{ s}^{-1}$, the calculated atmospheric lifetime $\tau = 0.23$ d under clear sky; $\tau = 0.18$ d under cloudy conditions at 298 K, reduced to 0.11 d due to the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis: no hydrolyzable functional groups (Smith et al. 1978).

Biodegradation: $t_{1/2} = 1\text{--}2$ d for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964)

Completely degraded by a soil microflora in one day (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate $k = 55.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2} = 12$ h in eutrophic lake for a point source continuously discharging $1.0 \mu\text{g/mL}$ predicted by one compartment model for all processes including dilution (Smith et al. 1978); laboratory determined $k = 5.2 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ at 25°C (Smith et al. 1978)

$k(\text{calc}) = 1.7 \text{ d}^{-1}$ in river water, $k = 0.8\text{--}4.7 \text{ d}^{-1}$ in estuary water and $k = 2.8\text{--}4.8 \text{ d}^{-1}$ in marine water after a lag period (Vashon & Schwab 1982; quoted, Battersby 1990);

$t_{1/2}(\text{aq. aerobic}) = 1\text{--}16$ h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; selected, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 240\text{--}672$ h, based on anaerobic screening test data (Boyd et al. 1983; Horowitz et al. 1982; selected, Howard et al. 1991);

$k = 1.72 \times 10^{-17}$ mol cell⁻¹ h⁻¹ in pure culture system (Banerjee et al. 1984).

Biotransformation: estimated $t_{1/2} = 12$ h in river, eutrophic lake and pond and $t_{1/2} > 10000$ h in oligotrophic lake, based on an average photolysis rate on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 10$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson et al. 1979; quoted, Howard 1989);

photooxidation $t_{1/2} = 1.5\text{--}15$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

calculated atmospheric lifetime $\tau = 0.23$ d under clear sky and $\tau = 0.18$ d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to $\tau = 0.11$ d due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: $t_{1/2} = 0.55$ h in river, $t_{1/2} = 12$ h in pond and eutrophic lake, and $t_{1/2} = 2400$ h in oligotrophic lake for a point source continuously discharging 1.0 µg/mL predicted by one compartment model for all processes including dilution (Smith et al. 1978; quoted, Howard 1989);

rate constant $k = (3.0 \pm 0.6) \times 10^4$ M⁻¹·s⁻¹ for the reaction with ozone at pH 1.5/2.0 in water (Hoigné & Bader 1983b);

$t_{1/2} = 1\text{--}16$ h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{1/2} = 500$ h for the reaction with singlet oxygen in water at pH 8 and $(19 \pm 2)^\circ\text{C}$ (Scully & Hoigné 1987).

Ground water: estimated half-life for cresols, $t_{1/2} = 0.01$ yr at Noordwijk (Zoeteman et al. 1981); $t_{1/2} = 2\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:

$t_{1/2} = 1\text{--}16$ h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{1/2} = 0.5$ d in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 1.0$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.1.4.1
Reported aqueous solubilities of *p*-cresol at various temperatures

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Dohnal & Fenclová 1995	
shake flask-synthetic method		shake flask-optical method		vapor-liquid equil.-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
40.2	22400	0	10000	25	21500
52.6	24900	20	17000	40.2	22840
63.5	28000	40	23000	75.9	43534
73.5	31900	60	30000	88.7	50064
84.0	37200	80	37000	98.5	54615
88.8	40600	100	48000	100	56146
94.0	44700	110	56000		
124.5	74200	120	72000		
139.4	151000	130	101000		
141.2	200700	140	177000		
143.5	301300	142	226000		
143.4	400800	143	264000		
141.5	506300	143.5	340000		
134.8	606100	148	380000		
111.6	719100				
77.9	704000				
37.4	836100				
27.5	844800				
17.2	852800				
8.7	868600				
9.2	879000				
10.8	900900				
17.1	946800				
20.3	960100				
24.0	922700				
27.5	983200				
29.9	990600				
33.8	1000000				
critical solution temp 143.5°C					
triple point 8.7°C					

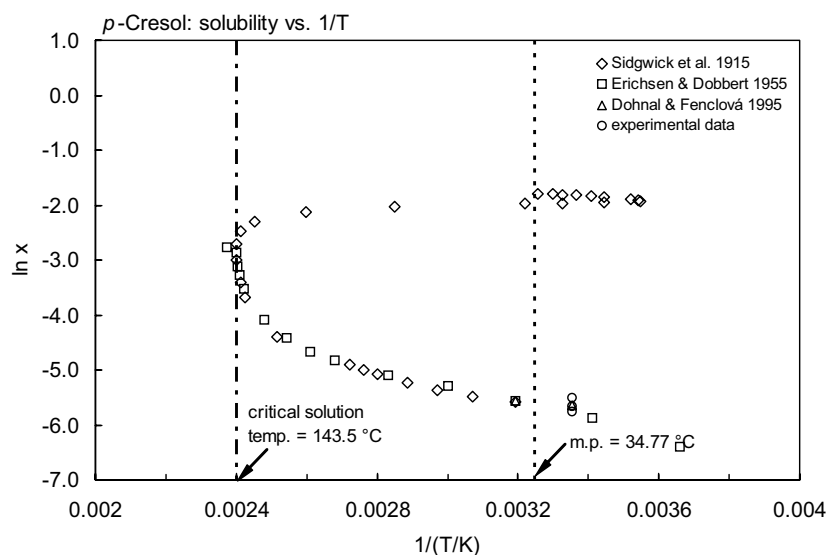


FIGURE 14.1.1.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *p*-cresol.

TABLE 14.1.1.4.2

Reported vapor pressures of *p*-cresol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1)$$

$$\ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2)$$

$$\ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log(T/K) \quad (4)$$

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
53.0	133.3	145.7	17599	128.65	7605	0	1.493	124.151	7518
76.5	666.6	163.6	32664	131.26	10114	4.75	1.640	138.025	13204
88.6	1333	171.6	42263	143.86	16500	8.60	2.653	145.593	17517
102.3	2666	179.2	53329	171.27	42066	10.8	4.066	155.395	24845
117.7	5333	187.2	67194	187.17	67661	13.9	4.880	162.723	31824
127.0	7999	193.7	80660	201.88	101325	16.8	7.199	168.937	38934
140.0	13332	200.8	98392			20.0	9.013	173.819	45366
157.7	26664	153.0	22931			22.0	12.08	178.598	52497
179.4	53329	183.8	61062	bp/°C	201.88	23.35	13.00	183.663	60995
201.8	101325	190.8	74261			28.85	21.86	186.521	66259
		197.1	88526			29.75	25.60	190.578	74355
mp/°C	35.5	200.8	98392			32.55	31.60	192.90	79336
						34.15	38.53	193.029	79631
		eq. 1	P/mmHg					197.102	89029
		A	8.308					198.609	92732
		B	2520			bp/°C	201.94	199.666	95395
								200.226	96828
						for temp range:		200.535	97964
						0–34°C		201.122	99164
						eq. 2	P/mmHg	201.719	100728
						A	12.0298	202.269	102205

TABLE 14.1.1.4.2 (Continued)

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						B	3861.98	202.985	104133
						C	273		
						$\Delta H_v/(kJ\ mol^{-1})$		for temp range:	
						at bp	49.534	110–200°C	
						at 25°C	73.931	eq. 2	P/mmHg
								A	7.11767
								B	1566.029
								C	167.680

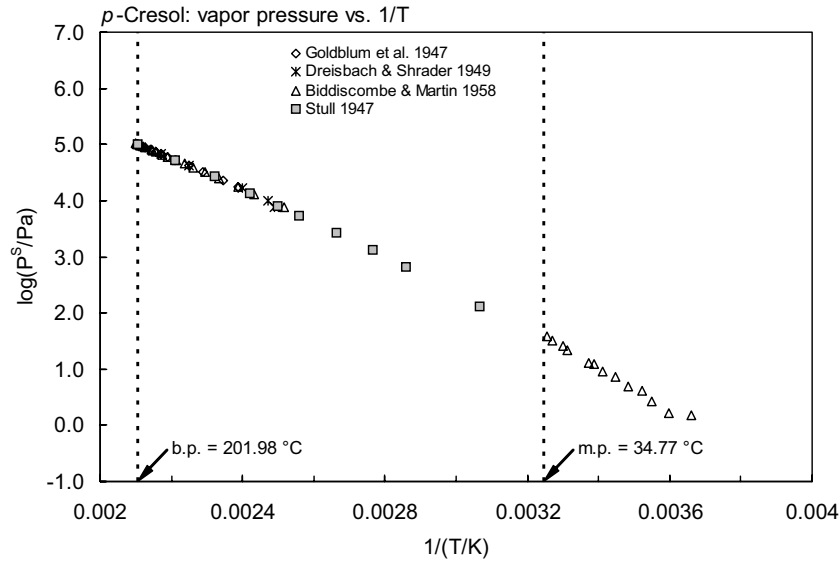


FIGURE 14.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for *p*-cresol.

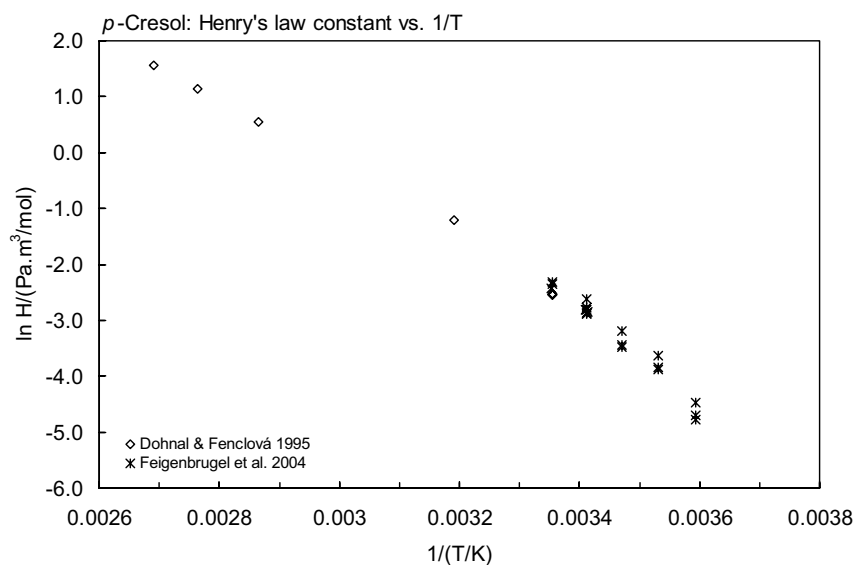
TABLE 14.1.1.4.3
Reported Henry’s law constants of *m*-cresol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/atm) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
Dohnal & Fenclová 1995		Feigenbrugel et al. 2004			
vapor-liquid equilibrium		gas stripping-GC/MS			
t/°C	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)		
25.0	0.0783*	278.25	0.00914		
40.2	0.297*	278.25	0.01148		
75.9	1.735	278.35	0.00846		

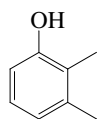
(Continued)

TABLE 14.1.1.4.3 (Continued)

Dohnal & Fenclová 1995		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-GC/MS	
t/°C	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)
88.7	3.144	283.15	0.0262
98.5	4.774	283.15	0.0215
25.0	0.0801#	283.25	0.0207
25.0	0.0792\$	288.10	0.0323
		288.15	0.0414
#calculated from eq. 1		288.20	0.0307
\$calculated from eq. 3		293.10	0.0557
*data from literature		293.15	0.0724
		293.15	0.0627
eq. 1	K _{AW}	293.15	0.0606
A	9.328	293.15	0.0563
B	5865	293.25	0.0602
		298.15	0.0943
enthalpy of hydration:		298.25	0.0875
$\Delta H_K/(\text{kJ mol}^{-1}) = 48.8 \pm 0.6$		293	0.0582
OR		298	0.0989
eq. 3	k _H /kPa		
A	22.071		
B	6138		
$\Delta H_K/(\text{kJ mol}^{-1}) = 51.0 \pm 0.6$			

FIGURE 14.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for *p*-cresol.

14.1.1.5 2,3-Dimethylphenol



Common Name: 2,3-Dimethylphenol

Synonym: 2,3-xylenol, 1-hydroxy-2,3-dimethylbenzene

Chemical Name: 2,3-dimethylphenol

CAS Registry No: 526-75-0

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

72.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

216.9 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.54 (Dohnal & Fenclová 1995)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.08, 47.32 ($25^{\circ}C$, normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F : 0.342 (mp at $72.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

40000* ($150^{\circ}C$, shake flask-optical method, measured range 150 – $208.8^{\circ}C$, Erichsen & Dobbert 1955)

3930 ($20^{\circ}C$, shake flask or batch contacting technique-UV, Dohnal & Fenclová 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

133.3* ($56^{\circ}C$, summary of literature data, temp range 56 – $219.0^{\circ}C$, Stull 1947)

1333* ($84.0^{\circ}C$, ebulliometry, measured range 84.0 – $219.0^{\circ}C$, Vonterres et al. 1955)

3.64* ($24.71^{\circ}C$, ebulliometry/gas saturation, measured range 10 – $45^{\circ}C$, Andon et al. 1960)

$\log(P/mmHg) = 13.1606 - 4389.99/(t/^{\circ}C + 273)$; temp range 10 – $50^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/mmHg) = 7.04268 - 1069.164/(t/^{\circ}C + 169.744)$; temp range 149 – $219^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/kPa) = 6.13887 - 1588.200/(167.385 + t/^{\circ}C)$; temp range 149 – $218^{\circ}C$ (Antoine eq. derived from experimental data of Andon et al. 1960, Boublik et al. 1984)

$\log(P/kPa) = 6.01592 - 1644.433/(192.286 + t/^{\circ}C)$, temp range 84 – $219^{\circ}C$ (Antoine eq. derived from experimental data of Vonterres et al. 1955, Boublik et al. 1984)

$\log(P_s/kPa) = 12.29616 - 4394.694/(T/K)$; temp range 282 – $323 K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.17998 - 1619.086/(-102.197 + T/K)$; temp range 433 – $492 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 82.92733 - 6.0367 \times 10^3/(T/K) - 26.948 \cdot \log(T/K) + 9.739 \times 10^{-3} \cdot (T/K) + 2.5196 \times 10^{-12} \cdot (T/K)^2$; temp range 346 – $723 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0631, 0.0952 (20 , $25^{\circ}C$, calculated-limiting activity coefficient γ^{∞} data, Dohnal & Fenclová 1995)

2.96, 5.656, 8.652 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

$\ln K_{AW} = 11.858 - 6567/(T/K)$; temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.48 (HPLC-RT correlation, Makovskaya et al. 1995b)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Half-Lives in the Environment:

TABLE 14.1.1.5.1

Reported aqueous solubilities of 2,3-dimethylphenol at various temperatures

Erichsen & Dobbert 1955

shake flask-optical method

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
150	40000
160	48000
170	58000
180	70000
190	94000
200	140000
202	156000
204	175000
206	200000
208	252000
208.8	365000

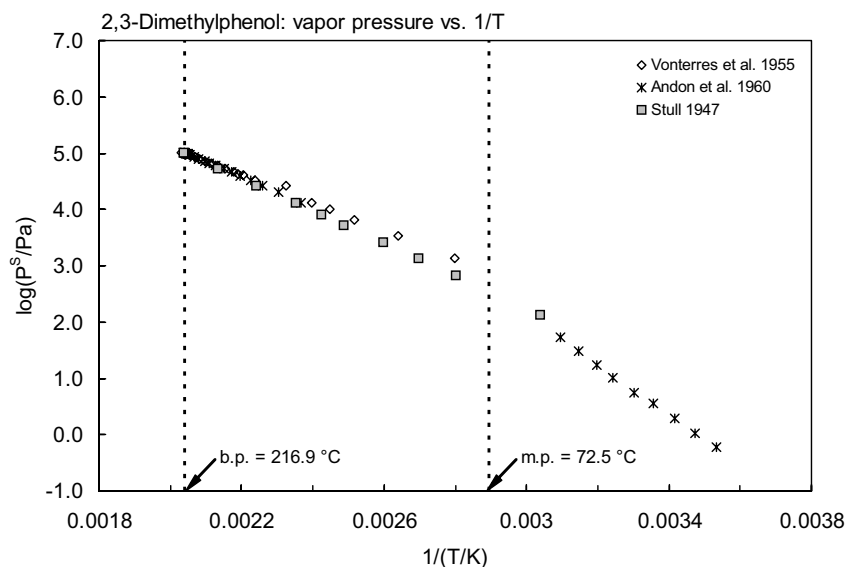


FIGURE 14.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylphenol.

TABLE 14.1.1.5.2

Reported vapor pressures of 2,3-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1)$$

$$\ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2)$$

$$\ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

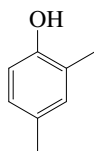
Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
56.0	133	84.0	1333	9.91	0.609	149.346	13304
83.8	666.6	105.6	3333	14.70	1.072	160.94	20045
97.6	1333	124.0	6666	19.70	1.933	169.634	26704
112.0	2666	135.2	9999	24.71	3.640	176.314	32963
129.2	5333	144.0	13332	29.58	5.650	182.500	39779
139.5	7999	157.0	26664	35.19	10.13	187.374	45920
152.2	13332	174.0	33330	39.54	17.33	192.094	53573
173.0	26664	180.2	39997	44.81	29.86	196.778	59919
196.0	53329	183.6	43330	49.88	52.93	200.752	66779
218.0	101325	186.1	46663			204.000	72842
		191.0	53329	mp/°C	72.57	207.54	79951
mp/°C	75.0	196.0	59995	bp/°C	216.87	210.672	86542
		200.0	66661			213.454	93026
		203.9	73327	for temp range:		214.137	94644
		207.0	79993	9–50°C		214.788	96151
		210.1	86659	eq. 2	P/mmHg	215.091	96929
		213.5	93325	A	13.1606	215.646	98283
		219.0	101325	B	4389.06	216.144	99513
				C	273	216.987	101613
						217.323	102400

(Continued)

TABLE 14.1.1.5.2 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				$\Delta H_v/(\text{kJ mol}^{-1})$		217.928	104010
				at 25°C	84.015		
				at bp	47.32	for temp range:	
						149–218°C	
						eq. 2	P/mmHg
						A	7.04268
						B	1609.184
						C	169.774

14.1.1.6 2,4-Dimethylphenol



Common Name: 2,4-Dimethylphenol

Synonym: 2,4-xylenol, *as-m*-xylenol, 1-hydroxy-2,4-dimethylbenzene

Chemical Name: 2,4-dimethylphenol

CAS Registry No: 105-67-9

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

24.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

210.98 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0202 (Andon et al. 1960)

0.9650 (Weast 1982–83)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

10.60 (Herington & Kynaston 1957; quoted, Callahan et al. 1979)

10.58 (Dean 1985)

10.63 (Riddick et al. 1986; Howard 1989)

10.10 (Kollig 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

47.15 (at normal boiling point, Andon et al. 1960)

65.86 (at $25^{\circ}C$, Andon et al. 1960; Dean 1992)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

8795 (shake flask-UV at pH 5.1, Blackman et al. 1955)

6200 (shake flask-UV at pH 6.5, Blackman et al. 1955)

6200* (synthetic method/shake flask-optical, extrapolated value, measured range 160 – $213.5^{\circ}C$, Ericksen & Dobbert 1955)

7868 (shake flask-LSC, Banerjee et al. 1980)

7888 (shake flask-radioactive analysis, Veith et al. 1980)

7819 (generator column-HPLC, Wasik et al. 1981)

4200 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

7929 (calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)

8200 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($51.8^{\circ}C$, summary of literature data, temp range 51.8 – $211.0^{\circ}C$, Stull 1947)

21.78 (calculated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.37688 - 1838.9/(1999.0 + t/^{\circ}C)$; temp range 115 – $245^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

- 1333* (89.50 °C, ebulliometry, measured range 89.50–211.0 °C, Vonterres et al. 1955)
 12.81* (24.87°C, ebulliometric and gas-saturation methods, measured range 9–45°C Andon et al. 1960)
 13.02 (interpolated-Antoine eq. derived from exptl. results, Andon et al. 1960)
 $\log (P/\text{mmHg}) = 10.5277 - 3439.99/(t/^{\circ}\text{C} + 273)$; temp range 9–45°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
 $\log (P/\text{mmHg}) = 7.04694 - 1581.391/(t/^{\circ}\text{C} + 168.652)$; temp range 114–212°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
 $\log (P/\text{mmHg}) = [-0.2185 \times 13130.2/(T/K)] + 8.867260$; temp range 51.8–211.5°C (Antoine eq., Weast 1972–73)
 10.28 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.05539 - 1587.459/(169.339 + t/^{\circ}\text{C})$; temp range 144.4–212.3°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)
 13.17 (calculated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 483.876/(T/K)] \times 10^{\{0.999891 - 8.94506 \times 10^{-4} \cdot (T/K) + 6.96026 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 298.02–707.95 K, (Cox eq., Chao et al. 1983)
 10.29, 20.22 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.18152 - 1588.34/(169.437 + t/^{\circ}\text{C})$, temp range 144.4–212.3°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 7.02271 - 2183.475/(225.488 + t/^{\circ}\text{C})$; temp range 89.5–211°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
 10.28 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.05539 - 1587.46/(169.34 + t/^{\circ}\text{C})$; temp range 144–212°C (Antoine eq., Dean 1985, 1992)
 12.87 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 9.65613 - 3442.574/(T/K)$; temp range 282–318 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.1672 - 1578.685/(-104.772 + T/K)$; temp range 429–486 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 12.96 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 86.11491 - 6138.775/(T/K) - 27.12977 \cdot \log (T/K) + 0.91169 \times 10^{-2} \cdot (T/K)$; temp range 418–485 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1960, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 53.3866 - 5.1516 \times 10^3/(T/K) - 15.095 \cdot \log (T/K) - 1.3196 \times 10^{-9} \cdot (T/K) + 2.8455 \times 10^{-6} \cdot (T/K)^2$; temp range 346–708 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1.722 (calculate-P/C, Mabey et al. 1982)
 500 (EPICS-GC, Ashworth et al. 1988)
 500* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm m}^3/\text{mol})] = -16.34 - 3307/(T/K)$, temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 0.0638 (8°C, Leuenberger et al. 1985)
 0.203, 0.0692 (calculated-P/C, estimated-bond contribution, Meylan & Howard 1991)
 0.1815 (calculated-P/C, Shiu et al. 1994)
 0.199* (calculated-limiting activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)
 4.338, 7.491, 11.46 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.202* (extrapolated-vapor liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{AW} = 10.077 - 5811/(T/K)$; temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 0.154 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)
 643 (20°C, selected from literature experimentally measured data - poor correlation coefficient, Staudinger & Roberts 2001)
 $\log K_{AW} = -5.192 + 1563/(T/K)$; poor correlation coefficient (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.30 (20°C, shake flask-UV, Korenman 1973)
 2.42 (23 ± 1.5°C, shake flask-LSC, Banerjee et al. 1980; Veith et al. 1980)

- 2.30 (shake flask, Korenman et al. 1980)
- 1.99, 2.54 (RP-HPLC-RT correlation, quoted calculated value, Veith et al. 1980)
- 2.54 (35°C, shake flask-UV, Rogers & Wong 1980)
- 2.34 (generator column-HPLC, Wasik et al. 1981)
- 2.37 (calculated-activity coeff. γ from UNIFAC not considering mutual solubility of octanol and water, Arbuckle 1983)
- 2.95 (calculated-activity coeff. γ from UNIFAC by considering mutual solubility of octanol and water, Arbuckle 1983)
- 2.14 (HPLC- k' correlation, Haky & Young 1984)
- 1.83 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
- 2.35 (recommended, Sangster 1989, 1993)
- 2.48 (calculated-UNIFAC activity coeff., Dallos et al. 1993)
- 2.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 1.18 (bluegill sunfish, Barrows et al. 1980)
- 2.18 (bluegill sunfish, Veith et al. 1980)
- 1.86 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.88 (calculated-MCI χ , Sabljic 1987a)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.98 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
- 2.63 (soil, calculated- K_{OW} , Lyman et al. 1982)
- 2.19 (activated carbon, Blum et al. 1994)
- 1.76 (calculated- K_{OW} , Kollig 1993)
- 2.62, 2.77 (average values for sediments, soils, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k < 4 \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, $1.1 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)
 photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$ in water, based on reported reaction rate constants for RO_2 radicals with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 8.0 \text{ h}$ in air, based on reaction with photochemically produced hydroxyl radical in air (GEMS 1986; selected, Howard 1989)

$k_{OH} = 71.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson 1989)

photooxidation $t_{1/2} = 1.19\text{--}11.9 \text{ h}$, based on estimated rate constant for the reaction with OH radical in air (Howard et al. 1991)

$k_{OH}(\text{calc}) = 51.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{OH}(\text{calc}) = 5.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 1.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation: average rate of biodegradation $28.2 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982); first-order rate constant $k = 1.0 \text{ d}^{-1}$ corresponding to $t_{1/2} = 0.7 \text{ d}$ in adapted activated sludge under aerobic conditions (Mills et al. 1982);

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168 \text{ h}$, based on aqueous aerobic screening test data (Petrasek et al. 1983; Chambers et al. 1963; selected, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 96\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

average $k(\text{exptl.}) = 0.0578 \text{ h}^{-1}$ compared to group contribution method predicted $k = 0.0758 \text{ h}^{-1}$ (nonlinear) and $k = 0.0646 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993).

Biotransformation: rate constant for bacterial transformation of 1×10^7 mL cell⁻¹ h⁻¹ in water (Mabey et al. 1982).
 Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 8.0$ h, based on reaction with photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989); photooxidation $t_{1/2} = 1.19$ – 11.9 h, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 77$ – 3840 h in water, based on reported reaction rate constants for RO₂ radical with the phenol class (Mill & Mabey 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 48$ – 336 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
 Sediment:

Soil: $t_{1/2} = 24$ – 168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 14.1.1.6.1

Reported aqueous solubilities and Henry's law constants of 2,4-dimethylphenol at various temperatures

Aqueous solubility		Henry's law constant			
Erichsen & Dobbert 1955		Ashworth et al. 1988		Dohnal & Fenclová 1995	
shake flask-optical method		EPICS-GC		vapor-liquid equilibrium	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
160	17000	10	840	75.9	4.338
170	33000	15	683	88.7	7.491
180	54000	20	1023	98.5	11.46
190	77000	25	500		
200	114000	30	380		
210	188000				
212	234000	log H = A – B/(T/K)			
213	279000		H/(atm m ³ /mol)		
213.5	335000	A	–16.34		
25	6200	B	–3307		
	extrapolated				

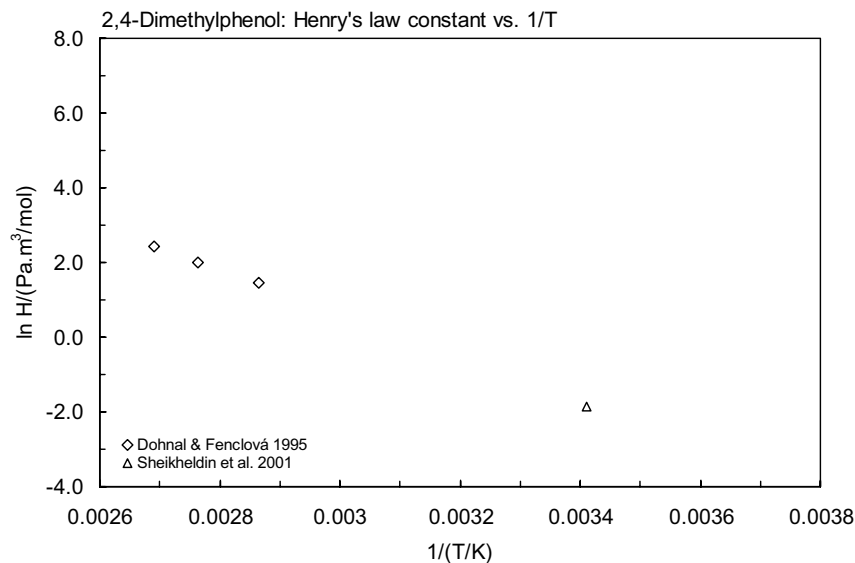


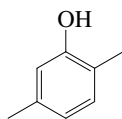
FIGURE 14.1.1.6.1 Logarithm of Henry’s law constant versus reciprocal temperature for 2,4-dimethylphenol.

TABLE 14.1.1.6.2
Reported vapor pressures of 2,4-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)					
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.8	133.3	89.50	1333	9.73	3.040	144.382	13195
78.0	666.6	109.9	3333	14.94	5.066	156.053	20024
91.3	1333	127.0	6666	20.13	8.279	164.129	26289
105	2666	137.4	9999	24.87	12.81	171.241	33051
131.5	5333	144.5	13332	29.91	20.13	176.700	39155
131	7999	156.0	19998	35.16	30.797	182.116	46078
143	13332	165.1	26664	39.41	43.73	186.169	52557
161.5	26664	171.2	33330	44.86	67.06	191.348	60131
184.5	53329	177.3	39997			194.795	66188
211.5	101325	180.0	46663	mp/°C	24.54	198.444	73115
		186.7	53329	bp/°C	210.931	201.747	79877
mp/°C	25.5	190.8	59995			204.809	86584
		194.4	66661	for temp range:		207.513	92867
		198.0	73327	9–45°C		208.299	94764
		201.0	79993	eq. 2	P/mmHg	208.898	97557
		204.0	86659	A	10.5277	209.314	97251
		206.6	93325	B	3499.99	209.847	98580
		211.0	101325	C	273	210.45	100102
						210.951	101381

(Continued)

14.1.1.7 2,5-Dimethylphenol



Common Name: 2,5-Dimethylphenol

Synonym: 2,5-xylenol, 1-hydroxy-2,5-dimethylbenzene

Chemical Name: 2,5-dimethyl phenol

CAS Registry No: 95-87-4

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

74.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

211.1 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.41 (Dohnal & Fenclová 1995)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.98, 46.94 ($25^{\circ}C$, normal bp, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.325 (mp at $74.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

3126 (shake flask-UV, pH 5.1, Blackman et al. 1955)

3122 ($20^{\circ}C$, shake flask-UV, Dohnal & Fenclová 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($51.8^{\circ}C$, summary of literature data, temp range 51.8 – $211.5^{\circ}C$, Stull 1947)

1333* ($89.40^{\circ}C$, ebulliometry, measured range 89.40 – $211.2^{\circ}C$, Vonterres et al. 1955)

1.213* ($24.82^{\circ}C$, ebulliometry/gas saturation, measured range 9.5 – $45^{\circ}C$, Andon et al. 1960)

$\log(P/mmHg) = 13.3705 - 4438.56/(t/^{\circ}C + 273)$; temp range 9 – $50^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/mmHg) = 7.03684 - 1581.906/(t/^{\circ}C + 169.497)$; temp range 143 – $212^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/kPa) = 6.1332 - 1560.465/(176.024 + t/^{\circ}C)$, temp range 144 – $211.2^{\circ}C$ (Antoine eq. derived from exptl data of Andon et al. 1960, Boublik et al. 1984)

$\log(P/kPa) = 6.04303 - 1383.881/(157.333 + t/^{\circ}C)$; temp range 89.4 – $211.2^{\circ}C$ (Antoine eq. derived from exptl data of Vonterres et al. 1955, Boublik et al. 1984)

$\log(P_s/kPa) = 12.51064 - 3950.681/(T/K)$, temp range 282 – $323 K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.17702 - 1593.804/(-102.241 + T/K)$; temp range 427 – $485 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 47.5888 - 4.8102 \times 10^3/(T/K) - 13.186 \cdot \log(T/K) - 1.0208 \times 10^{-9} \cdot (T/K) + 2.7045 \times 10^{-12} \cdot (T/K)^2$; temp range 348 – $707 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0873, 0.133 (20, 25°C, calculated-limiting activity coefficient γ^∞ data, Dohnal & Fenclová 1995)

4.353, 7.476, 11.20 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

$\ln K_{AW} = 12.004 - 6511/(T/K)$; temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.34 (shake flask, Korenman 1973)

2.33 (shake flask, Korenman et al. 1980)

2.35 (generator column-HPLC, Wasik et al. 1981)

2.34 (recommended, Sangster 1993)

2.48 (HPLC-RT correlation, Makovskaya et al. 1995b)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.1.7.1

Reported vapor pressures of 2,5-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)					
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Vonderres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.8	133.3	89.40	1333	9.42	0.60	143.024	12990
78.0	666.6	109.8	3333	15.01	1.215	154.805	19234
91.3	1333	126.8	6666	19.9	2.186	164.433	26584
105	2666	137.2	9999	24.82	3.946	171.549	33375
121.5	5333	144.5	13333	29.83	6.849	176.902	39361
131	7999	156.0	19998	35.33	12.59	182.455	46460
143	13332	164.8	26666	39.41	19.47	187.328	53509
161.5	26664	171.5	33330	44.79	34.53	191.46	60142
184.2	53329	177.4	39997	49.75	52.80	194.984	66312
211.5	101325	180.2	43330			198.93	73602
		182.5	46663			210.834	79735
mp/°C	74.5	186.6	53329	mp/°C	74.85	204.603	85737
		189.5	59995	bp/°C	211.132	207.748	92988
		194.2	66661			208.661	95182
		198.0	73327	for temp range:		209.138	96349
		201.0	79993	9–50°C		209.556	97373

(Continued)

TABLE 14.1.1.7.1 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		204.6	86659	eq. 2	P/mmHg	210.117	98764
		206.8	93325	A	13.3705	210.771	100257
		211.2	101325	B	4438.56	211.232	101580
				C	273	211.736	102870
				ΔH_v /(kJ mol ⁻¹)		for temp range:	
				at 25°C	84.98	143–212°C	
				at bp	46.94	eq. 2	P/mmHg
						A	7.03684
						B	1581.906
						C	169.497

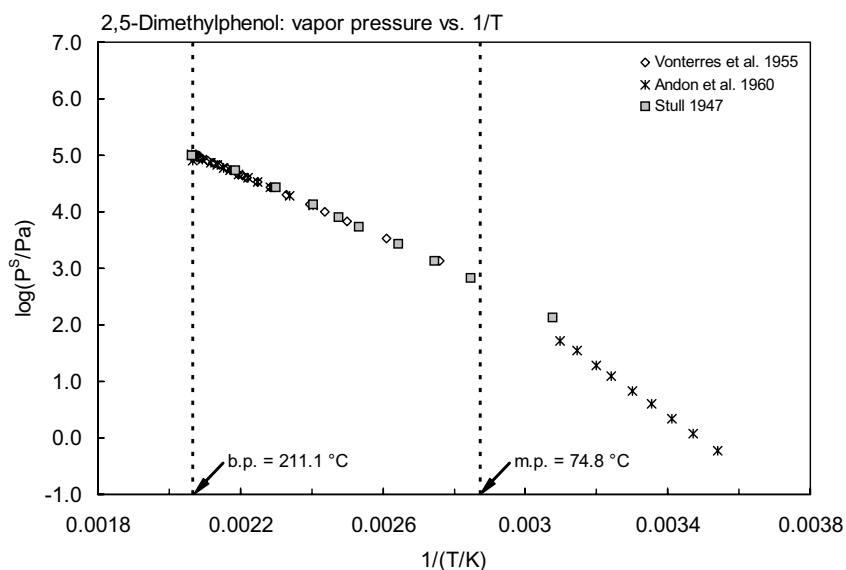
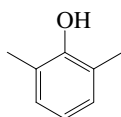


FIGURE 14.1.1.7.1 Logarithm of vapor pressure versus reciprocal temperature for 2,5-dimethylphenol.

14.1.1.8 2,6-Dimethylphenol



Common Name: 2,6-Dimethylphenol

Synonym: 2,6-xylenol, *vic-m*-xylenol

Chemical Name: 2,6-dimethylphenol

CAS Registry No: 576-26-1

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

45.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

201.07 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1320 ($25^{\circ}C$, Andon et al. 1960)

Molar Volume (cm^3/mol):

107.9 ($25^{\circ}C$, calculated-density)

147.8 calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

10.60 (McLeese et al. 1979; Dean 1985; Varhaníčková et al. 1995)

10.63 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

60.41, 46.97 ($25^{\circ}C$, bp, Dreisbach 1955)

44.52 (at normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

75.6 (at $25^{\circ}C$, Andon et al. 1960; Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.9; 16.3 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$.), F: 0.625 (mp at $45.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6230 (shake flask-UV at pH 5.1, Blackman et al. 1955)

13000* ($130^{\circ}C$, shake flask-optical method, measured range 130 – $241.2^{\circ}C$, Erichsen & Dobbett 1955)

9650 (generator column-HPLC, Wasik et al. 1981)

2900, 5900 (8 , $25^{\circ}C$, Leuenberger et al. 1985)

9560 ($20^{\circ}C$, shake flask-UV, Dohnal & Fenclová 1995)

6150 (shake flask-HPLC/UV at pH 6.3, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19.086 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.40318 - 1858.7/(199.0 + t/^{\circ}C)$; temp range 115 – $250^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* ($92.5^{\circ}C$, ebulliometry, measured range 92.5 – $212.0^{\circ}C$, Vonterres et al. 1955)

23.3* ($24.67^{\circ}C$, ebulliometric and gas-saturation methods, measured range 4.75 – $40^{\circ}C$, Andon et al. 1960)

24.31 (calculated-Antoine eq. from ebulliometry/gas saturation measurements, Andon et al. 1960)

$\log(P/mmHg) = 12.5036 - 3948.27/(t/^{\circ}C + 273)$; temp range 4 – $40^{\circ}C$ (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/mmHg) = 7.05753 - 1618.528/(t/^{\circ}C + 186.482)$; temp range 144 – $203^{\circ}C$ (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)

- 34.41 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.0707 - 1628.323/(187.603 + t/^{\circ}\text{C})$, temp range 144.8–203.5°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)
- 33.68 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 474.112/(T/K)] \times 10^{\{0.99333 - 9.96552 \times 10^{-4} \cdot (T/K) + 8.34247 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 321.81–701.65 K (Cox eq., Chao et al. 1983)
- 34.41, 10.37 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.19572 - 1628.413/(187.613 + t/^{\circ}\text{C})$, temp range 144.8–203.5°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.57979 - 1831.266/(188.83 + t/^{\circ}\text{C})$, temp range 97.5–212°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 34.4 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.00707 - 1628.32/(187.60 + t/^{\circ}\text{C})$; temp range 145–204°C (Antoine eq., Dean 1985, 1992)
- 19.09 (selected, Riddick et al. 1986)
- 24.0 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.6308 - 3950.681/(T/K)$; temp range 277–313 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19544 - 1629.621/(-85.358 + T/K)$; temp range 417–476 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
- 43.8 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 39.83138 - 4062.725/(T/K) - 10.16994 \cdot \log (T/K) + 0.20170 \times 10^{-2} \cdot (T/K)$; temp range: 418–477 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1960, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 87.1964 - 5.8721 \times 10^3/(T/K) - 28.853 \cdot \log (T/K) + 1.113 \times 10^{-2} \cdot (T/K) + 2.2316 \times 10^{-12} \cdot (T/K)^2$; temp range 319–701 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 0.684 (modified gas-stripping, Hawthorne et al. 1985)
 0.193 (8°C, Leuenberger et al. 1985)
 0.377 (calculated-P/C, Shiu et al. 1994)
 0.302 (calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)
 10.3, 17.81, 25.2 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.441 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{AW} = 11.176 - 5906/(T/K)$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 0.098 (calculated-group contribution, Lee et al. 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated:

- 2.36 (Leo et al. 1971; Hansch & Leo 1979)
 2.34 (LC- k' correlation; Carlson et al. 1975)
 2.40 (35°C, shake flask-UV, Rogers & Wong 1980)
 2.31 (generator column-HPLC, Wasik et al. 1981)
 2.07 (HPLC- k' correlation, Haky & Young 1984)
 2.51 (HPLC-RT correlation, Eadsforth 1986)
 2.36 (recommended, Sangster 1989, 1993)
 2.36 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 65.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 54.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated from Atmospheric Oxidation Program, $k_{OH}(\text{exptl}) = 65.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{OH}(\text{calc}) = 30.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated from Fate of Atmospheric Pollutants Program (Meylan & Howard 1993)

$k_{OH}(\text{calc}) = 49.48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital estimation method, Klamt 1993)

Hydrolysis:

Biodegradation: $t_{1/2} = 7\text{--}10 \text{ d}$ for bacteria to utilize 95% of 200 ppm in parent substrate (Tabak et al. 1964); average rate of biodegradation $9.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 14.1.1.8.1

Reported aqueous solubilities and vapor pressures of 2,6-dimethylphenol at various temperatures

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log (P/mmHg) = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log (P/Pa) = A – B/(C + T/K)		(3)					
log (P/mmHg) = A – B/(T/K) – C·log (T/K)		(4)					
Aqueous solubility		Vapor pressure					
Erichsen & Dobbert 1955		Vonterres et al. 1955		Andon et al. 1960			
shake flask-optical method		ebulliometry		gas saturation		ebulliometry	
t/°C	S/g·m ^{–3}	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
130	13000	92.5	1333	4.75	2.60	144.798	19813
140	16000	112.5	3333	9.46	4.48	153.385	26322
150	21000	129.0	6666	14.98	8.319	160.524	33079
160	27000	139.4	9999	19.78	13.87	166.759	39853
170	36000	147.1	13332	24.67	23.33	171.831	46274
180	47000	158.4	19998	30.2	39.86	176.276	52564
190	58000	167.0	26664	34.98	64.93	180.369	59847
200	71000	173.2	33330	39.66	100.3	184.792	66529
210	90000	179.1	39997			188.694	73851
220	120000	181.5	43330	mp/°C	74.85	191.754	80043
230	176000	188.0	53329	bp/°C	201.03	194.81	86616
232	191000	190.2	59995			196.676	90843
234	209000	196.3	66661	for temp range:		198.414	94918
236	229000	200.0	73327	4–40°C		198.937	96176
238	255000	202.5	79993	eq. 2	P/mmHg	199.432	97373
240	297000	205.6	86659	A	12.5036	199.983	98721
241.2	440000	208.0	93325	B	3948.27	200.45	99881
		212.0	101325	C	273	201.059	101400
						201.616	120808
					ΔH _v /(kJ mol ^{–1})	202.519	105117
				at 25°C	75.60	203.525	107738
				at bp	44.52		

TABLE 14.1.1.8.1 (Continued)

Aqueous solubility		Vapor pressure					
Erichsen & Dobbert 1955		Vonterres et al. 1955		Andon et al. 1960			
shake flask-optical method		ebulliometry		gas saturation		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
for temp range: 144–203°C							
eq. 2						P/mmHg	
A						7.05753	
B						1618.528	
C						186.492	

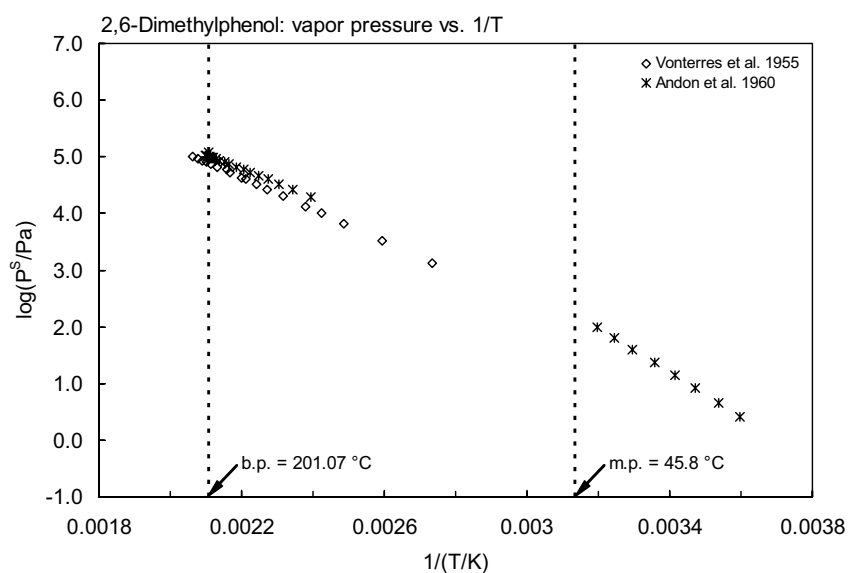
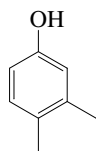


FIGURE 14.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dimethylphenol.

14.1.1.9 3,4-Dimethylphenol



Common Name: 3,4-Dimethylphenol

Synonym: 3,4-xylenol, *as-o*-xylenol

Chemical Name: 3,4-dimethylphenol

CAS Registry No: 95-65-8

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

65.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

227 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1380 ($25^{\circ}C$, Andon et al. 1960)

0.9830 (Weast 1982–83)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

10.40 (McLeese et al. 1979)

10.32 (Dean 1985)

10.36 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.67 (at normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

85.73 (at $25^{\circ}C$, Andon et al. 1960; Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.13; 17.0 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.404 (mp at $65.1^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5100 (shake flask-UV, Blackman et al. 1955)

5100* (synthetic method/shake flask-optical, extrapolated value, measured range 130 – $190.2^{\circ}C$, Ericksen & Dobbert 1955)

5000 (shake flask-spectrophotometry, Roberts et al. 1977)

12810 ($20^{\circ}C$, shake flask-UV, Dohnal & Fenclová 1995)

7250 (shake flask-HPLC/UV at pH 6.25, Varhaničková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($66.2^{\circ}C$, summary of literature data, temp range 66.2 – $225.2^{\circ}C$, Stull 1946)

5.160 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.70494 - 2030.9/(196.0 + t/^{\circ}C)$; temp range 130 – $265^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

- 1333* (105.7 °C, ebulliometry, measured range 105.7–226.0°C, Vonterres et al. 1955)
- 1.84* (24.88°C, ebulliometry/gas-saturation methods, measured range 9.89–49.36°C, Andon et al. 1960)
- 1.895 (interpolated-Antoine eq. from ebulliometry/gas saturation measurements, Andon et al. 1960)
- $\log (P/\text{mmHg}) = 13.1729 - 4478.23/(t/^{\circ}\text{C} + 273)$; temp range: 9–50°C, (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
- $\log (P/\text{mmHg}) = 7.07343 - 1617.202/(t/^{\circ}\text{C} + 158.778)$; temp range 171–229°C (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)
- $\log (P/\text{mmHg}) = [-0.2185 \times 13991.0/(T/\text{K})] + 9.02680$; temp range 66.2–225.2°C (Antoine eq., Weast 1972–73)
- 2.541 (extrapolated-Antoine eq., Boublik et al. 1973)
- $\log (P/\text{mmHg}) = 7.07979 - 1621.451/(159.261 + t/^{\circ}\text{C})$; temp range 172–228°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)
- 3.621 (extrapolated-Cox eq., Chao et al. 1983)
- $\log (P/\text{mmHg}) = [1 - 499.926/(T/\text{K})] \times 10^{[1.05062 - 10.2129 \times 10^{-4} \cdot (T/\text{K}) + 8.04338 \times 10^{-7} \cdot (T/\text{K})^2]}$; temp range: 353.20–729.65 K, (Cox eq., Chao et al. 1983)
- 7.327 (supercooled liquid P_L , extrapolated-Antoine eq., Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.20545 - 1622.411/(159.947 + t/^{\circ}\text{C})$; temp range 172–228°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 7.46831 - 2538.736/(239.359 + t/^{\circ}\text{C})$; temp range 105.7–226°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
- 2.540 (extrapolated-Antoine eq., Dean 1985)
- $\log (P/\text{mmHg}) = 7.07919 - 1621.45/(159.26 + t/^{\circ}\text{C})$; temp range 172–229°C (Antoine eq., Dean 1985, 1992)
- 5.160 (Riddick et al. 1986)
- 1.865 (solid P_S , interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_S/\text{kPa}) = 12.31521 - 4485.592/(T/\text{K})$; temp range 282–323 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.20617 - 1623.592/(-113.623 + T/\text{K})$; temp range 444–502 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
- 3.795 (extrapolated-four parameter vapor pressure eq., Nesterova et al. 1990)
- $\log (P/\text{Pa}) = 93.28460 - 6735.317/(T/\text{K}) - 29.48566 \cdot \log (T/\text{K}) + 0.95432 \times 10^{-2} \cdot (T/\text{K})$; temp range: 445–502 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1950, Nesterova et al. 1990)
- $\log (P/\text{mmHg}) = 68.6521 - 6.15 \times 10^3/(T/\text{K}) - 20.184 \cdot \log (T/\text{K}) - 1.1259 \times 10^{-10} \cdot (T/\text{K}) + 4.0266 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 338–730 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 0.00942 (Leuenberger et al. 1985)
- 0.0212 (calculated-P/C, Shiu et al. 1994)
- 0.0278 (20°C, calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)
- 1.416, 2.903, 4.619 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
- 0.0421 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
- $\ln K_{AW} = 11.854 - 6809/(T/\text{K})$, temp range 20–100°C (vapor-liquid equilibrium VLE measurements with additional lit. data, Dohnal & Fenclová 1995)
- 0.098 (calculated-group contribution, Lee et al. 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.23 (20°C, shake flask-UV, Korenman 1973)
- 2.23 (shake flask, Korenman et al. 1980)
- 2.23 (recommended, Sangster 1989, 1993)
- 2.23 (recommended, Hansch et al. 1995)
- 2.36 (HPLC-RT correlation, Makovskaya et al. 1995b)
- 2.26 (solid-phase micro-extraction, Dean et al. 1996)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 81.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 55.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital estimation method, Klamt 1993)

Biodegradation: average rate of biodegradation $13.4 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 14.1.1.9.1
Reported aqueous solubilities of 3,4-dimethylphenol at various temperatures

Erichsen & Dobbert 1955

shake flask-optical method

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
130	29000
140	36000
150	42000
160	59000
170	81000
180	124000
186	173000
188	200000
189	222000
190	278000
190.2	336000
25	5100*

*extrapolated

TABLE 14.1.1.9.2

Reported vapor pressures of 3,4-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1)$$

$$\ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2)$$

$$\ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947

Vonterres et al. 1955

Andon et al. 1960

summary of literature data		ebulliometry		gas saturation		ebulliometry	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
66.2	133.3	105.7	1333	9.89	0.293	171.933	20341
93.8	666.6	125.8	3333	14.78	0.543	180.131	26703
107.7	1333	142.6	6666	19.98	1.031	186.548	32749

(Continued)

TABLE 14.1.1.9.2 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
122	2666	152.9	9999	24.88	1.840	193.38	40369
138	5333	160.9	13332	29.8	3.240	197.879	46135
148	7999	172.3	19998	34.86	5.626	202.37	52526
162	13332	180.3	26664	39.67	9.386	207.376	60478
181.5	26664	187.7	33330	44.76	16.13	211.126	67049
203.6	53329	193.9	39997	49.36	25.46	213.126	72703
225.2	101325	196.3	43330			217.587	79685
		198.7	46663	mp/°C	65.11	200.898	86882
mp/°C	62.8	203.0	53339	bp/°C	221.692	223.649	93227
		212.5	66661			224.292	94764
		213.4	73327	for temp range:		224.799	95996
		216.5	79993	9–50°C		225.276	97153
		219.2	86659	eq. 2	P/mmHg	225.928	98771
		222.0	93325	A	13.1729	226.392	99920
		226.0	101325	B	4478.23	226.921	101242
				C	273	227.397	102474
						228.487	105289
				ΔH _v /(kJ mol ⁻¹)		228.899	106371
				at 25°C	85.73		
				at bp	49.67	for temp range:	
						171–229°C	
						eq. 2	P/mmHg
						A	7.07343
						B	1617.202
						C	158.778

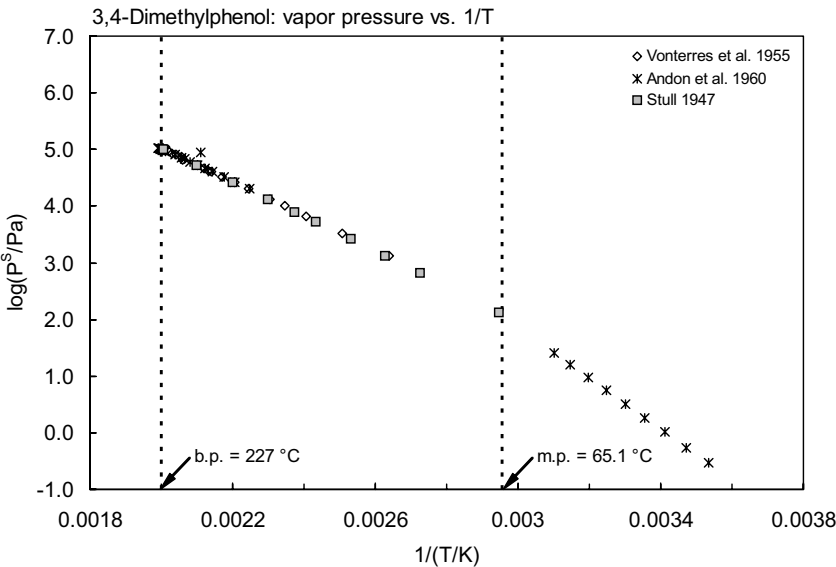
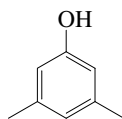


FIGURE 14.1.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for 3,4-dimethylphenol.

14.1.1.10 3,5-Dimethylphenol



Common Name: 3,5-Dimethylphenol

Synonym: 3,5-xilenol, 1-hydroxy-3,5-dimethylbenzene

Chemical Name: 3,5-dimethyl phenol

CAS Registry No: 108-68-9

Molecular Formula: $C_8H_{10}O$ $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

63.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

221.74 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constants, pK_a :

7.8 (McLeese et al. 1979)

10.19 (Dohnal & Fenclová 1995)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

82.84, 49.31 ($25^{\circ}C$, normal bp, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.420 (mp at $63.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4886 (shake flask-UV, pH 5.1, Blackman et al. 1955)

4425 ($20^{\circ}C$, shake flask-UV, Dohnal & Fenclová 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($62.0^{\circ}C$, summary of literature data, temp range 62 – $219.5^{\circ}C$, Stull 1947)

1333* ($102.8^{\circ}C$, ebulliometry, measured range 102.8 – $219.0^{\circ}C$, Vonterres et al. 1955)

2.63* ($24.95^{\circ}C$, ebulliometry/gas saturation, measured range 9 – $45^{\circ}C$, Andon et al. 1960)

$\log(P/mmHg) = 12.8271 - 4328.13/(t/^{\circ}C + 273)$; temp range 9 – $50^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/mmHg) = 7.11745 - 1630.124/(t/^{\circ}C + 163.076)$; temp range 154 – $224^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/kPa) = 6.25752 - 1641.206/(164.311 + t/^{\circ}C)$, temp range 154.7 – $223.3^{\circ}C$ (Antoine eq. derived from reported exptl data of Andon et al. 1960, Boublik et al. 1984)

$\log(P/kPa) = 8.27972 - 3182.232/(287.862 + t/^{\circ}C)$, temp range 102.8 – $219^{\circ}C$ (Antoine eq. derived from reported exptl data of Vonterres et al. 1960, Boublik et al. 1984)

$\log(P_s/kPa) = 11.97153 - 4336.025/(T/K)$; temp range 282 – $323\ K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.25292 - 1638.564/(-109.095 + T/K)$; temp range 427 – $497\ K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -44.915 - 2.8912 \times 10^3/(T/K) + 25.704 \cdot \log(T/K) - 3.9714 \times 10^{-2} \cdot (T/K) + 1.6464 \times 10^{-5} \cdot (T/K)^2$; temp range 337 – $716\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

0.0419, 0.0614 (20, 25°C , calculated-limiting activity coefficient γ^∞ data, Dohnal & Fenclová 1995)

1.95, 3.70, 6.12 (75.9, 88.7, 98.5°C , vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

$\ln K_{\text{AW}} = 11.654 - 6636/(T/\text{K})$; temp range $20\text{--}98.5^\circ\text{C}$ (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.31 (shake flask, Korenman 1972; Korenman et al. 1980)

2.55 (shake flask-UV, Rogers & Wong 1980)

2.38 (UNIFAC activity coefficient, Campbell & Luthy 1985)

2.54 (HPLC-RT correlation, Eadsforth 1986)

2.35 (shake flask, Log P Database, Hansch & Leo 1987)

2.35 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Half-Lives in the Environment:

TABLE 14.1.1.10.1

Reported vapor pressures of 3,5-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)					
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
62	133.3	102.8	1333	9.57	0.44	154.72	12984
89.2	666.6	122.5	3333	14.92	0.813	166.472	19760
102.4	1333	139.1	6666	20.35	1.587	175.126	26444
117.0	2666	149.0	9999	24.05	2.626	182.389	33392
133.3	5333	156.8	13332	30.42	4.866	187.937	39757
143.5	7999	168.1	19998	34.85	7.813	192.743	45815
156	13332	176.3	26664	39.94	13.32	197.298	52352
176.2	26664	182.9	33330	45.23	22.80	201.925	59794
197.8	53329	188.5	39997	49.97	35.33	205.601	66193
219.5	101325	191.0	43330			209.151	72942
		194.0	46663			212.159	79072
mp/°C	68.0	198.1	53329	mp/°C	63.27	215.799	87070
		202.0	59995	bp/°C	221.692	218.298	92904
		205.3	66661			219.146	94952
		208.3	73327	for temp range:		219.584	96027
		211.0	79993	9–50°C		220.097	97296
		214.0	86659	eq. 2	P/mmHg	220.692	98771

TABLE 14.1.1.10.1 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		216.2	93325	A	12.8271	221.309	100334
		219.0	101325	B	4328.13	221.709	101362
				C	273	222.269	102845
						222.724	104007
						223.321	105573
				ΔH_v /(kJ mol ⁻¹)			
				at 25°C			
				82.84			
				at bp			
				49.31		for temp range:	
						154–224°C	
						eq. 2	P/mmHg
						A	7.11745
						B	1630.124
						C	163.076

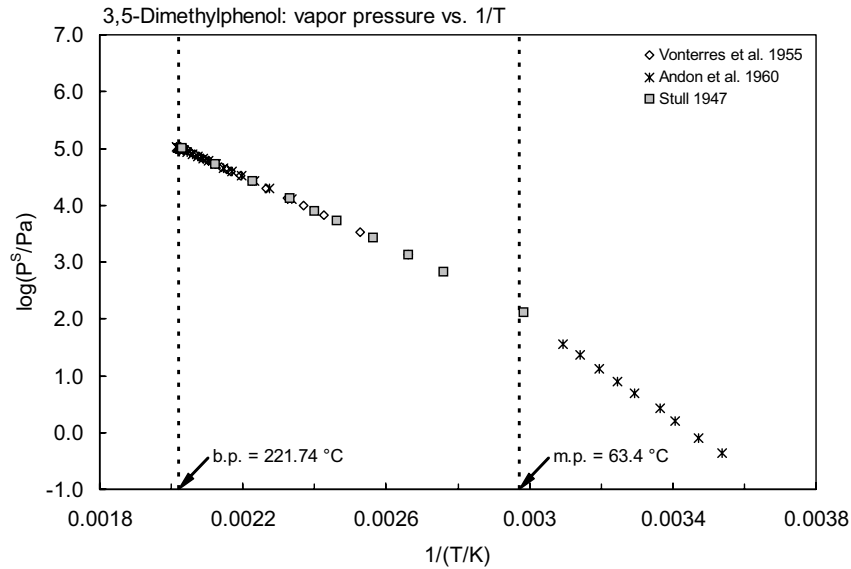
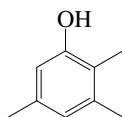


FIGURE 14.1.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for 3,5-dimethylphenol.

14.1.1.11 2,3,5-Trimethylphenol



Common Name: 2,3,5-Trimethylphenol

Synonym:

Chemical Name: 2,3,5-trimethylphenol

CAS Registry No: 697-82-5

Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

94.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

233 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.60 (Blackman et al. 1955)

Molar Volume (cm^3/mol):

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.208 (mp at $94.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

40000* (200 $^{\circ}C$, synthetic method/shake flask-optical, measured range 200–248 $^{\circ}C$, Erichsen & Dobbert 1955)

762 (shake flask-UV, Blackman et al. 1955)

855 (shake flask-HPLC/UV at pH 5.95, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.426* (extrapolated-Antoine eq., ebulliometry, measured range 186–247 $^{\circ}C$, Handley et al. 1964)

$\log (P/mmHg) = 7.08022 - 1685.973/(166.150 + t/^{\circ}C)$; temp range 186–247 $^{\circ}C$ (Antoine eq., ebulliometric method, Handley et al. 1964)

4.451 (extrapolated-Cox eq., Chao et al. 1983)

$\log (P/mmHg) = [1 - 508.477/(T/K)] \times 10^{0.932965 - 5.75276 \times 10^{-4} \cdot (T/K) + 3.29737 \times 10^{-7} \cdot (T/K)^2}$; temp range: 459.63–520.21 K, (Cox eq., Chao et al. 1983)

2.426 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 7.08012 - 1685.896/(166.141 + t/^{\circ}C)$, temp range 186.5–247 $^{\circ}C$ (Antoine eq. from reported exptl. data of Handley et al. 1964, Boublik et al. 1984)

2.43, 0.0234 (extrapolated from liquid, Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.02493 - 1685.528/(166.133 + t/^{\circ}C)$, temp range 186.5–247 $^{\circ}C$ (Antoine eq. from reported exptl. data of Handley et al. 1964, Boublik et al. 1984)

$\log (P/kPa) = 6.95436 - 889.02/(67.752 + t/^{\circ}C)$, temp range 106–233 $^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

2.43 extrapolated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 7.08012 - 1685.90/(166.14 + t/^{\circ}C)$, temp range 186–247 $^{\circ}C$ (Antoine eq., Dean 1985, 1992)

2.44 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.20676 - 1687.869/(-106.761 + T/K)$, temp range 459–531 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{Pa}) = 89.62984 - 6541.396/(T/\text{K}) - 28.26318 \cdot \log (T/\text{K}) + 0.92991 \times 10^{-2} \cdot (T/\text{K})$; temp range: 460–520 K
(four-parameter vapor pressure eq. derived using exptl data of Handley et al. 1964, Nesterova et al. 1990)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.404 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.06 (COMPUTOX databank, Kaiser 1993)

2.92 (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.61 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

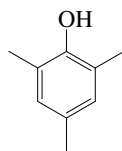
TABLE 14.1.1.11.1
Reported aqueous solubilities and vapor pressures of 2,3,5-trimethylphenol at various temperatures

Aqueous solubility		Vapor pressure	
Erichsen & Dobbert 1955		Handley et al. 1964	
shake flask-optical method		ebulliometry	
$t/^\circ\text{C}$	$S/\text{g} \cdot \text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa
200	40000	186.482	26547
210	54000	193.614	33021
220	79000	200.127	40002
230	128000	205.448	46560
240	200000	210.422	53453
242	224000	214.675	59972
244	250000	218.644	66623
246	291000	222.382	73417
257.8	420000	225.707	79909
		229.041	86877
		231.852	93116
		234.759	99940
		237.50	106735
		240.13	113587
		242.511	120090
		244.811	126646
		247.062	133344
		mp/ $^\circ\text{C}$	93.73
		bp/ $^\circ\text{C}$	235.329

TABLE 14.1.1.11.1 (Continued)

Aqueous solubility		Vapor pressure	
Erichsen & Dobbert 1955		Handley et al. 1964	
shake flask-optical method		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa
for temp range: 186–247°C			
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$			
			P/mmHg
A			7.08022
B			1685.973
C			166.150
$\Delta H_v/(\text{kJ mol}^{-1})$			
at bp			49.96

14.1.1.12 2,4,6-Trimethylphenol



Common Name: 2,4,6-Trimethylphenol

Synonym: Mesityl

Chemical Name: 2,4,6-Trimethylphenol

CAS Registry No: 527-60-6

Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

73 (Lide 2003)

Boiling Point ($^{\circ}C$):

220 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.90 (Blackman et al. 1955)

10.88 (Dean 1985)

Molar Volume (cm^3/mol):

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.338 (mp at $73^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1007 (shake flask-UV, Blackman et al. 1955; quoted, Varháníčková et al. 1995)

1420 (shake flask-HPLC/UV at pH 4.85, Varháníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.0 (extrapolated from liquid state, Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.91352 - 1481.329/(158.589 + t/^{\circ}C)$, temp range $94-220.6^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

19.6 (supercooled liquid P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.82395 - 2158.2/(-45.2 + T/K)$, temp range $367-494 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.2512 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.73 (generator column-HPLC/UV, Wasik et al. 1981)

2.73 (quoted and recommended, Sangster 1989; 1993)

2.7 3 (COMPUTOX databank, Kaiser 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

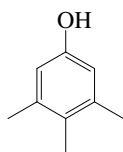
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.1.13 3,4,5-Trimethylphenol



Common Name: 3,4,5-Trimethylphenol

Synonym:

Chemical Name: 3,4,5-trimethylphenol

CAS Registry No: 527-54-8

Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

108 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

249 (Stephenson & Malanowski 1987)

248.5 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.25 (Dean 1985)

Molar Volume (cm^3/mol):

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.153 (mp at $108^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1538 (shake flask-HPLC/UV, Varhaníčková et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P_L/kPa) = 7.33216 - 2536.1/(-44.56 + T/K)$, temp range 396–521 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

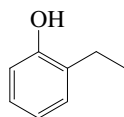
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.1.14 *o*-Ethylphenol

Common Name: 2-Ethylphenol

Synonym: *o*-ethylphenol

Chemical Name: 2-ethylphenol, *o*-ethylphenol

CAS Registry No: 90-00-6

Molecular Formula: C₈H₁₀O, C₂H₅C₆H₄OH

Molecular Weight: 122.164

Melting Point (°C):

18 (Lide 2003)

Boiling Point (°C): 204.52

204.5 (Lide 2003)

Density (g/cm³ at 20°C):

1.01885, 1.01459 (20°C, 25°C Biddiscombe et al. 1963)

1.0370 (Verschuereen 1983; 25°C, Dean 1985)

Molar Volume (cm³/mol):

117.8 (0°C, Stephenson & Malanowski 1987)

147.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a:

10.02 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

14040 (shake flask-HPLC/UV at pH 5.2, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (46.2 °C, summary of literature data, temp range 46.2–207.5°C, Stull 1947)

33.66 (calculated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 7.23343 – 1771.5/(200.0 + t/°C), temp range 105–245°C (Antoine eq. for liquid state, Dreisbach 1955)

20.84 (interpolated-Antoine eq., Biddiscombe et al. 1963)

20.4* (24.93°C, ebulliometric and gas transpiration measurements, measured range 5–45°C, Biddiscombe & Martin 1958)

log (P/mmHg) = 10.3131 – 3313.50/(t/°C + 273); temp range 5–45°C (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)

log (P/mmHg) = 7.00742 – 1648.923/(t/°C + 170.833); temp range 150–218°C (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)

log (P/mmHg) = [–0.2185 × 12516.7/(T/K)] + 8.586948; temp range 46.2–207.5°C (Antoine eq., Weast 1972–73)

log (P/mmHg) = [1– 480.731/(T/K)] × 10⁴{0.883881 – 6.07675 × 10^{–4}·(T/K) + 6.44264 × 10^{–7}·(T/K)²}; temp range: 319.35–480.65 K, (Cox eq., Chao et al. 1983)

16.7, 29 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.13214 – 1548.802/(170.82 + t/°C), temp range 150.4–215.05°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1963, Boublik et al. 1984)

log (P/kPa) = 6.97225 – 2178.815/(231.035 + t/°C), temp range 86–207.5°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

27.01 (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.8003 – 2140.4/(227 + t/°C), temp range 86–208°C (Antoine eq., Dean 1985, 1992)

20.87 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.13344 - 1550.409/(-102.103 + T/\text{K})$; temp range 423–491 K (Antoine eq.-I, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 9.44878 - 3318.181/(T/\text{K})$, temp range 277–318 K (Antoine eq.-II, Stephenson & Malanowski 1987)

19.55 (extrapolated-Antoine eq., Nesterova et al. 1990)

$\log (P/\text{Pa}) = 94.95377 - 6350.841/(T/\text{K}) - 30.56287 \cdot \log (T/\text{K}) + 1.09475 \times 10^{-2} \cdot (T/\text{K})$; temp range: 424–491 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.174 (calculated with selected-P/C)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.47 (shake flask, Hansch & Leo 1979)

2.64 (shake flask, Korenman 1980)

2.64 (HPLC-RT correlation, Butte et al. 1981)

2.47 (recommended, Sangster 1989, 1993)

2.46 (HPLC-RT correlation, Ritter et al. 1994)

2.47 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.1.14.1

Reported vapor pressures of *o*-ethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/\text{K})$	(1)	$\ln P = A - B/(T/\text{K})$	(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log (P/\text{Pa}) = A - B/(C + T/\text{K})$	(3)		
$\log (P/\text{mmHg}) = A - B/(T/\text{K}) - C \cdot \log (T/\text{K})$	(4)		

Stull 1947

Biddiscombe et al. 1963

summary of literature data		gas saturation		ebulliometry	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
46.2	133.3	4.98	3.346	150.425	20458
73.4	666.6	10.0	5.173	158.137	26542
87	1333	15.01	8.759	164.876	32996
101.5	2666	20.01	13.73	171.143	40086
117.9	5333	24.93	20.40	176.174	46627
127.9	7999	29.53	30.80	180.808	53390
141.8	13332	34.84	45.86	184.869	59946
161.6	26664	39.99	73.99	188.565	66460
184.5	53329	45.0	102.9	192.115	73235
207.5	101325			195.266	79702
				198.382	86528
mp/°C	−45	mp/°C	−3.31	200.845	92242

(Continued)

bp/°C		217.985	204.350	100866
TABLE 14.1.1.14.1 (Continued)				
Stull 1947		Biddiscombe et al. 1963		
summary of literature data		gas saturation		ebulliometry
t/°C	P/Pa	t/°C	P/Pa	t/°C P/Pa
				206.632 106865
		for temp range:		208.429 111753
		5–45°C		209.854 115762
		eq. 2	P/mmHg	212.651 123942
		A	10.3131	215.149 131641
		B	3313.50	218.047 142363
		C	273	
		ΔH _v /(kJ mol ⁻¹)		for temp range:
		at 25°C	63.60	150–218°C
		at bp	48.116	eq. 2 P/mmHg
				A 7.00742
				B 1548.923
				C 170.833

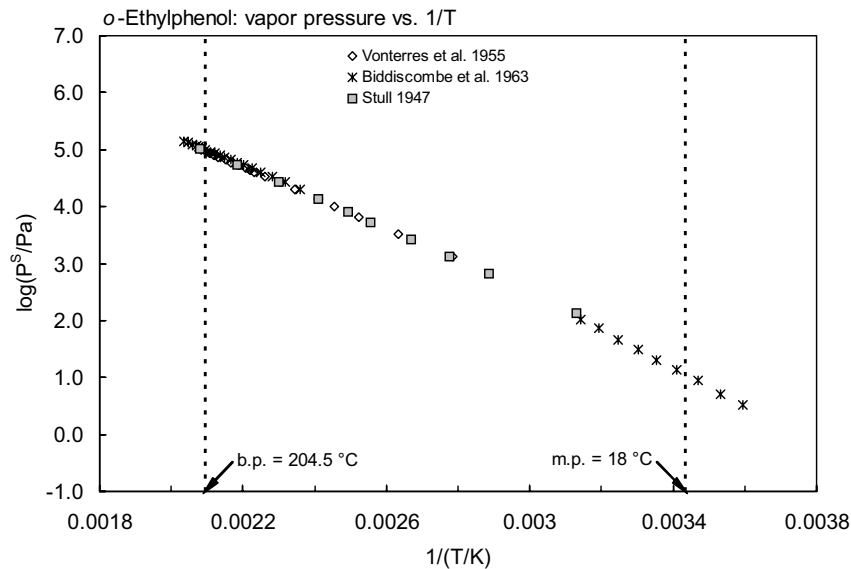
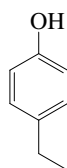


FIGURE 14.1.1.14.1 Logarithm of vapor pressure versus reciprocal temperature for o-ethylphenol.

14.1.1.15 *p*-Ethylphenol

Common Name: 4-Ethylphenol

Synonym: *p*-ethylphenol

Chemical Name: 2-ethylphenol, *p*-ethylphenol

CAS Registry No: 123-07-9

Molecular Formula: $C_8H_{10}O$, $C_2H_5C_6H_4OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

45 (Lide 2003)

Boiling Point ($^{\circ}C$):

217.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.054 ($25^{\circ}C$, Biddiscombe et al. 1963)

1.011 ($25^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

10.0 (Dean 1985)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

50.84 (at normal boiling point, Biddiscombe et al. 1963)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

80.33 (at $25^{\circ}C$, Andon et al. 1960)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F : 0.636 (mp at $45^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

24000* ($150^{\circ}C$, synthetic method-shake flask-optical, measured range 150 – $187^{\circ}C$, Erichsen & Dobbert 1955)

5000 (shake flask-spectrophotometry, Roberts et al. 1977)

7980 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($59.3^{\circ}C$, summary of literature data, temp range 59.3 – $219.0^{\circ}C$, Stull 1947)

9.67 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.55177 - 1943.1/(197.0 + t/^{\circ}C)$, temp range: 125 – $255^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1955)

1333* ($101.0^{\circ}C$, ebulliometry, measured range 101.0 – $218.2^{\circ}C$, Vonterres et al. 1955)

5.030 (calculated-Antoine eq., Biddiscombe et al. 1963)

4.96* ($25.03^{\circ}C$, ebulliometric and gas transpiration measurements, measured range 5 – $44^{\circ}C$, Biddiscombe et al. 1963)

$\log(P/mmHg) = 12.6090 - 4183.50/(t/^{\circ}C + 273)$; temp range 5 – $44^{\circ}C$ (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)

$\log(P/mmHg) = 7.01297 - 1548.923/(t/^{\circ}C + 156.820)$; temp range 171 – $229^{\circ}C$ (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)

$\log (P/\text{mmHg}) = [-0.2185 \times 13437.9/(T/K)] + 8.854990$; temp range 59.3–219°C (Antoine eq., Weast 1972–73)
 6.575 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.13614 - 1547.614/(156.677 + t/^\circ\text{C})$, temp range 171.8–229.1°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1963, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 7.59041 - 2575.507/(242.273 + t/^\circ\text{C})$, temp range 101–218.2°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
 7.530 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 8.291 - 2423/(229 + t/^\circ\text{C})$, temp range 101–218°C (Antoine eq., Dean 1985, 1992)
 4.95 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.74364 - 4188.624/(T/K)$, temp range 278–317 K, (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.13939 - 1550.479/(-116.1 + T/K)$, temp range: 444–503 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
 6.137 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 96.72774 - 6779.787/(T/K) - 30.80658 \cdot \log (T/K) + 1.101581 \times 10^{-2} \cdot (T/K)$; temp range: 445–502 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 16.9092 - 3.7255 \times 10^3/(T/K) - 1.7886 \cdot \log (T/K) - 4.2275 \times 10^{-3} \cdot (T/K) + 1.8002 \times 10^{-6} \cdot (T/K)^2$; temp range 318–716 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.132 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.75 (literature average, Leo et al. 1971)
 2.58 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
 2.26 (shake flask, Korenman 1972, Korenman et al. 1980)
 2.26, 2.58 (Hansch & Leo 1979)
 2.60 (shake flask-UV, Rogers & Wong 1980)
 2.37 (HPLC-RT correlation, Butte et al. 1981)
 2.12, 2.19 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 2.59 ± 0.07 ; 2.58 (HPLC-RV correlation-ALPM, selected best lit. value, Garst & Wilson 1984)
 2.50 (recommended, Sangster 1989, 1993)
 2.50 (COMPUTOX databank, Kaiser 1993)
 2.40; 2.58 (pH 7.4, pH 5.6, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.1.15.1

Reported aqueous solubilities of *p*-ethylphenol at various temperatures

Erichsen & Dobbert 1955

synthetic method, SF-optical	
t/°C	S/g·m ⁻³
150	24000
160	30000
170	45000
180	93000
182	112000
184	141000
186	197000
187.1	395000

TABLE 14.1.1.15.2

Reported vapor pressures of *p*-ethylphenol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log (P/\text{Pa}) = A - B/(C + T/K) & (3) & & \\ \log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

Stull 1947

Vonderres et al. 1955

Biddiscombe et al. 1963

summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
59.3	133.3	101.0	1333	5.0	0.480	171.757	26571
86.5	666.6	109.8	3333	10.0	0.907	178.525	33069
100.2	1333	137.5	6666	15.0	1.613	184.585	39942
115.0	2666	148.0	9999	19.99	2.813	189.724	46636
131.3	5333	155.5	13332	25.03	4.960	194.356	53416
141.7	7999	167.0	19998	30.02	8.426	198.419	59999
154.2	13332	177.2	26664	35.0	14.27	202.227	66736
175.0	26664	182.0	33330	39.99	23.33	205.607	73211
197.4	53329	187.7	39997	43.97	34.13	208.892	79979
219.0	101325	190.5	43330			211.911	86626
		192.6	46663			214.673	93090
mp/°C	46.5	197.0	53329	mp/°C	45.06	217.535	100174
		201.7	59995	bp/°C	217.985	220.026	106683
		204.0	66661			222.543	113599
		207.4	73327	for temp range:		224.769	119995
		210.9	79993	5–44°C		226.933	126484
		213.1	86659	eq. 2	P/mmHg	229.147	133418
		216.1	93325	A	12.6090		
		218.2	101325	B	4183.81	for temp range:	
				C	273	171–229°C	
						eq. 2	P/mmHg
				$\Delta H_v/(\text{kJ mol}^{-1})$		A	7.01297
				at 25°C	80.33	B	1548.754
				at bp	50.84	C	156.820

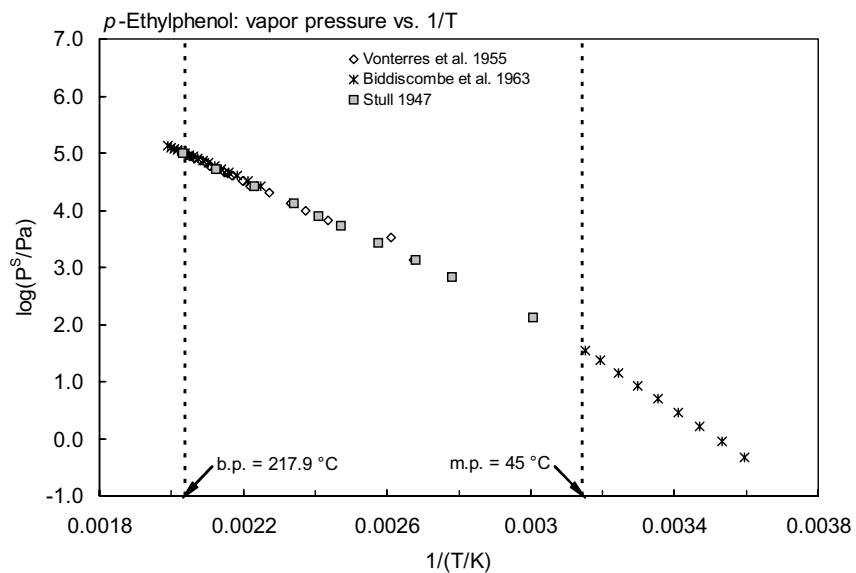
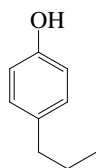


FIGURE 14.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-ethylphenol.

14.1.1.16 4-Propylphenol



Common Name: 4-Propylphenol

Synonym:

Chemical Name: 4-propylphenol

CAS Registry No: 645-56-7

Molecular Formula: $C_9H_{12}O$, $C_3H_7C_6H_4OH$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

22 (West 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

232.6 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.009 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1278 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P_L/kPa) = 7.32632 - 2550.1/(-28.65 + T/K)$, temp range 383–508 K, (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.1 (HPLC-RT correlation, McLeese et al. 1979)

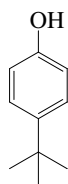
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.1.17 *p*-*tert*-Butylphenol

Common Name: 4-*tert*-Butylphenol

Synonym: *p*-*tert*-butylphenol, 4-(α,α -dimethylethylphenol)

Chemical Name: 4-*tert*-butylphenol, *p*-*tert*-butylphenol

CAS Registry No: 98-54-4

Molecular Formula: $C_{10}H_{14}O$, $(CH_3)_3CC_6H_4OH$

Molecular Weight: 150.217

Melting Point ($^{\circ}C$):

98 (Lide 2003)

Boiling Point ($^{\circ}C$):

237 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

152.0 ($20^{\circ}C$, Stephenson & Malanowski 1987)

192.2 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

9.90 (McLeese et al. 1979)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

67.33, 50.62 ($25^{\circ}C$, bp, Dreisbach 1955)

50.54 (at normal boiling point, Handley et al. 1964)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.192 (mp at $98^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

650 (20 – $25^{\circ}C$, Geyer et al. 1981)

1000 (Thomas 1982)

700 (Verschueren 1983)

580 (Yalkowsky et al. 1987)

580 (shake flask-UV, Ahel & Giger 1993a)

1850 (shake flask-HPLC/UV at pH 6.05, Varhanířková et al. 1995)

753 (calculated-group contribution, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6.402* (extrapolated-regression of tabulated data, temp range 70 – $238^{\circ}C$, Stull 1947)

3.688 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.49264 - 1999.8/(194.0 + t/^{\circ}C)$, temp range 140 – $370^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1.225* (liquid, extrapolated-Antoine eq., ebulliometry, measured range 198 – $251^{\circ}C$, Handley et al. 1964)

$\log(P/mmHg) = 11.5638 - 3586.36/(t/^{\circ}C + 273)$; temp range 198 – $251^{\circ}C$ (Antoine eq. from ebulliometric measurements, Handley et al. 1964)

$\log(P/mmHg) = [-0.2185 \times 13787.7/(T/K)] + 8.785696$; temp range 70 – $238^{\circ}C$ (Antoine eq., Weast 1972–73)

5.072 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/mmHg) = [1 - 512.693/(T/K)] \times 10^4 \{0.834403 - 2.10918 \times 10^{-4} \cdot (T/K) + 0.554077 \times 10^{-7} \cdot (T/K)^2\}$; temp range 343.15 – $524.76 K$ (Cox eq., Chao et al. 1983)

1.24 (supercooled liquid P_L , extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.12365 - 1626.256/(155.092 + t/^{\circ}\text{C})$; temp range 198–231.6°C (Antoine eq. from reported exptl. data of Handley et al. 1964, Boublik et al. 1984)

1.25 (extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.00038 - 1627.51/(155.24 + t/^{\circ}\text{C})$, temp range 198–252°C (Antoine eq., Dean 1985, 1992)

1.272 (extrapolated-liquid, Antoine eq., Stephenson & Malanowski 1987)

0.492 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 11.46945 - 4405.873/(T/\text{K})$; temp range 280–304 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.13162 - 1632.939/(-117.258 + T/\text{K})$, temp range: 471–525 K, (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log (P/\text{Pa}) = 122.26679 - 8003.926/(T/\text{K}) - 40.16380 \cdot \log (T/\text{K}) + 1.40155 \times 10^{-2} \cdot (T/\text{K})$; temp range 471–525 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)

$\log (P/\text{mmHg}) = -54.7404 - 2.4727 \times 10^3/(T/\text{K}) + 28.991 \cdot \log (T/\text{K}) - 3.9356 \times 10^{-3} \cdot (T/\text{K}) + 1.543 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 372–734 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.113 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

0.139; 3.750 (calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)

0.922 (calculated-P/C, Thomas 1982)

0.113, 0.375 (quoted, calculated-MCI χ , Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.04 (shake flask, Geyer et al. 1984)

2.94, 3.14 (shake flask-OECD 1981 Guideline, Geyer et al. 1984)

3.41 (HPLC-RT correlation, Butte et al. 1987)

3.04 (recommended, Sangster 1989)

3.31 (recommended, Hansch et al. 1995)

3.10 (HPLC-RT correlation, Makovskaya et al. 1995b)

2.95 (solid-phase microextraction, Dean et al. 1996)

Bioconcentration Factor, $\log \text{BCF}$:

1.53 (*Chlorella*, after exposure to 50 $\mu\text{g}/\text{L}$ for 24 h, Geyer et al. 1981)

1.88 (calculated-S, Geyer et al. 1981)

1.53; 2.08 (algae, golden *orfe*, Freitag et al. 1982)

2.38 (activated sludge, Freitag et al. 1982, 1985)

1.53 (Alga *Chlorella fusca*, wet weight basis, Geyer et al. 1984)

1.48; 2.07 (algae; golden ide, Freitag et al. 1985)

1.86 (zebrafish, Butte et al. 1987; quoted, Devillers et al. 1996)

2.38; 1.48; 2.07 (activated sludge; algae; fish; Freitag et al. 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: volatilization

$t_{1/2} = 117$ h from water body with depth of 1 m (Thomas 1982).

Half-Lives in the Environment:

TABLE 14.1.1.17.1

Reported vapor pressures of *p*-*tert*-butylphenyl at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Handley et al. 1964			
summary of literature data		ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70.0	133.3	198.21	33059	mp/°C	99.55
99.2	666.6	204.527	39955	bp/°C	239.83
114	1333	209.901	46592	for temp range: 198–251°C	
129.5	2666	214.892	53489		
146	5333	219.142	59984	eq. 2	P/mmHg
156	7999	223.088	66579	A	6.99455
170.2	13332	226.818	73350	B	1623.046
191.5	26664	230.203	79963	C	154.716
214	53329	233.457	86724	$\Delta H_v/(\text{kJ mol}^{-1})$	
238	101325	236.342	92123	at bp	50.54
		239.305	100052		
mp/°C	99.0	242.180	106758		
		244.560	113369		
		247.015	120049		
		249.336	126634		
		251.608	133354		

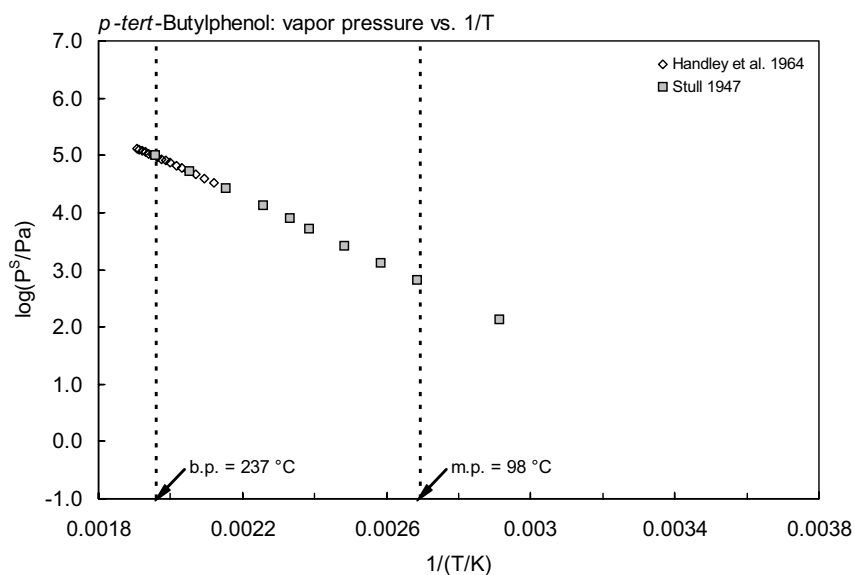
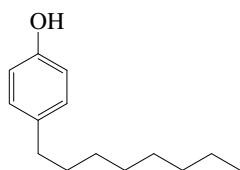


FIGURE 14.1.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-*tert*-butylphenol.

14.1.1.18 4-Octylphenol



Common Name: 4-Octylphenol

Synonym: *p*-octylphenol

Chemical Name: 4-octylphenol

CAS Registry No: 27193-28-8

Molecular Formula: $C_{14}H_{22}O$, $C_8H_{17}-C_6H_4OH$

Molecular Weight: 206.324

Melting Point ($^{\circ}C$):

43 (Lide 2003)

Boiling Point ($^{\circ}C$):

280-283 (Lewis 1996)

Density (g/cm^3 at $20^{\circ}C$):

0.941 (at $24^{\circ}C$, Lewis 1996)

Molar Volume (cm^3/mol):

281.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.666 (mp at $43^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

12.6 ± 0.50 (generator column-HPLC/fluo., Ahel & Giger 1993a)

14.1 ± 0.60 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

0.071 (quoted, Shiu et al. 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

0.4916 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.70 (calculated- π substituent const. or fragment const., McLeese et al. 1981)

4.12 ± 0.10 (shake flask-HPLC/fluo., Ahel & Giger 1993b)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

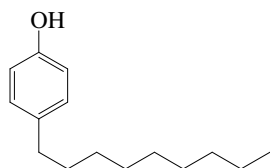
Biodegradation: average exptl. rate constant $k = 0.0894 h^{-1}$ compared to group contribution method predicted rate constants $k = 0.1124 h^{-1}$ (nonlinear) and $k = 0.0982 h^{-1}$ (Tabak & Govind 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

14.1.1.19 4-Nonylphenol



Common Name: 4-Nonylphenol

Synonym: *p*-nonylphenol

Chemical Name: 4-nonylphenol

CAS Registry No: 104-40-5; 25154-52-3

Molecular Formula: $C_{15}H_{24}O$, $C_9H_{19}C_6H_4OH$

Molecular Weight: 220.351

Melting Point ($^{\circ}C$):

42 (Lide 2003)

Boiling Point ($^{\circ}C$):

approx. 295 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.513 (Budavari 1989)

Molar Volume (cm^3/mol):

231.1 ($20^{\circ}C$, Stephenson & Malanowski 1987)

303.2 (calculated-Le Bas method at normal boiling)

Acid Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.681 (mp at $42^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.43 ± 0.17 (generator column-HPLC/fluor., Ahel & Giger 1993a)

4.90 ± 0.4 (shake flask-GC/FID, Brix et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0701* (ebulliometry, extrapolated, measured range 214.78 – $321.91^{\circ}C$, Hon et al. 1976)

$\log (P/mmHg) = 7.74950 - 2550.67/(260.28 + t/^{\circ}C)$; temp range 214.78 – $321.91^{\circ}C$ (Antoine eq., ebulliometry, Hon et al. 1976)

0.0720 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.8847 - 2560.53/(207.199 + t/^{\circ}C)$, temp range 214.8 – $321.8^{\circ}C$ (Antoine eq. from reported exptl. data of Hon et al. 1976, Boublik et al. 1984)

0.0691 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.87147 - 2547.289/(-67.246 + T/K)$, temp range 487 – $595 K$ (Antoine eq., Stephenson & Malanowski 1987)

0.174, 0.14, 0.109, 0.0908, 0.0802, 0.0556 (GC-RT correlation, 7 isomers, Bidleman & Renberg 1985)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1.5705 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.20 (calculated- π substituent const. or fragment const., McLeese et al. 1981)

4.10 (Geyer et al. 1982)

5.90 (selected, Yoshida et al. 1986)

5.76 (HPLC-RT correlation, Itokawa et al. 1989)

4.48 ± 0.12 (shake flask-HPLC/fluor., Ahel & Giger 1993b)

6.36 (calculated-CLOGP 3.51, Jaworska & Schultz 1993)

- 6.36 (COMPUTOX, Kaiser 1993)
 5.76 (Sangster 1993; Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 2.45 (salmon, McLeese et al. 1981)
 1.00 (mussel *mytilus edulis*, Geyer et al. 1982)
 2.40 (fish liver, Ahel & Giger 1993a)
 2.22; 2.45 (laboratory BCF data: killifish; salmon; Tsuda et al. 2000)
 1.49; 1.32; 1.40; 1.34; 1.32; 1.18; 1.11–2.61 (field BCF data: pale chub; Ayu sweetfish, dark chub, crucian carp; large-mouth bass; bluegill; fish tissue; Tsuda et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: average exptl. rate constant of 0.0894 h^{-1} compared to group contribution method predicted rate constants of 0.1124 h^{-1} (nonlinear) and 0.0982 h^{-1} (linear) (Tabak & Govind 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 45.0 \text{ d}^{-1}$ (McLeese et al. 1981)

$k_2 = 0.16 \text{ d}^{-1}$ (McLeese et al. 1981)

Half-Lives in the Environment:

Biota: $t_{1/2} = 4 \text{ d}$ in salmon before excretion (McLeese et al. 1981).

TABLE 14.1.1.19.1
Reported vapor pressures of 4-nonylphenol at various temperatures

Hon et al. 1976	
ebulliometry	
$t/^{\circ}\text{C}$	P/Pa
214.78	6557
251.33	19998
261.87	26679
274.76	37250
283.74	46663
289.28	53364
298.78	66656
303.76	74873
307.72	81628
310.82	87441
314.17	94271
317.1	100170
321.81	110655
bp/ $^{\circ}\text{C}$	317.61

(Continued)

TABLE 14.1.1.19.1 (*Continued*)**Hon et al. 1976****ebulliometry****t/°C****P/Pa** $\log P = A - B/(C + t/^{\circ}\text{C})$

P/mmHg

A 7.74950

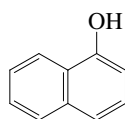
B 2550.67

C 260.28

 $\Delta H_v/(\text{kJ mol}^{-1})$

at bp 61.923

14.1.1.20 1-Naphthol



Common Name: 1-Naphthol

Synonym: α -naphthol, 1-naphthalenol, 1-hydroxynaphthalene

Chemical Name: 1-naphthol

CAS Registry No: 90-15-3

Molecular Formula: $C_{10}H_8O$, $C_{10}H_7OH$

Molecular Weight: 144.170

Melting Point ($^{\circ}C$):

95 (Lide 2003)

Boiling Point ($^{\circ}C$):

288.0 (sublimation, Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm^3):

1.0989 ($99^{\circ}C$, Weast 1982–83)

1.0954 ($99^{\circ}C$, Dean 1985)

Acid Dissociation Constant, pK_a :

9.20 (McLeese et al. 1979)

9.30 (Dean 1985)

Molar Volume (cm^3/mol):

131.2 ($99^{\circ}C$, Stephenson & Malanowski 1987)

155.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.47 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

63.6 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$, F: 0.206 (mp at $95^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

438 (quoted, Tsonopoulos & Prausnitz 1971)

870; 674 (exptl., calculated-group contribution, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.550* (extrapolated-regression of tabulated data, temp range 94 – $282.5^{\circ}C$, Stull 1947)

1333* ($141.5^{\circ}C$, ebulliometry, measured range 141.5 – $282.5^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 14205.6/(T/K)] + 8.476669$; temp range 94 – $282.5^{\circ}C$ (Antoine eq., Weast 1972–73)

0.509 (extrapolated-liquid, Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.69308 - 2275.566/(202.869 + t/^{\circ}C)$, temp range 141.5 – $282.5^{\circ}C$ (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

0.290 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.28421 - 2077.56/(184.0 + t/^{\circ}C)$; temp range 141 – $282^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_s/kPa) = 12.20753 - 4873.394/(T/K)$; temp range 298 – $312\ K$ (Antoine eq.-I, α form, solid, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.70115 - 4405.522/(T/K)$; temp range 314 – $324\ K$ (Antoine eq.-II, β form, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.53825 - 3083.8/(1.731 + T/K)$; temp range 399 – $556\ K$ (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.49 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.98	(shake flask-UV, Hansch & Anderson 1967)
2.98, 2.84, 2.31	(Hansch & Leo 1979)
2.28	(HPLC- k' correlation, Haky & Young 1984)
2.84	(recommended, Sangster 1989, 1993)
2.84	(CPC centrifugal partition chromatography, Gluck & Martin 1990)
3.13	(back-flushing-CPC centrifugal partition chromatography, Menges et al. 1990)
2.81	(shake flask-HPLC, Menges et al. 1991)
3.02	(concurrent chromatography, Berthod et al. 1988)
2.84	(COMPUTOX, Kaiser 1993)
2.43	(HPLC-RT correlation, Ritter et al. 1994)
2.84	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:Sorption Partition Coefficient, $\log K_{OC}$:

2.64	(soil and sediment, Hassett et al. 1981)
3.33	(soil, Means et al. 1982)
3.41	(soil, calculated-MCI χ , Sabljic 1987)
2.10–2.77	(soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987)
2.63–2.99	(soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987)
1.84–2.1	(soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987)
1.99–2.66	(soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987)
1.30–1.90	(soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987)
2.89	(soil, calculated-MCI χ , Bahnick & Doucette 1988)
2.52–2.96, 2.53	(soil: quoted, calculated- K_{OW} , Xing et al. 1994)
1.92–2.64	(organic sorbent: cellulose, lignin, Xing et al. 1994)
3.31, 2.91, 2.61	(RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
2.61; 3.48	(HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: average rate of biodegradation 38.4 mg COD $g^{-1} \cdot h^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

TABLE 14.1.1.20.1
Reported vapor pressures of 1-naphthol at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
94.0	133.3	141.5	1333
125.5	666.6	164.8	3333
142	1333	184.2	6666
158	2666	196.9	9999
177.8	5333	206.0	13332
190	7999	219.3	19998
206	13332	229.0	26664
229.6	26664	236.4	33330
255.8	53329	244.0	39997
282.5	101325	246.5	43330
		250.2	46663
mp/°C	96.0	255.1	53329
		260.3	59995
		264.8	66661
		265.7	73327
		272.0	79993
		275.2	86659
		278.3	93325
		282.5	101325

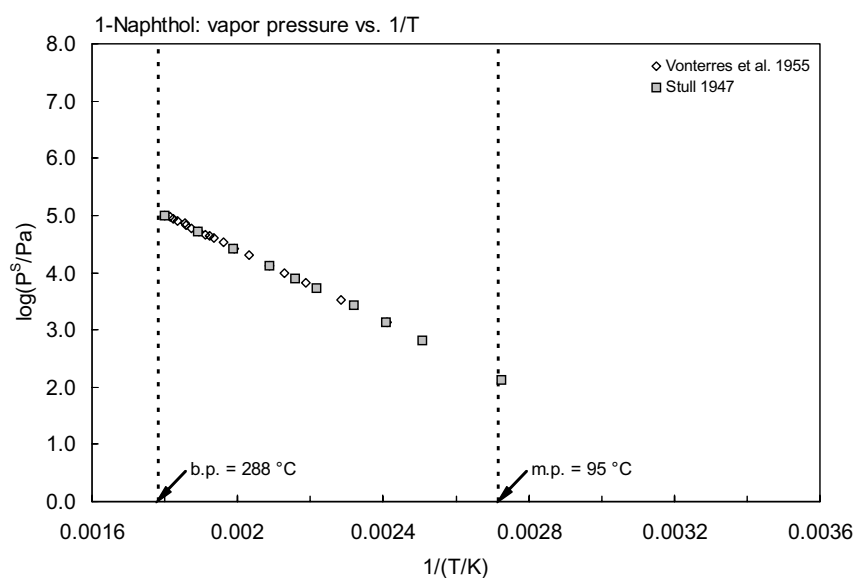
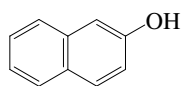


FIGURE 14.1.1.20.1 Logarithm of vapor pressure versus reciprocal temperature for 1-naphthol.

14.1.1.21 2-Naphthol



Common Name: 2-Naphthol

Synonym: β -naphthol, 2-naphthalenol, 2-hydroxynaphthalene

Chemical Name: 2-naphthol

CAS Registry No: 135-19-3

Molecular Formula: $C_{10}H_7OH$

Molecular Weight: 144.170

Melting Point ($^{\circ}C$):

121.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.280 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.57 (Dean 1985)

Molar Volume (cm^3/mol):

155.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.79 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

47.7 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$), F: 0.113 (mp at $121.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

680* ($23.20^{\circ}C$, shake flask, measured range 15.55–31.25, McCune & Wilhelm 1949)

700 (20 – $25^{\circ}C$, Seidell 1941; Lange 1973)

713* ($21.5^{\circ}C$, shake flask-UN spectrophotometry, measured range 6.9 – $75^{\circ}C$, Moyle & Tyner 1953)

754 (Tsonopoulos & Prausnitz 1971)

1000 (shake flask-UV spectrophotometry, Roberts et al. 1977)

740 (Verschuereen 1983)

477 (calculated-group contribution, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.430* (extrapolated-regression of tabulated data, temp range 128.5 – 288° , Stull 1947)

1333* ($144.0^{\circ}C$, ebulliometry, measured range 144.0 – $288.0^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 14138.5/(T/K)] + 8.391271$; temp range 128.6 – $288^{\circ}C$ (Antoine eq., Weast 1972–73)

0.386 (extrapolated-Antoine eq., supercooled liquid P_L , Boublik et al. 1984)

$\log(P/kPa) = 6.62476 - 2244.555/(198.594 + t/^{\circ}C)$, temp range 144 – $288^{\circ}C$ (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

0.160 (extrapolated-Antoine eq., supercooled liquid P_L , Dean 1985)

$\log(P/mmHg) = 7.34714 - 2135.0/(183.0 + t/^{\circ}C)$, temp range 144 – $288^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.0303 (interpolated-Antoine eq.-III, solid P_s , Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 12.48704 - 5110.333/(T/K)$, temp range 298 – $312\ K$ (Antoine eq.-I, α form, solid, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.80636 - 4586.029/(T/K)$, temp range 314 – $332\ K$ (Antoine eq.-II, β form, solid, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 9.273 - 4112/(T/K)$, temp range 283 – $323\ K$ (Antoine eq.-III, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.22927 - 2827.5/(-19.868 + T/K)$, temp range 401 – $561\ K$ (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.280 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.84 (shake flask-UV, Hansch & Anderson 1967)
 2.70, 2.84, 2.89 (Hansch & Leo 1979)
 2.01, 2.46 (HPLC- k' correlation, Eadsforth 1986)
 2.84 (recommended, Sangster 1989)
 2.85 (centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)
 2.70 (EPA CLOGP Data Base, Hulzebos et al. 1993)
 2.70 (COMPUTOX, Kaiser 1993)
 2.70 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.33 (soil, Means et al. 1982)
 3.41 (soil, calculated-MCI χ , Sabljic 1987)
 2.10–2.77 (soil, calculated- K_{OW} based on model of Karickhoff et al. 1979, Sabljic 1987)
 2.63–2.99 (soil, calculated- K_{OW} based on model of Kenaga & Goring 1980, Sabljic 1987)
 1.84–2.19 (soil, calculated- K_{OW} based on model of Briggs 1981, Sabljic 1987)
 1.99–2.66 (soil, calculated- K_{OW} based on model of Means et al. 1982, Sabljic 1987)
 1.30–1.90 (soil, calculated- K_{OW} based on model of Chiou et al. 1983, Sabljic 1987)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: average rate of biodegradation $39.2 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 14.1.1.21.1

Reported aqueous solubilities and vapor pressures of 2-naphthol at various temperatures

Aqueous solubility				Vapor pressure			
McCune & Wilhelm 1949		Moyle & Tyner 1953		Stull 1947		Vonterres et al. 1955	
shake flask		shake flask-UV spec.		summary of literature data		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
15.55	501	6.90	355	128.6	666.6	144.0	1333
16.24	526	13.45	487	145.5	1333	158.0	3333
23.20	680	17.7	561	161.8	2666	188.0	6666
31.25	928	21.5	713	181.7	5333	200.5	9999
		29.5	876	193.7	7999	210.0	13332
		33.3	985	209.8	13332	223.1	19998
log (100·C _w) = A – B/(T/K)		38.7	1304	234.0	26664	233.0	26664
C _w	g/100 mL	44.5	1609	260.6	53329	246.0	33330
A	5.8833	48.5	2001	288.0	101325	247.4	39997
B	1495.84	55.2	2460			251.0	43330
		60.0	3034	mp/°C	122.5	254.2	46663
		68.1	4222			260.2	53329
		75.0	5493			265.1	59995
						269.0	66661
						273.0	73327
						276.6	79993
						279.7	86659
						283.0	93325
						288.0	101325

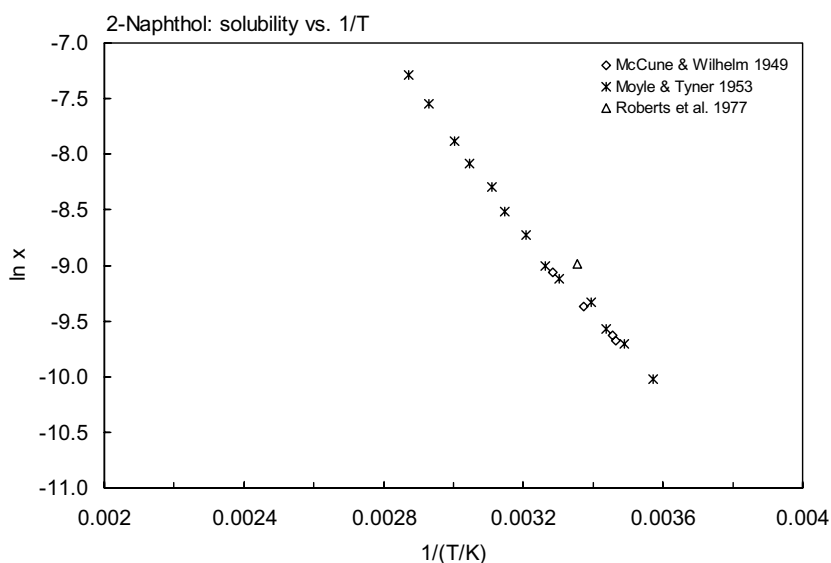


FIGURE 14.1.1.21.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-naphthol.

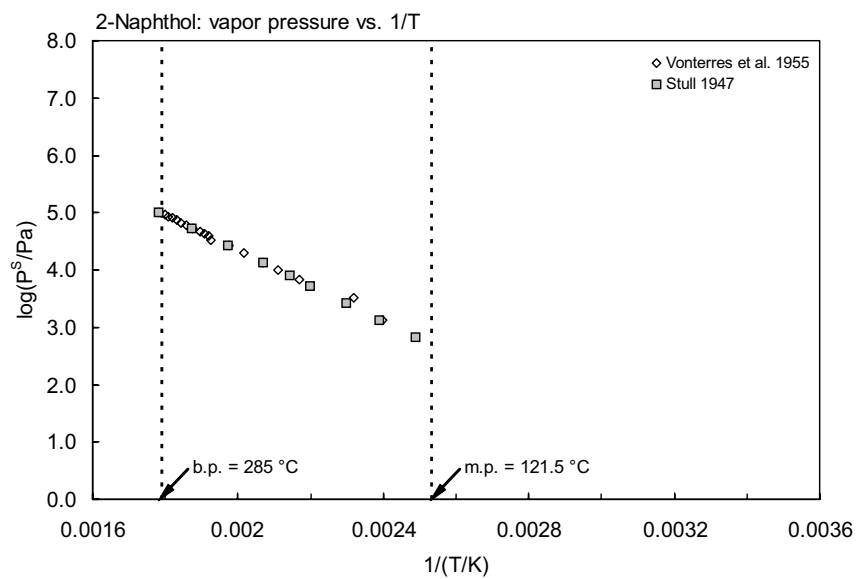
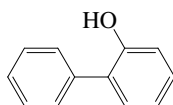


FIGURE 14.1.1.21.2 Logarithm of vapor pressure versus reciprocal temperature for 2-naphthol.

14.1.1.22 2-Phenylphenol (2-Hydroxybiphenyl)



Common Name: 2-Phenylphenol

Synonym: *o*-phenylphenol, 2-hydroxybiphenyl, [1,1'-biphenyl]-2-ol

Chemical Name: 2-phenylphenol

CAS Registry No: 90-43-7

Molecular Formula: $C_{12}H_{10}O$, $C_6H_5C_6H_4OH$

Molecular Weight: 170.206

Melting Point ($^{\circ}C$):

57.5 (Weast 1982–83)

Boiling Point ($^{\circ}C$):

286 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.213 (Dean 1985)

1.200 ($25^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

192.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

9.55 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.480 (mp at $57.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

700 (Verschueren 1983)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($100^{\circ}C$, summary of literature data, temp range 100 – $275^{\circ}C$, Stull 1947)

1333* ($161.9^{\circ}C$, ebulliometry, measured range 161.9 – $275.0^{\circ}C$, Vonterres et al. 1955)

$\log (P/mmHg) = [-0.2185 \times 15397.8/(T/K)] + 9.015370$; temp range 100 – $275^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [1 - 549.249/(T/K)] \times 10^{0.889463 - 4.72320 \times 10^{-4} \cdot (T/K) + 5.27654 \times 10^{-7} \cdot (T/K)^2}$; temp range 373.15 – $548.15 K$ (Cox eq., Chao et al. 1983)

2667, 13330 ($163^{\circ}C$, $206^{\circ}C$, Verschueren 1983)

$\log (P/kPa) = 5.50723 - 1137.035/(72.282 + t/^{\circ}C)$, temp range 161.9 – $275^{\circ}C$ (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

30.0 (interpolated-Antoine eq.-I, solid P_s , Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 10.8635 - 4326.754/(T/K)$, temp range 291 – $314 K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 4.1553 - 547.8/(-298.55 + T/K)$, temp range 434 – $547 K$ (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.09 (Hansch & Leo 1979)

3.09 (COMPUTOX, Kaiser 1993)

3.06 (HPLC-RT correlation, Ritter et al. 1994)

3.09 (recommended, Sangster 1993)

3.06 (HPLC-RT correlation, Ritter et al. 1994)

3.09 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 66\text{--}3840$ h in water, based on reported reaction rate constants for OH and RO_2 radicals to react with phenol class compounds (Mill & Mabey 1985; Guesten et al. 1981; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.1\text{--}22$ h, based on estimated reaction rate constant with OH radical (Atkinson 1987; quoted, Howard et al. 1991) and NO_3 radical in nighttime air to react with the phenol and cresol classes (Howard et al. 1991).

Hydrolysis:

Biodegradation: 100% degradation under aerobic and anaerobic conditions after 3 wk (504 h) at 22°C (Verschuereen 1983);

$t_{1/2}$ (aq. aerobic) = 24–168 h, based on a river die-away study in which a 50% degradation was observed over a one week period (Gonsior et al. 1984; quoted, Howard et al. 1991); $t_{1/2}$ (aq. anaerobic) = 96–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.1\text{--}22$ h, based on estimated reaction rate constant with OH radical (Atkinson 1987; quoted, Howard et al. 1991) and NO_3 radical in nighttime air to react with the phenol and cresol classes (Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 66\text{--}3840$ h in water, based on reported reaction rate constants for OH and RO_2 radicals to react with phenol class compounds (Mill & Mabey 1985; Güesten et al. 1981; quoted, Howard et al. 1991); $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 14.1.1.22.1
Reported vapor pressures of 2-phenylphenol at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
100	133.3	161.9	1333
131.6	666.6	168.0	3333
146.2	1333	188.1	6666
163.3	2666	198.0	9999
180.3	5333	206.8	13332
192.2	7999	219.0	19998
205.9	13332	228.1	26664
227.9	26664	235.2	33330
251.8	53329	241.6	39997
275.0	101325	244.0	43330
		247.4	46663

(Continued)

TABLE 14.1.1.22.1 (Continued)

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
mp/°C	56.6	252.0	53329
		257.0	59995
		261.0	66661
		264.0	73327
		268.0	79993
		270.0	86659
		273.8	93325
		275.0	101325
		bp/°C	278.004

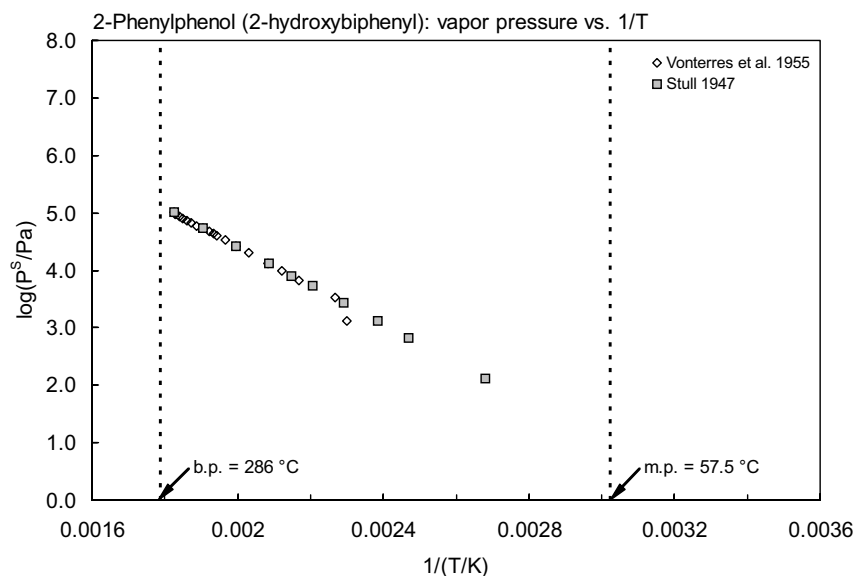
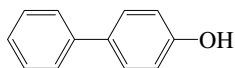


FIGURE 14.1.1.22.1 Logarithm of vapor pressure versus reciprocal temperature for 2-phenylphenol.

14.1.1.23 4-Phenylphenol (4-Hydroxybiphenyl)



Common Name: 4-Phenylphenol

Synonym: *p*-phenylphenol, 4-hydroxybiphenyl, [1,1'-biphenyl]-4-ol

Chemical Name: 4-phenylphenol

CAS Registry No: 92-69-3

Molecular Formula: $C_{12}H_{10}O$, $C_6H_5C_6H_4OH$

Molecular Weight: 170.206

Melting Point ($^{\circ}C$):

166 (Lide 2003)

Boiling Point ($^{\circ}C$):

305–308 (sublimation, Weast 1982–83; Stephenson & Malanowski 1987)

305 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

192.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

9.55 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.0414 (mp at $166^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9.79 (CESARS 1988)

56.4; 50.2 (quoted exptl.; calculated-group contribution, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1333* ($176.2^{\circ}C$, summary of literature data, temp range 176.2 – $308^{\circ}C$, Stull 1947)

1333* ($177.0^{\circ}C$, ebulliometry, measured range 177.0 – $308.0^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 16974.3/(T/K)] + 9.234838$; temp range 176.2 – $308^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [1 - 580.171/(T/K)] \times 10^{\{0.949514 - 5.554686 \times 10^{-4} \cdot (T/K) + 5.61184 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 450.15 – $581.15 K$, (Cox eq., Chao et al. 1983)

0.0278 (liquid, extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.97182 - 3214.349/(231.575 + t/^{\circ}C)$, temp range 177 – $308^{\circ}C$ (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

0.020 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 8.6575 - 3022.8/(216.1 + t/^{\circ}C)$; temp range: 177 – $308^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.00153 (extrapolated-Antoine eq., solid P_s , Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.17513 - 5066.004/(T/K)$; temp range 327 – $348 K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.41978 - 3684.9/(-5.81 + T/K)$, temp range 450 – $581 K$ (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.20 (shake flask-UV, Norrington et al. 1975)

3.63 (HPLC-RV correlation, Garst 1984)

2.88 (centrifugal partition chromatography (CPC), Terada et al. 1987)

3.20 (COMPUTOX databank, Kaiser 1993)

3.31 (HPLC-RT correlation, Ritter et al. 1994)

3.20 (recommended, Sangster 1993)

3.20 (recommended, Hansch et al. 1995)

2.60, 2.56, 2.70, 2.72 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

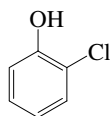
TABLE 14.1.1.23.1

Reported vapor pressures of 4-phenylphenol at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
176.2	1333	177.0	1333
193.8	2666	199.2	3333
213.0	5333	217.8	6666
225.3	7999	229.0	9999
240.9	13332	237.4	13332
263.2	26664	250.0	19998
285.5	53329	260.2	26664
308.0	101325	267.1	33330
		273.8	39997
mp/°C	164.5	276.0	43330
		278.8	46663
		283.0	53329
		287.1	59995
		291.0	66661
		294.7	73327
		297.8	79993
		300.6	86659
		303.5	93325
		308.0	101325
		bp/°C	307.194

14.1.2 CHLOROPHENOLS

14.1.2.1 2-Chlorophenol



Common Name: 2-Chlorophenol

Synonym: *o*-chlorophenol, 1-chloro-2-hydroxybenzene

Chemical Name: 2-chlorophenol

CAS Registry No: 95-57-8

Molecular Formula: $C_6H_4(OH)Cl$

Molecular Weight: 128.556

Melting Point ($^{\circ}C$):

9.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

174.9 (Dreisbach 1955; Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.2634 ($20^{\circ}C$, Weast 1982–83)

1.257 ($25^{\circ}C$, Krijgsheld & van der Gen 1986)

Acid Dissociation Constant, pK_a :

8.65 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)

8.48 (Pearce & Simkins 1968; Krijgsheld & van der Gen 1986)

8.52 (Drahonovsky & Vacek 1971)

8.29 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)

8.55 (Serjeant & Dempsey 1979)

8.30 (Hoigné & Bader 1983)

9.30 (HPLC, Miyake et al. 1987)

Molar Volume (cm^3/mol):

101.8 ($20^{\circ}C$, Stephenson & Malanowski 1987)

124.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.05, 49.25 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

13.50 (Dreisbach 1955)

10.75 (Tsonopoulos & Prausnitz 1971)

12.52 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

38.12 (Tsonopoulos & Prausnitz 1971)

44.24 (exptl., Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

25000* ($20^{\circ}C$, synthetic method, measured range -0.20 to $173.0^{\circ}C$, Sidgwick & Turner 1922)

29000 (20 – $25^{\circ}C$, Seidell 1941; Urano et al. 1982)

24650 ($20^{\circ}C$, shake flask-UV, Mully & Metcalf 1966)

22000 (shake flask-spectrophotometry, Roberts et al. 1977)

28500 ($20^{\circ}C$, Verschueren 1977, 1983)

11480 (shake flask-LSC, Banerjee et al. 1980)

11200 (shake flask-radioactive analysis, Veith et al. 1980)

20000 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

23260 (shake flask-HPLC/UV at pH 4.8, Ma et al. 1993)

28500 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

22660* (24.6°C, shake flask-conductimetry, measured range 15.4–34.5°C, Achard et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

316* (interpolated-regression of tabulated data, temp range 12.7–174.5°C, Stull 1947)

208 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/\text{mmHg}) = 7.05272 - 1589.1/(206.0 + t/^\circ\text{C})$, temp range 80–300°C (Antoine eq. for liquid state, Dreisbach 1955)

313 (extrapolated from Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 10341.1/(T/K)] + 7.952334$; temp range 12.1–174.5°C (Antoine eq., Weast 1972–73)

5532 (80°C, Verschueren 1977, 1983)

293, 180.7 (extrapolated, Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 6.87731 - 1471.61/(193.17 + t/^\circ\text{C})$; temp range 80–200°C (Antoine eq., Dean 1985, 1992)

131.8 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.78693 - 1314.9/(-101.95 + T/K)$, temp range 333–449 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.3685 - 1096.98/(-122.58 + T/K)$; temp range 354–448 K (Antoine eq.-II, Stephenson & Malanowski 1987)

737, 1329, 2278, 3736, 5907 (50, 60.24, 69.94, 79.95, 89.94°C, calculated-Antoine eq. of Stephenson & Malanowski 1987, Tabai et al. 1997)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

1.065 (calculated-P/C, Mabey et al. 1982)

0.688 (calculated-P/C, Shiu et al. 1994)

0.661 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

$k_H/\text{kPa} = 161.250 - 12658.0/(T/K) - 20.4027$; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.15 (shake flask-UV, Fujita et al. 1964;)

2.15, 2.19 (Leo et al. 1971)

2.20 (calculated using data from Fujita et al. 1964, Umeyama et al. 1971)

2.12 (20°C, shake flask, Korenman 1974)

2.15 (LC- k' correlation, Carson et al. 1975)

2.17 (Hansch & Leo 1979)

2.16 (shake flask-LSC, Banerjee et al. 1980)

0.83 (RP-HPLC-RT correlation, Veith et al. 1980)

2.11 (RP-HPLC-RT correlation, Butte et al. 1981)

2.03 (shake flask, Dearden & Bresnen 1981)

2.16 \pm 0.03 (HPLC- k' correlation, Hammers et al. 1982)

2.32 (RP-HPLC-RT correlation, Chin et al. 1986)

1.56, 1.99 (HPLC- k' correlation, Eadsforth 1986)

2.09 (HPLC-RT correlation, Miyake et al. 1986)

2.13 (shake flask-UV, Miyake et al. 1987)

2.16 (shake flask-CPC, Berthod et al. 1988)

2.24 (batch equilibration-UV, Beltrame et al. 1988)

2.11 (centrifugal partition chromatography, Gluck & Martin 1990)

2.25 (back flashing-CPC centrifugal partition chromatography; Menges et al. 1990)

2.05 (centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)

2.17 (counter-current chromatography, Berthod et al. 1992)

2.15 (recommended, Sangster 1993)

2.29 (shake flask-GC, Kishino & Kobayashi 1994)

2.15 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.33	(bluegill sunfish, Barrows et al. 1980)
2.33	(bluegill sunfish, Veith et al. 1980)
1.61	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
2.33	(bluegill sunfish, Bysshe 1982)
0.81	(gold fish, Kobayashi et al. 1979; quoted, Verschueren 1983; Howard 1989)
0.81	(Isnard & Lambert 1988)
0.28–1.40	(estimated from K_{OW} , Howard 1989)

Sorption Partition Coefficient, log K_{OC} :

3.70, 3.60	(sediment: fine, coarse; Isaacson & Frink 1984)
1.86	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)
1.71	(clay loam soil, Boyd 1982; quoted, Howard 1989)
3.69	(untreated fine sediment, Isaacson & Frink 1984)
3.60	(untreated coarse sediment, Isaacson & Frink 1984)
3.98	(treated fine sediment, Isaacson & Frink 1984)
4.36	(treated coarse sediment, Isaacson & Frink 1984)
1.20–2.55	(estimated from K_{OW} , Howard 1989)
1.82	(calculated- K_{OW} , Kollig 1993)
2.60	(soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 1.35, 1.60$ h from stirred and static water at 23.8°C (Chiou et al. 1980; Howard 1989);
 $t_{1/2} = 73$ d, based on estimation from a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1989).

Photolysis: vapor phase $t_{1/2} = 47$ h (Howard 1989);

first-order photolysis disappearance rate constant $k = 3.01 \times 10^{-2} \text{ min}^{-1}$ in the absence of DOM at 313 nm (Kawaguchi 1992).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k(aq.) < 7 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $1 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k(aq.) = 66 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, $k = (1.1 \pm 0.3) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species, $k = (0.2 \pm 0.1) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.8–4 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH} = 1.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in air (Bunce et al. 1991)

$k(aq.) = (9.2 \pm 9.4) \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991)

Hydrolysis:

Biodegradation: average rate $k = 25.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

time necessary for complete degradation of 16 mL in 14–25 d by wastewater (Haller 1978);

aerobic degradation in a non-sterile clay loam soil: 91% loss at 0°C after 8 d at the termination of the experiment, 94% loss at 4°C after 8 d and 100% loss at 20°C after 10–15 d all under same exptl. conditions (Baker et al. 1980);

rate constants $k = 1.0 \text{ d}^{-1}$ with $t_{1/2} = 0.7$ d in adopted activated sludge and $k = 0.3 \text{ d}^{-1}$ with $t_{1/2} = 2.3$ d in soil suspension under aerobic conditions (Mills et al. 1982);

completely degraded in soil suspensions in 14 d and by a soil microflora within 64 d (quoted, Verschueren 1983);

approximately 48 h in a column microcosm under aerobic conditions (Sufliata & Miller 1985);

degradation rate $k = 10^{-10} \text{ mol L}^{-1} \text{ d}^{-1}$ in freshwater and $k = 8^{-10} \text{ mol L}^{-1} \text{ d}^{-1}$ in saline water with acclimated sulfidogenic sediment cultures (Häggblom & Young 1990).

Biotransformation: rate constant for bacterial transformation of $1 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982);

microbial transformation $k = (7.1 \pm 1.6) \times 10^{-11} \text{ L organism}^{-1} \text{ h}^{-1}$ (Paris et al. 1983; quoted, Steen 1991);

degradation $k = 3.49 \times 10^{-17} (\pm 38\% \text{ SD}) \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies (Banerjee et al. 1984).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: half-life in the atmosphere was estimated to be 1.96 d (Howard 1989); tropospheric lifetime of 1 d, calculated based on reactions principally with OH radical on March 21 at 43°N (Bunce 1991).

Surface water: $t_{1/2} = 16.8$ d in sludge and $t_{1/2} = 55.2$ d in polluted river waters (Mills et al. 1982); rate constant of $(1.1 \pm 0.3) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 1.8–4.0 (Hoigné & Bader 1983b); photolysis disappearance $k = 3.01 \times 10^{-2} \text{ min}^{-1}$ in the absence of DOM at 313 nm (Kawaguchi 1992).

Groundwater:

Sediment:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 14 d in Dunkirk silt loam, 47 d in Mardin silt loam (Alexander & Aleem 1961)

$t_{1/2} = 51$ d in a coarse sandy soil, $t_{1/2} = 110$ d in sandy loam (Kjeldsen et al. 1990)

$t_{1/2} = 7.2$ d in an acidic clay soil with < 1.0% organic matter and $t_{1/2} = 1.7$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota: $t_{1/2} < 1$ d in tissue of bluegill sunfish (Barrows et al. 1980).

TABLE 14.1.2.1.1

Reported aqueous solubilities and vapor pressures of 2-chlorophenol at various temperatures

Aqueous solubility				Vapor pressure	
Sidgwick & Turner 1922		Achard et al. 1996		Stull 1947	
synthetic method		shake flask-conductimetry		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa
−0.20	15600	15.4	24007	12.1	133.3
−0.30	24400	24.6	22660	38.2	666.6
82.9	37600	34.5	24007	51.2	1333
106.3	51200			65.9	2666
159.1	135800			82.0	5333
165.8	169500			92.0	7999
170.7	225900			106.0	13332
173.0	330000			126.4	26664
172.9	450400			149.8	53329
170.1	549500			174.5	101325
166.2	607200				
156.6	706200			mp/°C	7.0
118.9	828200				
91.5	859000				
−2.0	877300				
−4.0	892500				
−5.0	896200				
−8.0	908700				
−8.2	922000				
−6.0	929200				
−1.50	967900				
2.0	983900				
7.0	1000000				
critical solution temp 173°C					

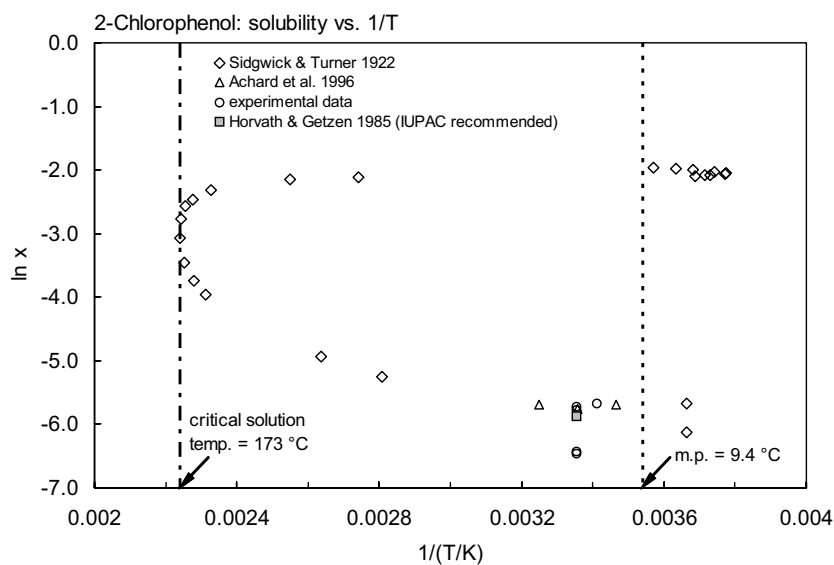


FIGURE 14.1.2.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-chlorophenol.

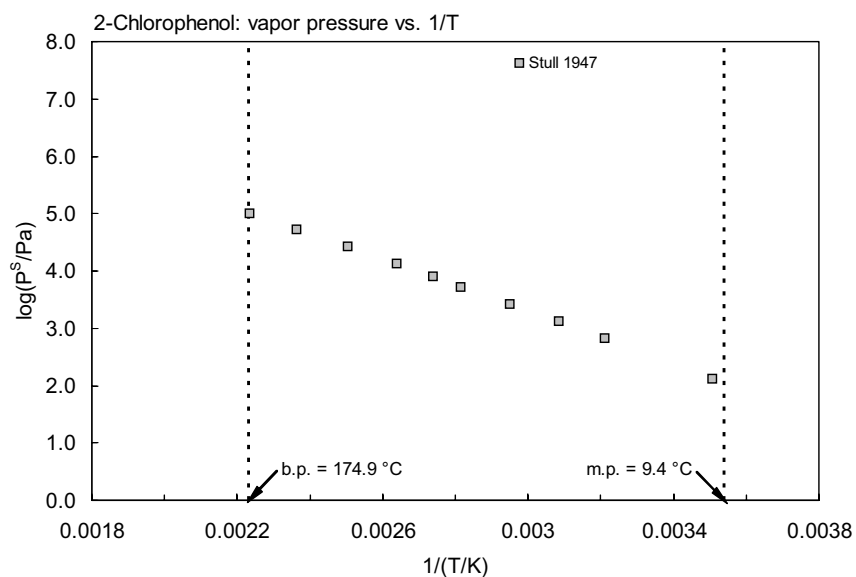
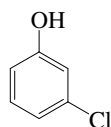


FIGURE 14.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for 2-chlorophenol.

14.1.2.2 3-Chlorophenol



Common Name: 3-Chlorophenol

Synonym: *m*-chlorophenol, 1-chloro-3-hydroxybenzene

Chemical Name: 3-chlorophenol

CAS Registry No: 108-43-0

Molecular Formula: C₆H₄ClOH

Molecular Weight: 128.556

Melting Point (°C):

32.6 (Lide 2003)

Boiling Point (°C):

214.0 (Sidgwick & Turner 1922; Stull 1947; Weast 1982–83; Lide 2003)

Density (g/cm³, 20°C):

1.268 (25°C, Weast 1982–83)

Acid Dissociation Constant, pK_a:

9.12 (Farquharson et al. 1958; Renner 1990)

8.85 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)

9.08 (Pearce & Simkins 1968)

8.78 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)

9.12 (Serjeant & Dempsey 1979; Howard 1989; Tratnyek & Hoigné 1991; Haderlein & Schwarzenbach 1993)

8.97 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Renner 1990; Ma et al. 1993)

9.10 (Dean 1985; Schultz & Cajina-Quezada 1987)

9.02 (Krijgsheld & van der Gen 1986)

9.37 (quoted from Ugland et al. 1981, Lagas 1988)

Molar Volume (cm³/mol):

103.3 (45°C, Stephenson & Malanowski 1987)

124.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.72 (Tsonopoulos & Prausnitz 1971)

14.91; 15.6 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

38.2 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol·K), F: 0.842 (mp at 9.4°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

26000* (20°C, synthetic method, measured range –0.20 to 130.8°C, Sidgwick & Turner 1922)

26000 (20–25°C, Seidell 1941; Urano et al. 1982; Shigeoka et al. 1988)

22420 (20°C, Mulley & Metcalf 1966)

22000 (recommended, Horvath & Getzen 1985)

22190 (shake flask-HPLC/UV at pH 4.6, Ma et al. 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

41.90* (extrapolated-regression of tabulated data, temp range 44.2–214°C, Stull 1947)

41.40 (extrapolated-Antoine eq., liquid value, Weast 1972–73)

log (P/mmHg) = [–0.2185 × 11979.7/(T/K)] + 8.276287; temp range 44.2–214°C (Antoine eq., Weast 1972–73)

667.0 (72°C, Verschueren 1983)

1.034 (extrapolated-Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 7.61412 - 3178.132/(T/\text{K})$, temp range 252–293 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

33.40 (extrapolated-Antoine eq., supercooled liquid P_L , Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.54908 - 1978.86/(-51.572 + T/\text{K})$, temp range 317–487 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$):

0.0567 (calculated, Hine & Mookerjee 1975)

0.2045 (calculated-P/C, Shiu et al. 1994)

$k_H/\text{kPa} = 22.0921 - 6444.46/(T/\text{K})$; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.50 (shake flask-UV, Fujita et al. 1964)

2.55 (calculated using data from Fujita et al. 1964, Umeyama et al. 1971)

2.52 (shake flask-UV, Korenman 1974)

2.17, 2.29 (calculated- π const., calculated-fragment const., Rekker 1977)

2.50 (Hansch & Leo 1979)

2.33 (HPLC- k' correlation, Butte et al. 1981, Butte et al. 1987)

2.44 (Dearden & Bresnen 1981)

2.36 (HPLC- k' correlation, Hammers et al. 1982)

2.55 (RP-HPLC- k' correlation, Miyake & Terada 1982)

1.87, 2.29 (HPLC- k' correlation, Eadsforth 1986)

2.36 (HPLC-RT correlation, Miyake et al. 1986)

2.55 (batch equilibration-UV, Beltrame et al. 1988)

2.50 (RP-HPLC-capacity ratio correlation, Minick et al. 1988)

2.48 (RP-HPLC, Shigeoka et al. 1988)

2.43; 2.63 (shake flask, HPLC-RT correlation, Wang et al. 1989)

2.50 (recommended, Sangster 1993)

2.64 (shake flask-GC, Kishino & Kobayashi 1994)

2.50; 2.57 (HPLC-RT correlation, electrometric titration, Slater et al. 1994)

2.50 (recommended, Hansch et al. 1995)

2.60 (solid-phase microextraction, Dean et al. 1996)

Bioconcentration Factor, $\log \text{BCF}$:

1.30 (Golden ide, Freitag et al. 1985)

1.25 (zebrafish, Butte et al. 1987)

0.845, 1.23 (earthworms *e. fetida andrei*: Kooyenberg soil, Holten soil, van Gestel & Ma 1988)

2.01, 2.09 (earthworms *I. rubellus*: Kooyenberg soil, Holten soil, van Gestel & Ma 1988)

1.17–2.55 (estimated from K_{OW} , Howard 1989)

1.00, 1.32, 2.17, 2.18 (earthworm system, from literature, Connell & Markwell 1990)

1.10, 1.40, 10.1, 16.3 (earthworm system, derived data, Connell & Markwell 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.20–2.74 (estimated from K_{OW} , Howard 1989)

2.54 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 73$ d for evaporation from a model river of 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: vapor phase $t_{1/2} = 1.96$ d (Howard 1989);

measured pseudo-first-order reaction $k = 0.048 \pm 0.001 \text{ min}^{-1}$ for direct photolysis in aqueous solutions (Peijnenburg et al. 1992).

Oxidation: rate constant $k = (5.4 \pm 1.0) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991).

Hydrolysis: will not be an important degradation process (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);

completely degraded in soil suspensions within 72 d and by a soil microflora within 64 d (quoted, Verschuieren 1983);

time necessary for complete degradation of 16 mg/L in 14–25 d by wastewater (Haller 1978); degradation rate of $15 \text{ -mol L}^{-1} \text{ d}^{-1}$ in freshwater and $18 \text{ }\mu\text{mol L}^{-1} \text{ d}^{-1}$ in saline water with acclimated sulfidogenic sediment cultures (Hägglom & Young 1990).

Biotransformation: degradation rate of $4.32 \times 10^{-17} (\pm 47\% \text{ SD}) \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: vapor phase half-life was estimated to be 1.96 d (Howard 1989).

Surface water: $t_{1/2} = (14.5 \pm 0.3) \text{ min}$ for direct photolysis in aqueous solutions (Peijnenburg et al. 1992).

Ground water:

Sediment: half-life was approximately 30 d in sediment from a farm stream at 20°C (Howard 1989).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 + d in Dunkirk silt loam, 47 + d in Mardin silt loam (Alexander & Aleem 1961)

disappearance $t_{1/2} = 2.5 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 5.4 \text{ d}$ from Holten soil with earthworms *e. fetida andrei* and $t_{1/2} = 2.6 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 2.1 \text{ d}$ from Holten soil with earthworms *I. rubellus* (van Gestel & Ma 1988);

$t_{1/2} = 15.1 \text{ d}$ in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 21.8 \text{ d}$ in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.2.2.1

Reported aqueous solubilities and vapor pressures of 3-chlorophenol at various temperatures

Aqueous solubility				Vapor pressure	
Sidgwick & Turner 1922				Stull 1947	
synthetic method				summary of literature data	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa
−0.18	7300	3.2	844700	44.2	133.3
1.20	12500	−0.90	−*	72.0	666.6
2.5	18500	4.5	871900	86.1	1333
82.25	51200	−4.8	886600*	101.7	2666
118.0	111300	−8.2	901100*	118.0	5333
123.0	135600	−13.2	917300*	129.4	7999
127.5	178400	10.8	922300	143.0	13332
130.8	320200	−17.0	−*	164.8	26664
130.7	388900	17.0	951000	188.7	53329
130.5	461200	22.2	971100	214.0	101325
129.1	536500	32.5	1000000		
109.8	712300			mp/ $^\circ\text{C}$	32.5
23.1	823000	critical solution temp 130.8°C			
11.8	829000	*metastable point			

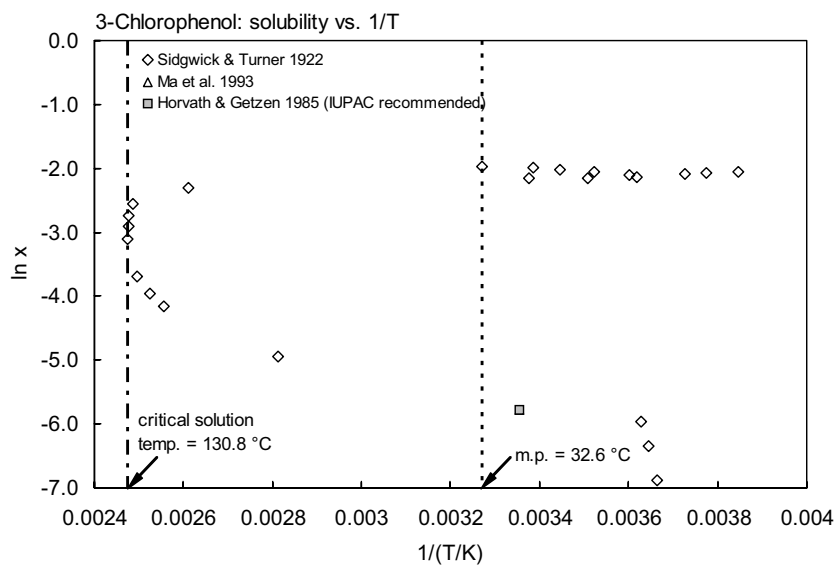


FIGURE 14.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-chlorophenol.

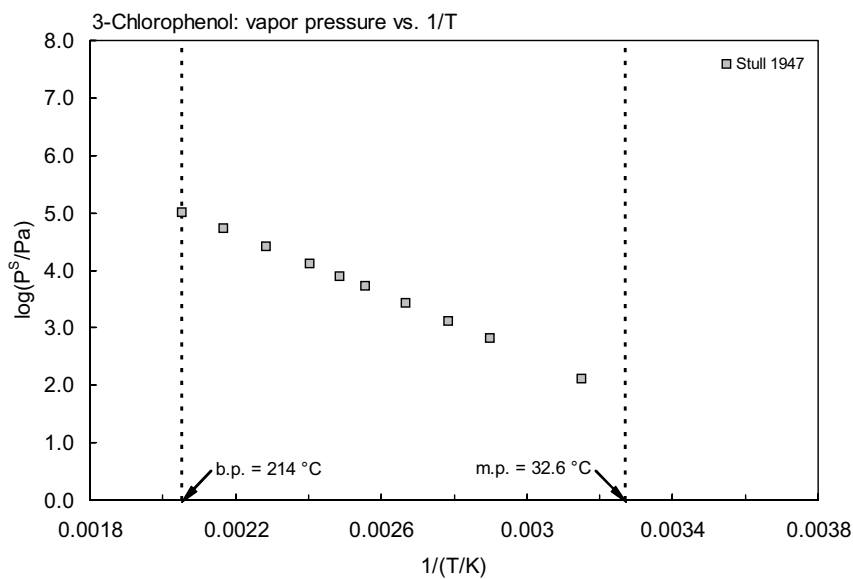
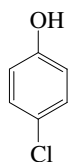


FIGURE 14.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 3-chlorophenol.

14.1.2.3 4-Chlorophenol



Common Name: 4-chlorophenol

Synonym: *p*-chlorophenol, 1-chloro-4-hydroxybenzene

Chemical Name: 4-chlorophenol

CAS Registry No: 106-48-9

Molecular Formula: $\text{ClC}_6\text{H}_4\text{OH}$

Molecular Weight: 128.556

Melting Point ($^{\circ}\text{C}$):

42.8 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

220 (Lide 2003)

Density (g/cm^3 at 20°C):

1.2651 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.37 (Farquharson et al. 1958; Ugland et al. 1981; Saarikoski & Viluksela 1982; Renner 1990)

9.18 (Doedens 1967)

9.42 (Pearce & Simkins 1968)

9.14 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988; Argese et al. 1999)

9.41 (Serjeant & Dempsey 1979)

9.38 (Paris et al. 1982; Krijgsheld & van der Gen 1986)

9.20 (Hoigné & Bader 1983)

9.43 (Dean 1985; Schultz & Cajina-Quezada 1987)

9.37 ± 0.01 (potentiometric partition, Hersey et al. 1989)

9.57 ± 0.01 (UV with pH profile, Hersey et al. 1989)

Molar Volume (cm^3/mol):

101.6 (40°C , Stephenson & Malanowski 1987)

124.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.69 (Tsonopoulos & Prausnitz 1971)

14.07; 16.2 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

46.44 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F : 0.669 (mp at 42.8°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

27000* (20°C , synthetic method, measured range -0.20 to 128.7°C , Sidgwick & Turner 1922)

27000 (20 – 25°C , Seidell 1941; Urano et al. 1982)

27000 (shake flask-UV at pH 5.1, Blackman et al. 1955)

26250 (20°C , shake flask-UV, Mulley & Metcalf 1966)

24000 (shake flask-spectrophotometry, Roberts et al. 1977)

27000 (recommended, Horvath & Getzen 1985)

26390 (shake flask-HPLC/UV at pH 4.6, Ma et al. 1993)

25540* (25.2°C , shake flask-conductimetry, measured range 15.1 – 34.5°C , Achard et al. 1996)

20712* (11.05°C , shake flask-optical method, measured range 282.2 – 386.1 K , Jaoui et al. 1999)

25519* (24.85°C , shake flask-optical method, measured range 298 – 341.9 K , Jaoui et al. 2002)

$\ln [\text{S}/(\text{mol kg}^{-1})] = 5.6451 - 716.81/(T/\text{K})$; temp range 282 – 342 K (eq. derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 28.6* (extrapolated-regression of tabulated data, temp range 49.8–220°C, Stull 1947)
- 28.0 (extrapolated-Antoine eq., liquid value, Weast 1972–73)
- $\log (P/\text{mmHg}) = [-0.2185 \times 12281.6/(T/K)] + 8.331937$; temp range 49.8–220°C (Antoine eq., Weast 1972–73)
- 13.3, 33.3 (20°C, 30°C, Verschueren 1977, 1983)
- 3.47 (extrapolated liquid value, Antoine eq., Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 8.83238 - 1385.1/(-131.1 + T/K)$, temp range 373–493 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):

- 0.0567 (calculated, Hine & Mookerjee 1975; Howard 1989)
- 0.0471 (calculated-P/C, Leuenberger et al. 1985)
- 0.0952 (calculated-P/C, Shiu et al. 1994)
- $k_H/\text{kPa} = 2017.07 - 110385.0/(T/K) - 290.078$; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.39 (shake flask-UV, Fujita et al. 1964)
- 2.53 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
- 2.37 (HPLC-RT correlation, Carlson et al. 1975)
- 2.40 (HPLC-RT correlation, Mirrlees et al. 1976)
- 2.17, 2.29 (calculated- π const., calculated-fragment const., Rekker 1977)
- 2.35, 2.39, 2.44, 2.40 (lit. values, Hansch & Leo 1979)
- 2.51 (calculated- π const. or fragment const., McLeese et al. 1979)
- 2.55 (20°C, shake flask-UV, Rogers & Wong 1980)
- 2.35 (HPLC- k' correlation, Hammers et al. 1982)
- 2.51 (RP-HPLC- k' , correlation Miyake & Terada 1982)
- 2.46 ± 0.06 (HPLC-RV correlation.-ALPM, Garst & Wilson 1984)
- 2.88 (CPC-RV, Terada et al. 1987)
- 2.43 (batch equilibration-UV, Beltrame et al. 1988, Beltrame et al. 1989)
- 2.39 (RP-HPLC-capacity ratio, Minick et al. 1988)
- 2.41 (shake flask, Shigeoka et al. 1988)
- 2.42; 2.46; 2.34, 2.45 (filter chamber-UV; potentiometric partition; Hersey et al. 1989)
- 2.52; 2.59 (shake flask; HPLC-RT correlation, Wang et al. 1989)
- 2.39 (recommended, Sangster 1993)
- 2.63 (shake flask-GC, Kishino & Kobayashi 1994)
- 2.41; 2.45 (HPLC-RT correlation, electrometric titration, Slater et al. 1994)
- 2.39 (recommended, Hansch et al. 1995)
- 1.82, 1.83, 2.01, 1.98 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, $\log BCF$:

- 1.18 (goldfish, Kobayashi et al. 1979)
- 0.30–1.59 (estimated from K_{OW} , Howard 1989)
- 1.05–1.50 (estimated, NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.85 (clay loam soil, Boyd 1982; Howard 1989)
- 1.20–2.68 (estimated from K_{OW} , Howard 1989)
- 2.377, 2.686, 2.025, 2.222, 2.332 (soils, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 2.142, 1.966, 1.966, 2.289, 1.952 (soils, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: half-lives of 12.8 h, 17.4 h for evaporation from stirred and static water at a depth of 0.38 cm at 23.6°C (Chiou et al. 1980; Howard 1989); $t_{1/2} = 73$ d was estimated for evaporation from a river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1989).

Photolysis:

photo-transformation rate constants: $k = 0.011 \text{ h}^{-1}$ with $t_{1/2} = 63$ h for distilled water in summer (mean temp 25°C) and $k = 0.007 \text{ h}^{-1}$ with $t_{1/2} = 99$ h in winter (mean temp 14°C); $k = 0.03 \text{ h}^{-1}$ with $t_{1/2} = 28$ h for estuarine water in summer and $k = 0.011 \text{ h}^{-1}$ with $t_{1/2} = 63$ h in winter exposed to full sunlight and microbes (Hwang et al. 1986)

photo-mineralization rate constants: $k = 0.012 \text{ h}^{-1}$ with $t_{1/2} = 58$ d for distilled water in summer and $k = 0.003 \text{ h}^{-1}$ with $t_{1/2} = 224$ d in winter; $k = 0.07 \text{ h}^{-1}$ with $t_{1/2} = 10$ d in summer and $k = 0.007 \text{ h}^{-1}$ with $t_{1/2} = 95$ d in winter for surface estuarine water exposed to full sunlight and microbes (Hwang et al. 1986);

photo-degradation $k = 564 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 1.1$ min for direct UV radiation in aqueous solutions (Benitez et al. 2000).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k(\text{aq.}) = (600 \pm 100) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM PrOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983a)

$k(\text{aq.}) = 34 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, and $k = (600 \pm 100) \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species, $k = (0.6 \pm 0.2) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.5–6 and 20–23°C (Hoigné & Bader 1983b)

$k(\text{aq.}) = (6.0 \pm 3.6) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991)

72.1 mg/L total organic carbon (TOC) degraded to 98% TOC after 5 h illumination with 250 watt tungsten lamp by the photo-Fenton reaction (Ruppert et al. 1993)

$k = 1877 \times 10^3 \text{ min}^{-1}$ with a half-life of 0.4 min for reaction with Fenton's reagent; $k_{\text{O}_3} = 17 \times 10^3 \text{ min}^{-1}$ with a half-life of 38.15 min at pH 2; and $k_{\text{O}_3} = 239 \times 10^3 \text{ min}^{-1}$ with a half-life of 3.4 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000)

Hydrolysis:

Biodegradation: 95% degradation in 3–6 d in a mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $11.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

time necessary for complete degradation of 16 mg/L in 7–14 d by wastewater and in 14–25 d by soil (Haller 1978);

$t_{1/2} = 475$ h in river waters with a calculated first-order $k = 0.035 \text{ d}^{-1}$ (Lee & Ryan 1979; quoted, Battersby 1990); aerobic degradation in a non-sterile clay-loam soil: 77% loss at 0°C at the termination of the experiment after 14 d, 84% loss at 4°C after 12 d and 100% loss at 20°C after 30 d all under same experimental conditions (Baker et al. 1980);

$t_{1/2} = 216$ –480 h and 72–1080 h for 75% degradation in mineral medium and seawater (de Kreuk & Hanstveit 1981);

biodegradation first order rate constant $k = 0.23 \text{ d}^{-1}$ in aquatic systems (Scow 1982);

completely degraded in soil suspensions in 9 d and by a soil microflora in 16 d (quoted, Verschueren 1983);

microbial degradation is the primary transformation process; transformation $k = 0.06 \text{ h}^{-1}$ with $t_{1/2} = 11$ h for estuarine water in summer and $t_{1/2} = 0.006 \text{ h}^{-1}$ with $t_{1/2} = 116$ h in winter in the darkness (Hwang et al. 1986) mineralization $k = 0.293 \text{ h}^{-1}$ with $t_{1/2} = 2$ d for estuarine water in summer and $k = 0.003 \text{ h}^{-1}$ with $t_{1/2} = 231$ d in winter in the darkness (Hwang et al. 1986); degradation rate constants $k = 0.035 \text{ d}^{-1}$ with $t_{1/2} = 480$ d in Skidway River water and 0.23 d^{-1} with a half-life of 72 h in Skidway River water-sediment slurry (Pritchard 1987); degradation rate constant of $37 \mu\text{mol L}^{-1} \text{ d}^{-1}$ in freshwater and $22 \mu\text{mol L}^{-1} \text{ d}^{-1}$ in saline water with acclimated sulfidogenic sediment cultures (Häggblom & Young 1990);

average transformation rate of $53 \mu\text{mol L}^{-1} \text{ d}^{-1}$ at 31°C for anaerobic degradation in freshwater sediments with an average adaptation time of 37 d (Zhang & Wiegel 1990);

70% degradation within 1–2 d in soil and completely degraded within 15 d in river water (NCASI 1992)

Degradation constant $k = 8.5 \mu\text{M/h}$ for aerobic dechlorination in shake flask experiments;; $k = 10 \mu\text{M/h}$ in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999).

Biotransformation: microbial transformation rate constant of $(1.7 \pm 0.9) \times 10^{-12}$ L organism⁻¹ h⁻¹ (Paris et al. 1982); microbial transformation rate constant of $(4.7 \pm 1.6 \times 10^{-11}$ L organism⁻¹ h⁻¹ to $(9.0 \pm 1.7) \times 10^{-11}$ L organism⁻¹ h⁻¹ in pond and river samples at five different sites (Paris et al. 1983); degradation rate $k = 5.44 \times 10^{-17}$ ($\pm 32\%$ SD) mol cell⁻¹ h⁻¹ from pure culture studies and 0.3×10^{-12} mol cell⁻¹ h⁻¹ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 1.96$ d in the atmosphere (Howard 1989)

Surface water: $t_{1/2} = 475$ h for biodegradation in river waters with a calculated first-order rate constant of 0.035 d⁻¹ (Lee & Ryan 1979; quoted, Battersby 1990);

$t_{1/2} = 216$ –624 h and 72–1080 h for 75% degradation in mineral medium and seawater, respectively (de Kreuk & Hanstveit 1981);

rate constant $k = 600 \pm 100$ M⁻¹ s⁻¹ for the reaction with ozone at pH 1.5–6.0 (Hoigné & Bader 1983);

$t_{1/2} = 63$ h in summer at season temp., 25°C, $t_{1/2} = 99$ h in winter at season temp., 14°C in distilled water and 28 h in summer, $t_{1/2} = 63$ h in winter in estuary surface water, based on photo-transformation rate (Hwang et al. 1986);

$t_{1/2} = 58$ d in summer, $t_{1/2} = 224$ d in winter in distilled water; and $t_{1/2} = 10$ d in summer, $t_{1/2} = 95$ d in winter in surface estuarine water, based on photo-mineralization rate (Hwang et al. 1986);

$t_{1/2} = 216$ h at 21°C in Skidway River water (Pritchard 1987);

$t_{1/2} = 20$ d in water (Howard 1989);

at a concentration of 1 mg/L, 4-CP was degraded completely within 15 d in river waters (NCASI 1992);

photo-oxidation $t_{1/2} = 0.4$ min for reaction with Fenton's reagent; $t_{1/2} = 38.15$ min at pH 2, and $t_{1/2} = 3.4$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water:

Sediment: $t_{1/2} = 72$ h at 22°C in Skidway River water-sediment slurry (Pritchard 1987);

$t_{1/2} = 3$ d in sediment and seawater (Howard 1989).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 9 d in Dunkirk silt loam, 3 d in Mardin silt loam (Alexander & Aleem 1961)

$t_{1/2} = 2.5$ d in an acidic clay soil with < 1.0% organic matter and $t_{1/2} = 1.0$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992);

70% degradation with 1 to 2 d (NCASI 1992).

Biota:

TABLE 14.1.2.3.1

Reported aqueous solubilities of 4-chlorophenol at various temperatures

Sidgwick & Turner 1922		Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002	
synthetic method		shake flask-conductivity		shake flask-optical method		shake flask-optical method*	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	S/g·m ⁻³
–0.20	20700	15.1	23337	282.2	17856.	298.0	25519
65.0	39100	25.2	25540	284.2	20712	305.2	27010
113.8	106600	34.6	28499	308.3	27855	315.3	29389
125.0	205000			311.2	29283	319.7	30057
128.2	291600			324.2	32140	323.8	30919
128.7	425700			341.9	35711	332.7	32809
125.8	534900			354.7	41425	341.2	34608
122.4	596200			359.9	44282	298.0	25519
115.5	650500			362.7	48567	305.2	27010
107.7	693600			364.4	52852	315.3	29132
97.0	740300			365.7	54261	332.7	32809

(Continued)

TABLE 14.1.2.3.1 (Continued)

Sidgwick & Turner 1922		Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002	
synthetic method		shake flask-conductivity		shake flask-optical method		shake flask-optical method*	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	S/g·m ⁻³
35.5	840200			366.7	57852	339.5	34248
17.0	854200			386.1	117132	298.3	25583
5.5	861900					309.3	27872
0.5	889200					315.8	29235
6.2	924800					324.8	31124
11.0	944800					329.0	32024
14.2	957000					341.9	34763
18.0	968200						
19.5	972900						
41.0	1000000						
critical solution temp 129°C							
triple point −0.30°							

*some data from Achard et al.
1996, Jaoui et al. 1999

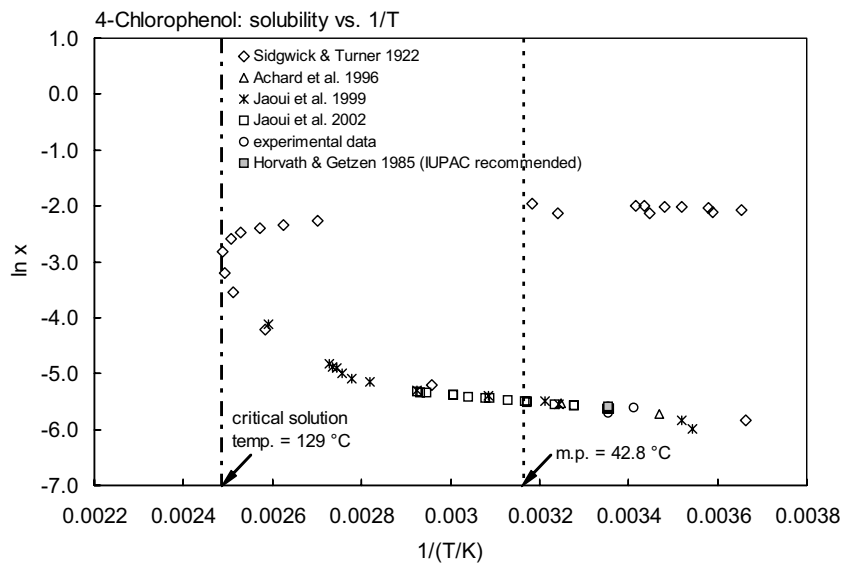


FIGURE 14.1.2.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-chlorophenol.

TABLE 14.1.2.3.2
Reported vapor pressures of 4-chlorophenol at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
49.8	133.3
78.2	666.6
92.2	1333
108.1	2666
125.0	5333
136.1	7999
150.0	13332
172.0	26664
196.0	53329
220.0	101325
mp/°C	42.0

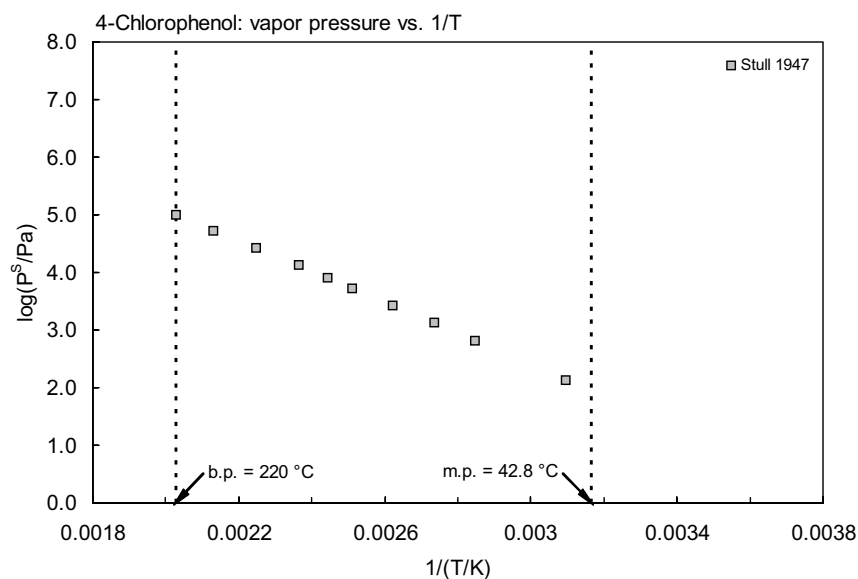
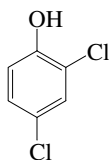


FIGURE 14.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-chlorophenol.

14.1.2.4 2,4-Dichlorophenol



Common Name: 2,4-Dichlorophenol

Synonym: 2,4-DCP

Chemical Name: 2,4-dichlorophenol

CAS Registry No: 120-83-2

Molecular Formula: $C_6H_4Cl_2O$, $C_6H_3Cl_2OH$

Molecular Weight: 163.001

Melting Point ($^{\circ}C$):

45.0 (Stull 1947; Verschuereen 1977, 1983; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

210.0 (Stull 1947; Verschuereen 1977, 1983; Weast 1982–83; Lide 2003)

Density (g/cm^3):1.383 (at 60/ $25^{\circ}C$, Verschuereen 1983)Acid Dissociation Constant, pK_a :

7.80 (Blackman et al. 1955; Hoigné & Bader 1983; Scully & Hoigné 1987)

7.85 (Farquharson et al. 1958; Pearce & Simkins 1968)

7.68 (Doedens 1967)

7.89 (Sillén & Martell 1971; Serjeant & Dempsey)

8.01, 8.04, 8.09 (measured values, Xie & Dyrssen 1984)

8.09 (Shigeoka et al. 1988)

Molar Volume (cm^3/mol):

145.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.09; 16.7 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.636 (mp at $45^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4500 (gravimetric, Mosso 1887)

6194 (shake flask-UV at pH 5.1, Blackman et al. 1955)

5000 (shake flask-spectrophotometry, Roberts et al. 1977)

2650 (shake flask-GC, Jones et al. 1977/1978)

4600 ($20^{\circ}C$, Verschuereen 1977, 1983)

5547 (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)

4600 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

5517* ($25.2^{\circ}C$, shake flask-conductimetry, measured range 15.3 – $35.1^{\circ}C$, Achard et al. 1996)6339* ($37.35^{\circ}C$, shake flask-optical method, measured range 310.5 – $423.2 K$, Jaoui et al. 1999)

4980 (shake flask-HPLC/UV, pH 4.98, Huang et al. 2000)

4841* ($21.45^{\circ}C$, shake flask-optical method, measured range 296.4 – $337.7 K$, Jaoui et al. 2002)

$\ln [S/(mol kg^{-1})] = 11.846 - 3025.1/(T/K)$; temp range 288 – $298 K$ (eq.-I derived using reported exptl. data, Jaoui et al. 2002)

$\ln [S/(mol kg^{-1})] = 5.0497 - 981.37/(T/K)$; temp range 298 – $347 K$ (eq.-II derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 20.6* (extrapolated-regression of tabulated data, temp range 53–210°C, Stull 1947)
- 11.9 (extrapolated-Antoine eq., Weast 1972–73)
- $\log(P/\text{mmHg}) = [-0.2185 \times 13230.4/(T/K)] + 8.884810$; temp range 53–210°C (Antoine eq., Weast 1972–73)
- 18.0 (supercooled liquid value, GC-RT correlation, Hamilton 1980)
- 15.4 (capillary GC-RT, Bidleman & Renberg 1985)
- 2.40, 11.87 (8°C, 25°C, extrapolated, Leuenberger et al. 1985)
- $\log(P_L/\text{kPa}) = 6.75941 - 1945.1/(-73.987 + T/K)$; temp range 326–483 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.32554 - 1807.32/(-69.17 + T/K)$; temp range 391–474 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 0.284 (calculated-P/C, Mabey et al. 1982)
- 0.110 (8°C, calculated-P/C, Leuenberger et al. 1985)
- 0.435 (calculated-P/C, Shiu et al. 1994)
- $k_H/\text{kPa} = 24.9070 - 6791.07/(T/K)$; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)
- 0.292 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.08 (Leo et al. 1971)
- 3.06 (shake flask-UV, Stockdale & Selwyn 1971)
- 3.06, 3.08 (Hansch & Leo 1979)
- 2.92 (HPLC- k' correlation, Hammers et al. 1982)
- 3.14 (RP-HPLC- k' correlation, Miyake & Terada 1982)
- 3.41 (shake flask-UV, Beltrame et al. 1984)
- 3.23 (shake flask-HPLC/UV, Schellenberg et al. 1984)
- 3.20, 3.17, 3.17 (20°C, shake flask-GC-calculated-regression, Xie & Dyrssen 1984)
- 3.21, 3.23 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)
- 3.23 (OECD 1981 guidelines, Leuenberger et al. 1985)
- 2.87 (RP-HPLC-RT correlation, Chin et al. 1986)
- 2.97 (HPLC-RT correlation, Miyake et al. 1986)
- 3.61 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
- 3.21 (shake flask, Shigeoka et al. 1988; quoted, Saito et al. 1993)
- 3.16 (shake flask/batch equilibrium-UV, Beltrame et al. 1988)
- 3.06 (EPA CLOGP Data Base, Hulzebos et al. 1993)
- 3.17 (recommended, Sangster 1993)
- 3.07 (calculated-QSAR, Kollig 1993)
- 3.20 (shake flask-GC, Kishino & Kobayashi 1994)
- 3.06 (recommended, Hansch et al. 1995)
- 3.34 (solid-phase microextraction; Dean et al. 1996)

Bioconcentration Factor, $\log BCF$:

- 1.53 (goldfish, Kobayashi 1979)
- 1.00 (trout, Hattula et al. 1981)
- 2.27 (microorganism-water, calculated- K_{OW} , Mabey et al. 1982)
- 2.00 (golden ide, after 3 d, Freitag et al. 1985)
- 2.42 (algae, after 1 d, Freitag et al. 1985)
- 2.53 (activated sludge, after 5 d, Freitag et al. 1985)
- 1.00 (quoted, brown trout, Walden et al. 1986)
- 1.80 (correlated, Isnard & Lambert 1988)
- 1.41–1.65 (estimated, NCASI 1992)

Sorption Partition Coefficient, log K_{OC} :

- 2.59 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 2.59–3.02 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
 2.89–3.12 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
 2.10–2.32 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
 2.48–2.91 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
 1.74–2.13 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
 3.60, 3.50 (untreated fine and coarse sediment, Isaacson & Frink 1984)
 3.71, 3.98 (treated fine and coarse sediment, Isaacson & Frink 1984)
 2.75 (sediment, Schenllenberg et al. 1984; quoted, Sabljic 1987a,b)
 2.76 (soil, calculated-MCI χ , Sabljic 1987a,b)
 2.49 (calculated- K_{OW} , Kollig 1993)
 2.75 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.47, 2.53 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 2.609, 2.654, 2.460, 2.346, 2.540 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
 2.49, 2.57, 2.77, 2.33 (soils: organic carbon OC -0.1% and pH 2.0–7.4, OC -0.1% and pH \leq 5.8, OC -0.5%, $0.1 \leq$ OC < 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

photolysis:

$k_p = 0.82 \text{ h}^{-1}$ with $t_{1/2} = 0.8 \text{ h}$ for distilled water in summer at mean temp. 25°C , and $k_p = 0.21 \text{ h}^{-1}$ with $t_{1/2} = 3 \text{ h}$ in winter at mean temp. 11°C ; $k_p = 1.16 \text{ h}^{-1}$ with $t_{1/2} = 0.6 \text{ h}$ for estuarine water in summer and $k_p = 0.44 \text{ h}^{-1}$ with $t_{1/2} = 2 \text{ h}$ in winter; $k_p = 1.0 \text{ h}^{-1}$ with $t_{1/2} = 0.7 \text{ h}$ in summer and $k_p = 0.38 \text{ h}^{-1}$ with $t_{1/2} = 2 \text{ h}$ in winter for poisoned estuarine water when exposed to full sunlight and microbes (photo-transformation, Hwang et al. 1986)

$k_p = 0.09 \text{ h}^{-1}$ with $t_{1/2} = 8 \text{ d}$ in summer and $k_p = 0.049 \text{ h}^{-1}$ with $t_{1/2} = 14 \text{ d}$ in winter for distilled water; $k_p = 0.20 \text{ h}^{-1}$ with $t_{1/2} = 4 \text{ d}$ in summer and $k_p = 0.04 \text{ h}^{-1}$ with $t_{1/2} = 17 \text{ d}$ in winter for estuarine water; $k_p = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 6 \text{ d}$ in summer and $k_p = 0.05 \text{ h}^{-1}$ with $t_{1/2} = 14 \text{ d}$ in winter for poisoned estuarine water when exposed to full sunlight and microbes (photo-mineralization rate, Hwang et al. 1986)

photochemical-transformation $t_{1/2} = 2.5$ – 2.6 h in Xenotest 1200 (Svenson & Björndal 1988)

atmospheric and aqueous photolysis $t_{1/2} = 0.8$ – 3 h based on measured rate of photolysis in distilled water under sunlight in summer and winter (Howard et al. 1991)

$k_p = 38 \times 10^3 \text{ min}^{-1}$ with a $t_{1/2} = 17.5 \text{ min}$ for direct UV radiation aqueous solutions (Benitez et al. 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k < 7 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, and $1 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k = 5 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, $k < 1.5 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species, $k = (8 \pm 4) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.3–1.5 and 20 – 23°C (Hoigné & Bader 1983b)

$k = 7 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ at pH 5.5, $k = 2 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 6.0, $k = 10 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 6.6, $k = 15 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.0, $k = 76 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.9, $k = 120 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 9.0 and pH 9.6 for the reaction with singlet oxygen in water at $19 \pm 2^\circ\text{C}$ (Scully & Hoigné 1987)

$k_{OH} = 1.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{OH} = 3.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Bunce et al. 1991)

$k = (5.1 \pm 4.7) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991)

$k_{OH}(\text{calc}) = 1.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital estimation method, Klamt 1993)

$k = 209 \times 10^3 \text{ min}^{-1}$ with a half-life of 2.4 min for reaction with Fenton's reagent; and $k = 24 \times 10^3 \text{ min}^{-1}$ with a half-life of 30.4 min at pH 2, and $k = 315 \times 10^3 \text{ min}^{-1}$ with a half-life of 3.3 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: 7 to 10 d for bacteria to utilize 95% of 200 ppm in parent substrate (Tabak et al. 1964);

aqueous aerobic $t_{1/2} = 66.7\text{--}199$ h, based on aerobic lake die-away test data (Aly & Faust 1964; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 324\text{--}1032$ h, based on anaerobic lake die-away test data (Aly & Faust 1964; selected, Howard et al. 1991);

completely degraded in soil suspensions in 9 d (Woodcock 1971; quoted, Verschueren 1983);

average rate of biodegradation $10.5 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

aerobic degradation in a non-sterile clay-loam soil: 79% loss at 0°C at the termination of the experiment after 14 days, 82% loss at 4°C after 12 d and 84% loss at 20°C after 40 d all under same experimental conditions (Baker et al. 1980);

rate constants $k = 0.5 \text{ d}^{-1}$ with $t_{1/2} = 1.4$ d in adapted activated sludge and $k = 0.1 \text{ d}^{-1}$ with $t_{1/2} = 6$ d in natural waters under anaerobic conditions (Mills et al. 1982);

microbial degradation negligible in darkness (Hwang et al. 1986);

$k = 0.223 \text{ h}^{-1}$ for maximum removal by activated sludge microorganisms (Chudoba et al. 1989);

biodegradation first-order rate of hydroxylation, $k = 0.017 \text{ min}^{-1}$ by *pseudomonas putida* Fl (Spain et al. 1989; quoted, Neilson et al. 1991);

15% reduction in concn ($2 \mu\text{M}$) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

transformation rate of $245 \text{ -mol L}^{-1} \text{ d}^{-1}$ at 31°C for anaerobic degradation in freshwater sediments with an average of 7 d adaptation time (Zhang & Wiegel 1990);

complete biodegradation in water, seawater, sludge and lagoon within 16 to 23 d (NCASI 1992).

Degradation constant $k = 1.6 \mu\text{M/h}$ for anaerobic batch experiment in serum bottles; $k = 1.2 \mu\text{M/h}$ for dechlorination in anaerobic batch or continuous bioreactor; $k = 1.9 \mu\text{M/h}$ in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999)

Biotransformation: for bacterial transformation $k = 1 \times 10^7 \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982);

degradation rate $k = 3.76 \times 10^{-19} \text{ mol cell}^{-1} \text{ h}^{-1}$ ($\pm 47\%$ SD) from pure culture studies, $k = 0.02 \times 10^{-14}$ to $2 \times 10^{-14} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 3 d for reaction with OH radical on March 21 at 43°N ; lifetime varies from 2 to 20 d at the latitude of Toronto depending on seasons; at latitude of 43.7°N , tropospheric lifetimes are: 20 d on December 21, 5 d on February 21, 2.2 d on April 21 and 1.5 d on June 21; and at different geographical locations on March 21, lifetimes are 1.7 d at latitude 0° , 2.2 d at 25°S , 6.7 d at 55°S and 680 at 85°S (Bunce et al. 1991);

$t_{1/2} = 21.2\text{--}212$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: rate constant $k < 1.5 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 1.5–3.0 (Hoigné & Bader 1983);

$t_{1/2} = 0.8$ h in summer, $t_{1/2} = 3.0$ h in winter for distilled water; $t_{1/2} = 0.7$ h in summer, $t_{1/2} = 2.0$ h in winter for poisoned estuarine water; $t_{1/2} = 0.6$ h in summer, $t_{1/2} = 2.0$ h in winter for estuarine water, all based on photo-transformation rate under full sunlight and microbes; $t_{1/2} = 8.0$ d in summer, $t_{1/2} = 14$ d in winter for distilled water; $t_{1/2} = 6$ d in summer, $t_{1/2} = 14$ d in winter for poisoned estuarine water and $t_{1/2} = 4$ d in summer, $t_{1/2} = 17$ d in winter for estuarine water, based on photo-mineralization rate under full sunlight and microbes (Hwang et al. 1986);

$t_{1/2} = 62$ h in water at pH 8 and $19 \pm 2^\circ\text{C}$ for the reaction with singlet oxygen (Scully & Hoigné 1987);

$t_{1/2} = 2.5\text{--}2.6$ h for photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{1/2} = 0.8\text{--}3$ h based on measured rate of photolysis in distilled water under sunlight in summer and winter (Howard et al. 1991);

complete biodegradation within 5–23 d in seawater (NCASI 1992);

photo-oxidation $t_{1/2} = 2.4$ min for reaction with Fenton's reagent; $t_{1/2} = 30.4$ min at pH 2 and $t_{1/2} = 3.3$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water: $t_{1/2} = 133\text{--}1032$ h, based on unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: mean half-life of dechlorination: $t_{1/2} = 116$ d in July and $t_{1/2} = 47$ d in November (Hale et al. 1991).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 9 d in Dunkirk silt loam, 3 d in Mardin silt loam (Alexander & Aleem 1961)

$t_{1/2}$ = 176–1680 h, based on aerobic soil die-away test data (Baker et al. 1980; Haider et al. 1974; selected, Howard et al. 1991);
 $t_{1/2}$ = 3.5 d in an acidic clay soil with < 1.0% organic matter and 1.5 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).
Biota:

TABLE 14.1.2.4.1
Reported aqueous solubilities and vapor pressures of 2,4-dichlorophenol at various temperatures

Aqueous solubility						Vapor pressure	
Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002		Stull 1947	
shake flask-conductivity		shake flask-optical method		shake flask-optical method*		summary of literature data	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	S/g·m ⁻³	t/°C	P/Pa
15.3	3896	310.5	6339	294.6	4841	53.0	133.3
25.2	5517	327.1	7244	303.1	6129	80.0	666.6
29.8	6075	338.1	8150	311.5	6683	92.8	1333
35.1	6501	347.2	9056	322.4	7433	107.7	2666
		355.1	9961	336.7	8460	123.4	5333
		363.5	10867	295.2	4939	133.5	7999
		373.7	10867	303.7	6161	146.0	13332
		382.1	11772	312.4	6748	165.2	26664
		393.5	12678	318.1	7139	187.5	53329
		401.5	13583	232.2	7482	210.0	101325
		408.4	14489	291.4	4320		
		423.2	15394	302.0	6047	mp/°C	45.0
				308.8	6504		
				321.0	7335		
				337.7	8525		

*some data from Achard et al.
1996, Jaoui et al. 1999

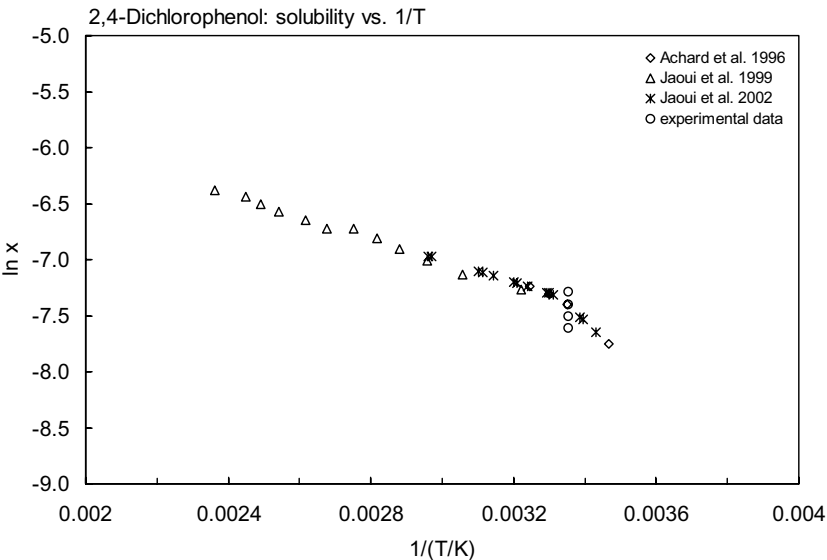


FIGURE 14.1.2.4.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2,4-dichlorophenol.

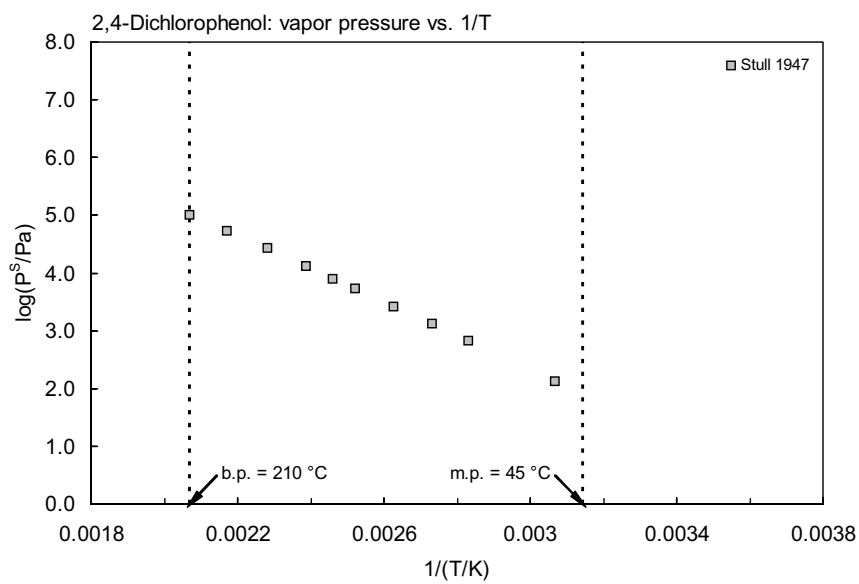
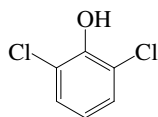


FIGURE 14.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dichlorophenol.

14.1.2.5 2,6-Dichlorophenol



Common Name: 2,6-Dichlorophenol

Synonym: 2,6-DCP

Chemical Name: 2,6-dichlorophenol

CAS Registry No: 87-65-0

Molecular Formula: $C_6H_3Cl_2OH$

Molecular Weight: 163.001

Melting Point ($^{\circ}C$):

68.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

220 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.91 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)

6.80 (Doedens 1967; McLeese et al. 1979)

6.79 (Pearce & Simkins 1968)

6.79 (Sillén & Martell 1971; Kaiser et al. 1984; Xie & Dyrssen 1984; Shigeoka et al. 1988)

6.78 (Ugland et al. 1981; Dean 1985)

6.54 (Nendza & Seydel 1988)

Molar Volume (cm^3/mol):

145.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

22.14 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$, F: 0.374 (mp at $68.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2625 (shake flask-HPLC/UV at pH 4.5, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

13.1* (extrapolated-regression of tabulated data, temp range 59.5 – $220^{\circ}C$, Stull 1947)

12.9 (extrapolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 13472.0/(T/K)] + 8.864007$; temp range 59.5 – $220^{\circ}C$ (Antoine eq., Weast 1972–73)

12.2 (supercooled liq. value, GC-RT correlation, Hamilton 1980)

12.7 (capillary GC-RT, Bidleman & Renberg 1985)

11.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.32845 - 2436.59/(-35.584 + T/K)$; temp range 333 – $493\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.2254 - 1106.4/(-151.42 + T/K)$; temp range 353 – $493\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.7376 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.86 (Hansch & Leo 1979)

2.34 (HPLC-RT correlation, Butte et al. 1981)

2.64 (HPLC- k' correlation, Hammers et al. 1982)

3.36	(shake flask-UV, Beltrame et al. 1984)
2.84, 2.92	(shake flask-GC, HPLC-k' correlation, Xie et al. 1984)
2.84	(shake flask, Shigeoka et al. 1988)
2.80	(batch equilibration-UV, Beltrame et al. 1988)
2.64	(recommended, Sangster 1993)
2.92	(shake flask-GC, Kishino & Kobayashi 1994)
2.75	(recommended, Hansch et al. 1995)
2.57	(HPLC-RT correlation, Makovskaya et al. 1995b)

Bioconcentration Factor, log BCF:

1.44–1.56 (estimated, NCASI 1992)

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: 1920 - ∞ h and 144–360 h for 75% degradation in mineral medium and seawater batch experiments respectively (de Kreuk & Hanstveit 1981)

81% reduction in concn (2 μ M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ = 1920 - ∞ h and 144–360 h for 75% degradation in mineral medium and seawater batch experiments, respectively (de Kreuk & Hanstveit 1981).

Ground water:

Sediment:

Soil: $t_{1/2}$ = 16.2 d in an acidic clay soil with < 1.0% organic matter and $t_{1/2}$ = 2.4 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.2.5.1
Reported vapor pressures of 2,6-dichlorophenol at various temperatures

Stull 1947

summary of literature data

t/°C	P/Pa
59.5	133.3
87.5	666.6
101.0	1333
115.5	2666
131.5	5333
141.8	7999
154.6	13332
175.5	26664
197.7	53329
220.0	101325
mp/°C	-

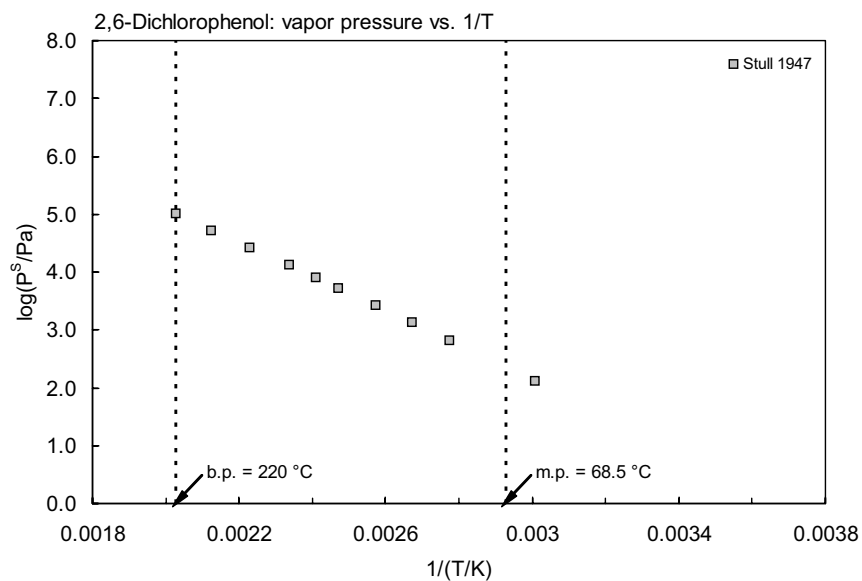
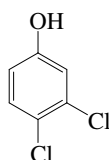


FIGURE 14.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dichlorophenol.

14.1.2.6 3,4-Dichlorophenol



Common Name: 3,4-Dichlorophenol

Synonym: 3,4-DCP

Chemical Name: 3,4-dichlorophenol

CAS Registry No: 95-77-2

Molecular Formula: $C_6H_3Cl_2OH$

Molecular Weight: 163.001

Melting Point ($^{\circ}C$):

68.0 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

253 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.39 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)

8.59 (Pearce & Simkins 1968; Serjeant & Dempsey 1979; Hammers et al. 1982)

8.59 (Sillén & Martell 1971; Kaiser et al. 1984)

8.62 (Ugland et al. 1981; Lagas 1988; Renner 1990; Ma et al. 1993)

8.68 (Xie & Dyrssen 1984; Shigeoka et al. 1988; Sangster 1993)

8.63 (Dean 1985)

Molar Volume (cm^3/mol):

145.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.93 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$), F : 0.379 (mp at $68^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9256 (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa\cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.37 (Hansch & Leo 1979)

3.05 (HPLC- k' correlation, Hammers et al. 1982)

3.33 (HPLC-RT correlation, Banerjee et al. 1984)

3.47 (shake flask-UV, Beltrame et al. 1984)

3.44, 3.41 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)

3.44 (shake flask, Shigeoka et al. 1988)

3.68 (shake flask/batch equilibration-UV, Beltrame et al. 1988)

3.33 (recommended, Sangster 1993)

3.27; 3.39 (HPLC-RT correlation; electrometric titration, Slater et al. 1994)

3.33 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.43, 1.38 (earthworm *E. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)

1.30, 1.61 (earthworm *L. rubellus*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)

1.79, 1.8, 1.94, 2.04 (earthworm system, collated from literature, Connell & Markwell 1990)
 0.8, 1.3, 1.4, 1.80 (earthworm system, derived data, Connell & Markwell 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

3.09 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 3.03 (2.93–3.13) (soil: organic carbon OC $\geq 0.5\%$ and pH ≤ 6.0 , average, Delle Site 2001)

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

Photolysis:

oxidation:

Hydrolysis:

Biodegradation: biodegradation first-order rate of hydroxylation of 0.008 min^{-1} by *Pseudomonas putida* Fl (Spain et al. 1989; quoted, Neilson et al. 1991).

Biotransformation: degradation rate of $6.84 \times 10^{-19} (\pm 38\% \text{ SD}) \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

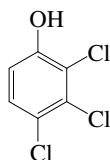
Sediment: mean half-life of dechlorination: $t_{1/2} = 115 \text{ d}$ in July and $t_{1/2} = 86 \text{ d}$ in November with relatively long $t_{1/2} = 66 \text{ d}$ reported from site 1, $t_{1/2} = 64 \text{ d}$ from site 3 and $t_{1/2} = 132 \text{ d}$ from site 5 in January (Hale et al. 1991).

Soil: disappearance $t_{1/2} = 10.1 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 11.2 \text{ d}$ from Holten soil with earthworms *E. fetida andrei* and $t_{1/2} = 24.7 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 49.5 \text{ d}$ from Holten soil with earthworms *L. rebellus* (van Gestel & Ma 1988);

$t_{1/2} = 18.3 \text{ d}$ in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 3.2 \text{ d}$ in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab experiments (Loehr & Matthews 1992).

Biota:

14.1.2.7 2,3,4-Trichlorophenol



Common Name: 2,3,4-Trichlorophenol

Synonym:

Chemical Name: 2,3,4-trichlorophenol

CAS Registry No: 1595-06-0

Molecular Formula: $C_6H_3Cl_3O$, $C_6H_2Cl_3OH$

Molecular Weight: 197.446

Melting Point ($^{\circ}C$):

83.5 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.66 (Doedens 1967)

6.50 (Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984; Shigeoka et al. 1988; Sangster 1993)

6.97 (Ugland et al. 1981; Dean 1985; Renner 1990; Ma et al. 1993)

7.18 (Schellenberg et al. 1984)

Molar Volume (cm^3/mol):

166.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$), F : 0.267 (mp at $83.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

500 (estimated, Ma et al. 1990)

915 (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

1.00 (selected, Ma et al. 1990)

3.48 (selected P_L , Shiu et al. 1994)

Henry's Law Constant ($Pa\cdot m^3/mol$):

0.3959 (calculated- P/C , Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.07 (Hansch & Leo 1979)

3.51 (HPLC-RT correlation, Butte et al. 1981)

3.54 (HPLC- k' correlation, Hammers et al. 1982)

3.80 (shake flask-UV, Beltrame et al. 1984)

3.80 (shake flask, Shigeoka et al. 1988)

3.82 (shake flask/batch equilibration-UV, Beltrame et al. 1988)

3.61 (recommended, Sangster 1993)

3.51, 3.54, 3.80 (lit. values, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

Photolysis: photochemical-transformation $t_{1/2} = 1.7$ h in Xenotest 1200 (Svenson & Björndal 1988).

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: 1.7 h for photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988).

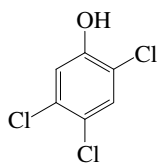
Ground water:

Sediment:

Soil:

Biota:

14.1.2.8 2,4,5-Trichlorophenol



Common Name: 2,4,5-Trichlorophenol

Synonym: 245-TCP

Chemical Name: 2,4,5-trichlorophenol

CAS Registry No: 95-95-4

Molecular Formula: $C_6H_2Cl_3OH$

Molecular Weight: 197.446

Melting Point ($^{\circ}C$):

69 (Lide 2003)

Boiling Point ($^{\circ}C$):

247 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.500 ($75^{\circ}C$, Verschueren 1983)

Acid Dissociation Constant, pK_a :

7.00 (Blackman et al. 1955, Sillén & Martell 1971; Kaiser et al. 1984)

7.07 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)

7.43 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)

6.72 (Ugland et al. 1981; Dean 1985; Lagas 1988; Renner 1990; Ma et al. 1993)

6.90 (Hoigné & Bader 1983)

6.94 (Schellenberg et al. 1984; Sangster 1993)

6.83 (Nendza & Seydel 1988)

Molar Volume (cm^3/mol):

166.1 (calculated-Le Bas method at normal boiling point)

165.5 (calculated- χ , Sabljic 1987b)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.59 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.370 (mp at $69^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

948 (shake flask-UV at pH 5.1, Blackman et al. 1955)

990 (IUPAC recommended at pH 5.1, Horvath & Getzen 1985)

700 ($8^{\circ}C$, Leuenberger et al. 1985)

649 (shake flask-HPLC/UV at pH 4.9, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6.69* (extrapolated-regression of tabulated data, temp range $72-251.8^{\circ}C$, Stull 1947)

6.60 (extrapolated liquid value, Antoine eq, Weast 1972-73)

$\log(P/mmHg) = [-0.2185 \times 13237.0/(T/K)] + 8.401072$; temp range $72-251.8^{\circ}C$ (Antoine eq., Weast 1972-73)

6.12 (supercooled liquid, GC-RT correlation, Hamilton 1980)

2.66 (capillary GC-RT, Bidleman & Renberg 1985)

2.93 (selected, Leuenberger et al. 1985)

7.64 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.38179 - 2812.25/(-2.091 + T/K)$; temp range $345-525 K$ (Antoine eq., Stephenson & Malanowski 1987)

2.93 (calculated, Howard 1991)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.132	(8°C , Leuenberger et al. 1985)
0.590	(calculated, Howard 1991)
0.521	(calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.72	(Leo et al. 1971; Hansch & Leo 1979; 1982)
2.39	(estimated-HPLC-RT correlation, Veith et al. 1979)
3.63	(HPLC- k' correlation, Hammers et al. 1982)
3.80	(shake flask-GC, Saarikoski & Viluksela 1982)
4.19	(shake flask-HPLC/UV, Schellenberg et al. 1984)
4.10, 3.96	(shake flask-GC, HPLC- k' correlation, Xie et al. 1984)
3.73	(HPLC-RT correlation, Miyake et al. 1986)
3.84	(shake flask/batch equilibration-UV, Beltrame et al. 1988)
4.10	(shake flask, Shigeoka et al. 1988)
3.52; 3.55	(shake flask; HPLC-RT correlation, Wang et al. 1989)
3.72	(recommended, Sangster 1993)
4.02	(shake flask-GC, Kishino & Kobayashi 1994)
3.72	(recommended, Hansch et al. 1995)
3.83	(HPLC-RT correlation, Makovskaya et al. 1995b)

Bioconcentration Factor, $\log \text{BCF}$:

3.28	(fathead minnow-28 d exposure, Veith et al. 1979b)
3.28, 2.70	(total ^{14}C in fathead minnows, observed, calculated, mean exposure level $0.0048 \mu\text{g}\cdot\text{mL}^{-1}$, Call et al. 1980)
3.26, 2.82	(total ^{14}C in fathead minnows, observed, calculated, mean exposure level $0.0493 \mu\text{g}\cdot\text{mL}^{-1}$, Call et al. 1980)
3.27	(total ^{14}C in fathead minnows, mean value, Call et al. 1980)
2.40	(calculated- K_{OW} , Mackay 1982)
2.88	(calculated-MCI χ , Sabljic 1987a)
1.79	(fish, van Gestel & Ma 1988)
1.81, 1.53	(earthworms <i>E. fetida andrei</i> : Kooyenburt soil, Holten soil, van Gestel & Ma 1988)
2.04, 2.82	(earthworms <i>L. rubellus</i> : Kooyenburt soil, Holten soil, van Gestel & Ma 1988)
2.04, 2.39, 2.61, 3.36	(earthworm system, collated from literature, Connell & Markwell 1990)
0.40, 1.50, 2.50, 8.40	(earthworm system, derived data, Connell & Markwell 1990)
3.28; 3.61	(fathead minnows; fish, Howard 1991)
2.14	(estimated, NCASI 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.49–3.98	(soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
3.38–3.64	(soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
2.56–2.82	(soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
3.38–3.87	(soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
2.55–2.99	(soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
3.36	(sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
2.99	(soil, calculated-MCI χ , Sabljic 1987a,b)
3.25, 3.12, 3.38, 2.56	(quoted:lake sediment, river sediment, aquifer material, soil, Howard 1991)
3.34, 3.30	(soils, Howard 1991)
2.93	(calculated- K_{OW} , Kollig 1993)
3.36	(soil, calculated-MCI χ , Sabljic et al. 1995)
3.11 (2.81–3.41), 3.35 (3.30–3.40)	(soils: organic carbon $\text{OC} \geq 0.1\%$ and $\text{pH} 3.4\text{--}6.0$, $\text{OC} \geq 0.5\%$ and $\text{pH} \leq 4.9$ undissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} \sim 9.0$ d from a model river 1 m deep, flowing 1 m/s with a wind speed of 3 m/s, and $t_{1/2} = 207$ d from a model pond (Howard 1991).

Photolysis:

$k_p = 1.30 \text{ h}^{-1}$ with $t_{1/2} = 0.6$ h in summer at mean temp. 25°C and $k_p = 0.61 \text{ h}^{-1}$ with $t_{1/2} = 1.0$ h in winter at mean temp 18°C in distilled water; $k_p = 1.2 \text{ h}^{-1}$ with $t_{1/2} = 0.6$ d in summer and $k_p = 0.65 \text{ h}^{-1}$ with $t_{1/2} = 1.0$ h in winter in poisoned estuarine water; and $k_p = 1.4 \text{ h}^{-1}$ with $t_{1/2} = 0.5$ h in summer and $k_p = 0.65 \text{ h}^{-1}$ with $t_{1/2} = 1.0$ h in winter for estuarine water under full sunlight and microbes (photo-transformation, Hwang et al. 1986)

$k_p = 1.30 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 0.5$ h in summer, $k_p = 0.61 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 1.0$ h in winter in distilled water and $k_p = 1.20 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 0.6$ h in summer, $k_p = 0.65 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 1.0$ h in winter in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993)

$t_{1/2} = 0.5\text{--}336$ h, based on photolysis rate constants for transformation and mineralization under summer and winter, sunlight conditions (Howard et al. 1991)

photolysis $t_{1/2} = 0.6$ and 1.0 h in natural water (and distilled water) exposed to midday sunlight during summer and winter respectively (Howard 1991)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

aqueous photooxidation $t_{1/2} = 66\text{--}3480$ h in water, based on reported reaction constants for OH and RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991)

$k(\text{aq.}) > 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, and $k < 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species, $k > 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.2–1.5 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983b)

$k_{\text{OH}} = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Bunce et al. 1991)

Hydrolysis: $t_{1/2} > 8 \times 10^6$ yr, based on hydrolysis rate constant is zero at pH 7.0 (Kollig et al. 1987; selected, Howard et al. 1991).

Biodegradation: decomposition in suspended soils: > 72 d for complete disappearance (Woodcock 1971; quoted, Verschueren 1983);

840 h for 75% degradation in mineral medium (de Kreuk & Hanstveit 1981);

aqueous aerobic $t_{1/2} = 552\text{--}16560$ h, based on unacclimated aerobic river die-away test data (Lee & Ryan 1979; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 3028\text{--}43690$ h, based on unacclimated anaerobic grab sample data for soil and ground water (Gibson & Suflita 1986; Baker & Mayfield 1980; selected, Howard et al. 1991);

degradation with microbes in darkness negligible (Hwang et al. 1986);

degradation $k = 0.00010 \text{ d}^{-1}$ with a $t_{1/2} = 16560$ h and $k = 0.030 \text{ d}^{-1}$ with a $t_{1/2} = 552$ h for Skidway River water and water-sediment slurry, respectively (Pritchard 1987);

biodegradation $t_{1/2} = 690$ d in river water (Howard 1991)

70% reduction in concn ($2 \mu\text{M}$) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

$t_{1/2}(\text{aerobic}) = 25$ d, $t_{1/2}(\text{anaerobic}) = 130$ d in natural waters (Capel & Larson 1995)

Biotransformation: degradation rate $k = 1.43 \times 10^{-20}$ ($\pm 77\%$ SD) $\text{mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies and $k = 5 \times 10^{-15} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime of 4 d on March 21 at 43°N (Bunce et al. 1991);

$t_{1/2} = 30.1\text{--}301$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

$t_{1/2} \sim 7.5$ d for reactions with OH radical (estimated, Howard 1991);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: 840 h for 75% degradation in mineral medium (de Kreuk & Hanstveit 1981);

Rate constant $k < 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with O_3 at pH 1.2–1.5 (Hoigné & Bader 1983);

$t_{1/2} = 0.5$ h (summer), $t_{1/2} = 1.0$ h (winter) in distilled water and $t_{1/2} = 0.5$ h (summer), $t_{1/2} = 1.0$ h (winter) in surface estuarine water based on photo-transformation rate under full sunlight and microbes (Hwang et al. 1986);

- $t_{1/2} = 7$ d (summer), $t_{1/2} = 14$ d (winter) in distilled water and $t_{1/2} = 3$ d (summer), $t_{1/2} = 8$ d (winter) in estuarine water based on photo-mineralization rate under full sunlight and microbes (Hwang et al. 1986);
- $t_{1/2} = 0.6$ h (summer), $t_{1/2} = 1.0$ h (winter) in poisoned estuarine water based on photo-transformation rate and $t_{1/2} = 6$ d (summer), $t_{1/2} = 14$ d (winter) in poisoned estuarine water based on photomineralization rate (Hwang et al. 1986);
- $t_{1/2} = 16560$ h at 21°C in Skidway River water (Pritchard 1987);
- photodegradation $t_{1/2} = 0.5$ h (summer), $t_{1/2} = 1.0$ h (winter) in distilled water and $t_{1/2} = 0.6$ h (summer), $t_{1/2} = 1.0$ h (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993);
- $t_{1/2} = 0.5$ –336 h, based on aqueous photolysis half-life (Howard et al. 1991); rapidly photolyze with a $t_{1/2} = 0.6$ –1.0 h at water surfaces, $t_{1/2} = 690$ d in water column (Howard 1991)
- t_2 (aerobic) = 25 d, t_2 (anaerobic) = 130 d in natural waters (Capel & Larson 1995)
- Ground water: $t_{1/2} = 1104$ –43690 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).
- Sediment: $t_{1/2} = 23$ d from calculated degradation rate constant $k = 0.0030$ d⁻¹ for radiolabeled 2,4,5-TCP in Skidway River water-sediment slurry (Lee & Ryan 1979; quoted, Pritchard 1987);
- biodegradation $t_{1/2} = 23$ d in sediments (Howard 1991).
- Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 + d in Dunkirk silt loam, 47 + d in Mardin silt loam (Alexander & Aleem 1961)
- disappearance $t_{1/2} = 3.4$ d from Kooyenburg soil and $t_{1/2} = 6.6$ d from Holten soil with earthworms *E. fetida andrei* and $t_{1/2} = 39.6$ d from Kooyenburg soil, $t_{1/2} = 13.9$ d from Holten soil with earthworm *L. rubellus* (van Gestel & Ma 1988);
- $t_{1/2} = 33$ d in sandy loam (Kjeldsen et al. 1990)
- $t_{1/2} = 552$ –16560 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); under aerobic conditions biodegradation $t_{1/2} = 15$ d in a soil suspension (Howard 1991);
- $t_{1/2} = 22.3$ d in an acidic clay soil with < 1.0% organic matter and $t_{1/2} = 14.6$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).
- Biota: depuration $t_{1/2}$ (obs.) = 12 h, $t_{1/2}$ (calc) = 9.2 h for mean exposure level of 0.0048 µg·mL⁻¹ and $t_{1/2}$ (obs) = 12 h, $t_{1/2}$ (calc) = 6.6 h for mean exposure level of 0.0493 µg·mL⁻¹ (fathead minnow, Call et al. 1980).

TABLE 14.1.2.8.1

Reported vapor pressures of 2,4,5-trichlorophenol at various temperatures

Stull 1947	
summary of literature data	
t/°C	P/Pa
72.0	133.3
102.1	666.6
117.3	1333
134.0	2666
151.5	5333
162.5	7999
178.0	13332
201.5	26664
226.5	53329
251.8	101325
mp/°C	62

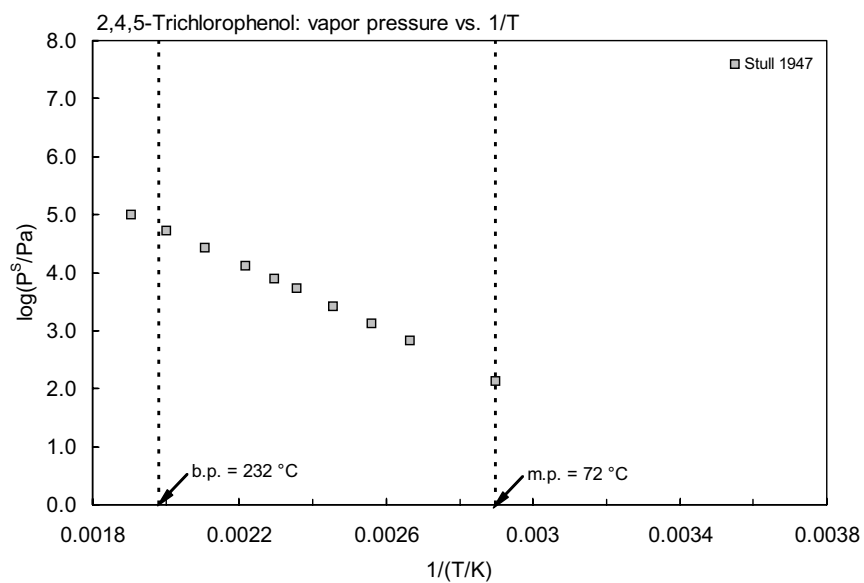
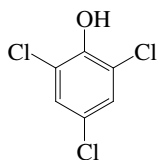


FIGURE 14.1.2.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,5-trichlorophenol.

14.1.2.9 2,4,6-Trichlorophenol



Common Name: 2,4,6-Trichlorophenol

Synonym: 2,4,6 TCP

Chemical Name: 2,4,6-trichlorophenol

CAS Registry No: 88-06-2

Molecular Formula: $C_6H_2Cl_3OH$

Molecular Weight: 197.446

Melting Point ($^{\circ}C$):

69 (Lide 2003)

Boiling Point ($^{\circ}C$):

246.0 (Stull 1947; Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.675 (Schmidt-Bleek et al. 1982)

1.491 ($75^{\circ}C$, Weast 1982–83)

Acid Dissociation Constant, pK_a :

6.10 (Blackman et al 1955)

6.22 (Farquharson et al. 1958; Saarikoski & Viluksela 1982)

5.99 (Dean 1985)

6.23 (Serjeant & Dempsey 1979; Tratnyek & Hoigné 1991)

6.00 (Xie 1983, Yoshida et al. 1987)

6.15 (Schellenberg et al. 1984; Leuenberger et al. 1985)

6.18 (Sangster 1993)

Molar Volume (cm^3/mol):

166.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.370 (mp at $69^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

858 (gravimetric method, Dacomo 1885)

434 (shake flask-UV at pH 5.1, Blackman et al. 1955)

900 (shake flask-spectrophotometry, Roberts et al. 1977)

430 (IUPAC recommended at pH 5.1, Horvath & Getzen 1985)

312 ($20^{\circ}C$, phenol form, shake flask-HPLC/UV, Yoshida et al. 1987)

$312 \times (1 + 10^{pH-6.06})$ ($20^{\circ}C$, measured at pH 4, 5, 6 and 7, shake flask-HPLC/UV, Yoshida et al. 1987)

300, 580, 270000 (river, oligotrophic lake, eutrophic lake, Yoshida et al. 1987)

708 (shake flask-HPLC/UV at pH 4.7, Ma et al. 1993)

800 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

692* ($24.9^{\circ}C$, shake flask-conductimetry, measured range 19.5 – $30.0^{\circ}C$, Achard et al. 1996)

1144* ($41.05^{\circ}C$, shake flask-optical method, measured range 314.2 – $420.6 K$, Jaoui et al. 1999)

503 (shake flask-HPLC/UV, pH 5.03, Huang et al. 2000)

439.6* ($21.75^{\circ}C$, shake flask-optical method, measured range 294.9 – $317.2 K$, Jaoui et al. 2002)

$\ln [S/(mol kg^{-1})] = 23.367 - 7096.7/(T/K)$; temp range 292 – $303 K$ (eq. derived using reported exptl. data, Jaoui et al. 2002)

$\ln [S/(mol kg^{-1})] = 6.6069 - 2029.9/(T/K)$; temp range 303 – $334 K$ (eq. derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 4.17* (extrapolated-regression of tabulated data, temp range 76.5–246°C, Stull 1947)
- 4.00 (20–25°C, extrapolated, Jordan 1954)
- 4.12 (extrapolated liquid, Antoine eq., Weast 1972–73)
- $\log(P/\text{mmHg}) = [-0.2185 \times 14092.8/(T/K)] + 8.82338$; temp range 76.5–246°C (Antoine eq., Weast 1972–73)
- 3.83 (supercooled liquid, GC-RT correlation, Hamilton 1980)
- 1.12 (gas saturation, Politzki et al. 1982)
- 1.30 (20°C, Schmidt-Bleek et al. 1982)
- 1.60 (extrapolated, Mabey et al. 1982)
- 2.67 (Leuenberger et al. 1985)
- 3.26 (capillary GC-RT correlation, supercooled liquid P_L , Bidleman & Renberg 1985)
- 4.28 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 7.67323 - 2876.7/(-11.682 + T/K)$, temp range 349–519 K (Antoine eq., Stephenson & Malanowski 1987)
- 0.827 (GC-RT correlation, solid phase, Yoshida et al. 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 0.405 (calculated-P/C, Mabey et al. 1982)
- 0.132 (8°C, calculated-P/C, Leuenberger et al. 1985)
- $0.523/(1 + 10^{\text{pH} + 6.06})$ (20°C, calculated-P/C, Yoshida et al. 1987)
- 0.5687 (calculated-P/C, Shiu et al. 1994)
- 0.428 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.06 (Leo et al. 1971)
- 3.69 (Leo et al. 1971)
- 3.69, 3.62, 4.02 (Hansch & Leo 1979)
- 3.76 (HPLC-RT correlation, Butte et al. 1981)
- 3.48 (RP-HPLC- k' correlation, Miyake & Terada 1982)
- 4.03 (shake flask-GC, Saarikoski & Viluksela 1982)
- 3.72 (shake flask-HPLC/UV, Schellenberg et al. 1984)
- 2.97, 2.80 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
- 3.75, 3.69 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)
- 3.72 (OECD 1981 guidelines, Leuenberger et al. 1985)
- 3.29 (RP-HPLC-RT correlation, Chin et al. 1986)
- 3.97 (CPC-RV, Terada et al. 1987)
- 3.75 (HPLC-RT correlation, Shigeoka et al. 1988)
- 3.68 (batch equilibration-UV, Beltrame et al. 1988)
- 3.96; 3.60 (shake flask; HPLC-RT correlation, Wang et al. 1989)
- 3.69 (recommended, Sangster 1993)
- 2.67 (shake flask-GC, Kishino & Kobayashi 1994)
- 3.69 (recommended, Hansch et al. 1995)
- 3.84, 3.76, 3.65, 3.54 (pH 3.0, 6.1, 7.0, 8.0, shake flask-GC (octanol phase)/HPLC (aqueous phase) measured range pH 2.1 to 13.3, Nowosielski & Fein 1998)

Bioconcentration Factor, $\log BCF$:

- 2.00–2.32 (Landner et al. 1977; Laake 1982)
- 2.40 (fish, Körte et al. 1978)
- 1.60, 1.71, 2.49 (activated sludge, algae, golden orfe, Freitag et al. 1982)
- 1.71; 1.81 (algae: exptl; calculated, Geyer et al. 1981)
- 1.54–1.78, 1.60 (mussel *mytilus edulis*, Geyer et al. 1982)
- 2.92 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 3.24, 3.48, 3.1–4.09 (algae, snail, guppy, Virtanen & Hattula 1982)
- 1.71, 2.49, 1.60 (algae, fish, activated sludge, Klein et al. 1984)

- 1.71, 2.13 (algae: exptl., calculated- K_{OW} , Geyer et al. 1984)
 1.78, 1.70, 2.49 (activated sludge, algae, golden ide, Freitag et al. 1985)
 1.48–2.08 (rainbow trout, Oikari et al. 1985)
 2.75; 2.84 (Atlantic salmon fry: humic water; lake water, Carlberg et al. 1986)
 1.30 (Isnard & Lambert 1988)
 1.94; 2.83 (flagfish: whole fish; fish lipid, Smith et al. 1990)
 1.87–2.16 (estimated, NCASI 1992)
 1.48–2.08, 3.01–4.09, 2.49, 3.48, 1.60, 1.70–3.24 (trout, guppy, fish, snail, mussel, algae, quoted from literature, NCASI 1992)
 3.6, 5.4, 5.0 (perch bile to water, Söderström et al. 1994)
 2.84 (*Salmo salar*, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC} :

- 2.34 (sediment, Virtanen & Hattula 1982)
 3.30 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 2.52 (soil, Seip et al. 1986)
 3.41–3.84 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
 3.33–3.57 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
 2.52–2.75 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
 3.30–3.73 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
 2.48–2.87 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
 3.02 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
 3.03 (sediment, Leuenberger et al. 1985)
 2.99 (soil, calculated, Sabljic 1987a,b)
 3.34, 2.79, 2.23 (average values, soil at pH 6, 7, and 7.7, Yoshida et al. 1987)
 2.79, 3.34, 2.04 (river, oligotrophic lake, eutrophic lake, Yoshida et al. 1987)
 2.50 (soil, calculated-MCI χ , Bahnick & Doucette 1988)
 2.92–3.12; 3.03 (lit. range, mean value, Robinson & Novak 1994)
 2.82–3.02 (log K_{OM} , organic matter, Robinson & Novak 1994)
 2.81, 3.03 (log K_{HA} , humic acid, Robinson & Novak 1994)
 2.25 (calculated- K_{OW} , Kollig 1993)
 3.02 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.59; 3.08 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
 2.52 (1.97–3.01), 2.88 (2.33–3.39) (soils: organic carbon OC \geq 0.1% and pH $>$ 4.2, OC \geq 0.1% and pH \leq 4.2 undissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization: volatilization and sorption $t_{1/2} \sim 192$ h from natural pond (Schauerte et al. 1982);
 volatilization rate constant from water $k = 3.90 \times 10^{-3} / (1 + 10^{pH-6.06}) / L_w$ h $^{-1}$, L_w , depth of water phase (Yoshida et al. 1987).
 Photolysis: aqueous photolysis $t_{1/2} = 2$ –96 h, based on laboratory photolysis rate constants for an environmental pond at noon under fall sunlight conditions at 40°N latitude (Sugiura et al. 1984; quoted, Howard et al. 1991);
 photo-degradation rate constants $k_p = (0.156 + 9.16 \times 10^{pH-5.86}) / (1 + 10^{pH-5.86})^{-1}$ in water, for summer, fine day, and $k_p = (0.042 + 1.40 \times 10^{pH-6.09}) / ((1 + 10^{pH-6.09})^{-1})$ h $^{-1}$ in water, for winter, fine day; $k = 0.72$ d $^{-1}$ for river, $k = 2.2$ d $^{-1}$ for oligotrophic lake and $k = 0.776$ d $^{-1}$ for eutrophic lake (Yoshida et al. 1987);
 photochemical-transformation $t_{1/2} = 1.2$ h in Xenotest 1200 (Svenson & Björndal 1988);
 photolysis $t_{1/2} = 24$ h (Paasivirta 1992);
 photo-degradation rate constant $k = 26 \times 10^3$ min $^{-1}$ with $t_{1/2} = 25.2$ min for direct UV radiation aqueous solutions (Benitez et al. 2000).
 Oxidation: aqueous oxidation rate constant $k < 7 \times 10^4$ M $^{-1}$ h $^{-1}$ for singlet oxygen and $k = 1 \times 10^6$ M $^{-1}$ h $^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);
 apparent reaction rate constant $k > 10^8$ M $^{-1}$ s $^{-1}$ at pH 8, and rate constants $k < 10^4$ M $^{-1}$ s $^{-1}$ for non-protonated species, $k > 10^8$ M $^{-1}$ s $^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.3–1.5 and 20–23°C (Hoigné & Bader 1983b);

photooxidation $t_{1/2} = 123.4\text{--}1234$ h, based on an estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 20.3\text{--}2027$ h, based on measured rate data for reaction with singlet oxygen in aqueous solution (Scully & Hoigne 1987; quoted, Howard et al. 1991);

rate constants: $k = 2 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 4.2, $k = 6 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 4.8, $k = 1.5 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 5.2, $k = 2.6 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 5.5, $k = 5.5 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 6.0, $k = 9.50 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7 and $k = 1.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ at pH 9 for the reaction with singlet oxygen in aqueous solution at $(19 \pm 2)^\circ\text{C}$ (Scully & Hoigné 1987);

rate constant $k = (1.7 \pm 0.7) \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991);

photo-oxidation rate constant $k = 98 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 5.1$ min for reaction with Fenton's reagent; and $k = 44 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 20.6$ min at pH 2 and $k = 314 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 3.1$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Hydrolysis: $t_{1/2} > 8 \times 10^6$ yr, based on hydrolysis rate constant of zero at pH 7 (Kollig et al. 1987; quoted, Howard et al. 1991).

Biodegradation: $t_{1/2} = 7\text{--}10$ d for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964); decompositions in soil suspensions: 5 d for complete disappearance (Woodcock 1971; quoted, Verschueren 1983); $t_{1/2} = 216\text{--}432$ h and $624\text{--}1560$ h for 75% degradation in mineral medium and seawater batch experiment, respectively (de Kreuk & Hanstveit 1981);

aqueous aerobic $t_{1/2} = 168\text{--}1680$ h, based on unacclimated aerobic river die-away test and soil grab sample data (Blades-Fillmore et al. 1982; Haider et al. 1974; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 4050\text{--}43690$ h, based on unacclimated anaerobic grab sample data for soil (Baker & Mayfield 1980; quoted, Howard et al. 1991);

92% aerobic biodegraded after 28 d by both Sturm of OECD and sealed vessel tests (Birch & Fletcher 1991);

biodegradation rate constant $k = 3.5 \times 10^{-11} \text{ L cell}^{-1} \text{ h}^{-1}$ at 20°C and pH 7;

biodegradation rate constants $k = 8.4 \times 10^{-5} \text{ d}^{-1}$ in river, $k = 8.2 \times 10^{-6} \text{ d}^{-1}$ in oligotrophic lake and $k = 8.4 \times 10^{-4} \text{ d}^{-1}$ in eutrophic lake in water compartment, $k = 8.4 \times 10^{-4} \text{ d}^{-1}$ in river, $k = 8.2 \times 10^{-5} \text{ d}^{-1}$ in oligotrophic lake and $k = 8.4 \times 10^{-3} \text{ d}^{-1}$ in eutrophic lake in soil compartment (Yoshida et al. 1987);

94% reduction in concn (2 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

up to 60% can be mineralized by acclimated bacteria *pseudomonas aeruginosa* in 48 h but decreased with increasing humic acid concentration (Robinson & Novak 1994)

Degradation constant $k = 3.2\text{-M/h}$ for anaerobic batch experiment in serum bottles; $k = 2.4 \text{-M/h}$ for dechlorination in anaerobic batch or continuous bioreactor; $k = 2.4 \text{-M/h}$ in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999)

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^9 \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 421 \text{ d}^{-1}$, 3573 d^{-1} (flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 4.78 \text{ d}^{-1}$, 5.26 d^{-1} (flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 4.78 \text{ d}^{-1}$, 2.54 d^{-1} (fish: bioconcentration based; toxicity based, Smith et al. 1990)

Half-Lives in the Environment:

Air: $t_{1/2} = 123.4\text{--}1234$ h, based on an estimated rate constant for the vapor phase reaction with OH radical (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $> 5\text{d}$ (Kelly et al. 1994).

Surface water: $t_{1/2} = 216\text{--}432$ h and $624\text{--}1560$ h for 75% degradation in mineral medium and seawater batch experiment, respectively (de Kreuk & Hanstveit 1981);

$t_{1/2} = 1.2$ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{1/2} = 2\text{--}96$ h, based on aqueous photolysis half-life (Sugiura et al. 1984; quoted, Howard et al. 1991);

$t_{1/2} = 62$ h for the reaction with singlet oxygen at pH 8 and $(19 \pm 2)^\circ\text{C}$ in water (Scully & Hoigné 1987)

photolysis $t_{1/2} = 24$ h (Paasivirta 1992);

photo-oxidation $t_{1/2} = 5.1$ min for reaction with Fenton's reagent; $t_{1/2} = 20.6$ min at pH 2 and $t_{1/2} = 3.1$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water: $t_{1/2}$ = 336–43690 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 5 d in Dunkirk silt loam, 13 d in Mardin silt loam (Alexander & Aleem 1961)

$t_{1/2}$ = 168–1680 h, based on estimated unacclimated aqueous aerobic biodegradation half-life including soil grab sample data (Haider et al. 1974; quoted, Howard et al. 1991);

$t_{1/2}$ = 6.3 d in an acidic clay soil with < 1.0% organic matter and $t_{1/2}$ = 5.3 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch laboratory microcosm experiments (Loehr & Matthews 1992);

$t_{1/2}$ = 6720 h (Paasivirta 1992).

Biota: $t_{1/2}$ = 0.15 d of clearance from whole flagfish; $t_{1/2}$ = 0.13 d of clearance from flagfish lipid (Smith et al. 1990).

TABLE 14.1.2.9.1

Reported aqueous solubilities and vapor pressures of 2,4,6-trichlorophenol at various temperatures

Aqueous solubility						Vapor pressure	
Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002		Stull 1947	
shake flask-conductivity		shake flask-optical method		shake flask-optical method*		summary of literature data	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	S/g·m ⁻³	t/°C	P/Pa
19.5	410	314.2	1144	294.9	493.6	76.5	133.3
20.1	427	334.3	1376	304.6	947.8	105.9	666.6
24.9	692	335.3	1377	308.6	933.1	120.2	1333
30.0	928	337.6	1733	314.6	1362	135.8	2666
		342.3	2116	320.9	1323	152.2	5333
		345.3	2377	294.9	493.6	163.5	7999
		352.2	2832	297.7	631.8	177.8	13332
		369.9	3391	302.4	908.3	199.0	26664
		383.8	5419	307.5	1007	222.5	53329
		408.1	7086	313.7	1145	246.0	101325
		420.6	7777	292.8	414.6		
				302.2	888.5	mp/°C	68.5
				308.0	1007		
				317.2	1224		
some data from Achard et al. 1996, Jaoui et al. 1999							

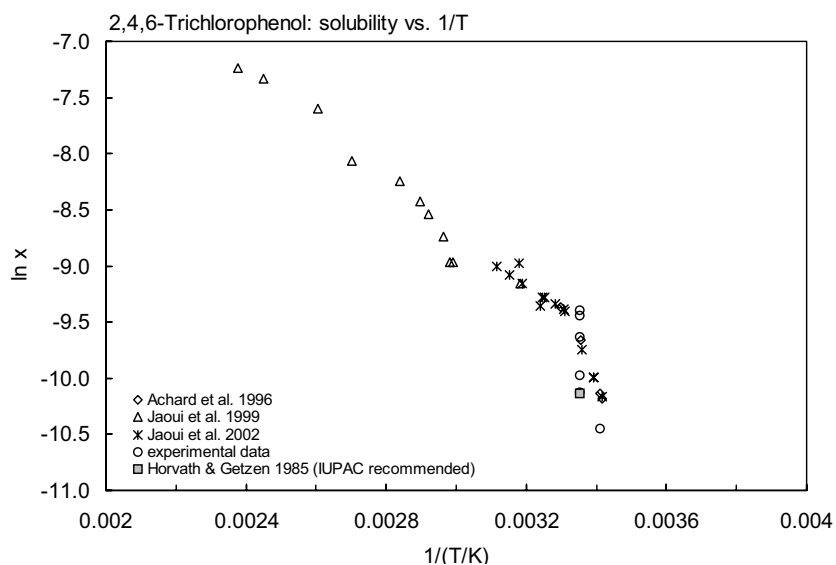


FIGURE 14.1.2.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,4,6-trichlorophenol.

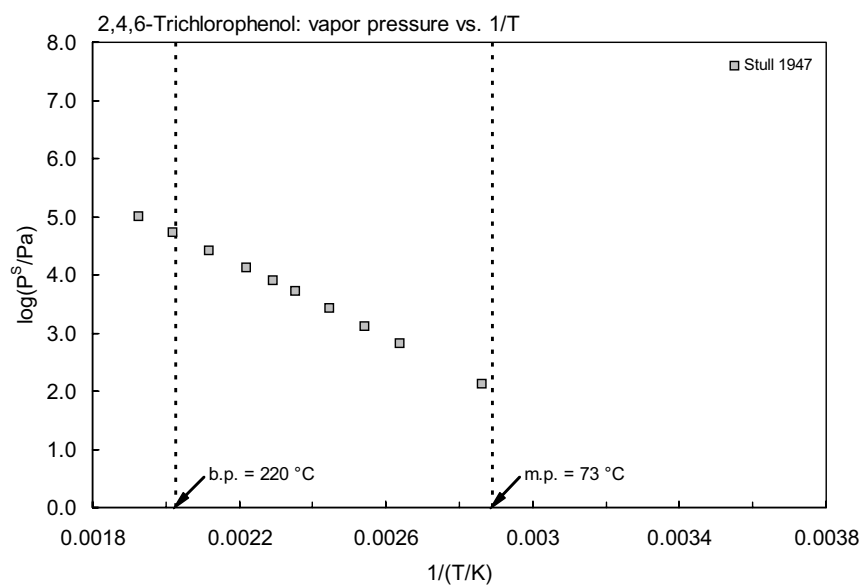
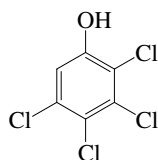


FIGURE 14.1.2.9.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trichlorophenol.

14.1.2.10 2,3,4,5-Tetrachlorophenol



Common Name: 2,3,4,5-Tetrachlorophenol

Synonym:

Chemical Name: 2,3,4,5-tetrachlorophenol

CAS Registry No: 4901-51-3

Molecular Formula: C_6HCl_4OH

Molecular Weight: 231.891

Melting Point ($^{\circ}C$):

116.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.96 (Doedens 1967)

5.30 (Sillén & Martell 1971; Kaiser et al. 1984)

5.64 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Dean 1985; Renner 1990)

6.35 (Schellenberg et al. 1984)

6.61 (Xie & Dyrssen 1984)

6.12 (Nendza & Seydel 1988)

6.48 (Sangster 1993)

Molar Volume (cm^3/mol):

187.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.127 (mp at $116.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

166 (shake flask-HPLC/UV at pH 4.9, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol):

0.140 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.95 (Hansch & Leo 1979)

5.03 (HPLC-RT correlation, Banerjee et al. 1984)

4.21 (shake flask-UV, Beltrame et al. 1984)

4.87 ($20^{\circ}C$, shake flask-HPLC, Schellenberg et al. 1984)

4.82, 4.68 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)

4.71 (shake flask-GC, Xie & Dyrssen 1984)

4.54 (batch equilibration-UV, Beltrame et al. 1988)

4.21 (recommended, Sangster 1993)

4.21 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

- 1.61, 1.60 (earthworm *E. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
 2.55, 2.33 (earthworm *L. rubellus*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
 2.61, 2.73, 3.49, 3.53 (earthworm system, collated from literature, Connell & Markwell 1990)
 0.40, 0.50, 2.30, 4.10 (earthworm system, derived data, Connell & Markwell 1990)

Sorption Partition Coefficient, log K_{OC} :

- 4.21–4.66 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
 3.77–4.01 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
 2.94–3.17 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
 4.11–4.55 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
 3.20–3.60 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
 4.12 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
 3.32 (soil, calculated-MCI χ , Sabljic 1987a,b)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photochemical transformation $t_{1/2} = 0.88$ h in Xenotest 1200 (Svenson & Björndal 1988).

Oxidation:

Hydrolysis:

Biodegradation: 100% reduction in concn (2 μ M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

Biotransformation: degradation rate constant $k = 7.14 \times 10^{-22}$ ($\pm 41\%$ SD) $\text{mol}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ from pure culture studies and $k = 5 \times 10^{-16}$ $\text{mol}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 0.88$ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988).

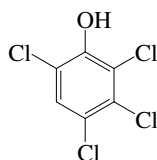
Ground water:

Sediment:

Soil: disappearance $t_{1/2} = 43.4$ d from Kooyenburg soil, $t_{1/2} = 29.1$ d from Holten soil with earthworm *E. fetida andrei* and $t_{1/2} = 26.8$ d from Kooyenburg soil, $t_{1/2} = 42.5$ d from Holten soil with earthworm *L. rebellus* (van Gestel & Ma 1988).

Biota:

14.1.2.11 2,3,4,6-Tetrachlorophenol



Common Name: 2,3,4,6-Tetrachlorophenol

Synonym:

Chemical Name: 2,3,4,6-tetrachlorophenol

CAS Registry No: 58-90-3

Molecular Formula: C_6HCl_4OH

Molecular Weight: 231.891

Melting Point ($^{\circ}C$):

70.0 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

150 (at 15 mm Hg, Weast 1982–83)

Density (g/cm^3):

1.60 (at $60^{\circ}C$, Verschueren 1983)

Acid Dissociation Constant, pK_a :

5.40 (Blackman et al. 1955; Xie 1983; Schellenberg et al. 1984; Sangster 1993)

5.46 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)

5.30 (Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)

5.22 (Ugland et al. 1981; Dean 1985; Lagas 1988; Renner 1990; Ma et al. 1993)

5.62 (Xie & Dyrssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)

Molar Volume (cm^3/mol):

187.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} , (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.362 (mp at $70^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

183 (shake flask-UV at pH 5.1, Blackman et al. 1955)

180 (recommended at pH 5.1, IUPAC Solubility Data Series, Horvath & Getzen 1985)

166 (shake flask-HPLC/UV, pH 4.62, Huang et al. 2000)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.763 (extrapolated-regression of tabulated data, temp range 100 – $275^{\circ}C$, Stull 1947)

0.750 (extrapolated liquid, Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 15362.7/(T/K)] + 9.016052$; temp range 100 – $275^{\circ}C$ (Antoine eq., Weast 1972–73)

0.692 (supercooled liq. value, GC-RT correlation, Hamilton 1980)

0.564 (capillary GC-RT correlation, Bidleman & Renberg 1985)

0.810 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.96172 - 3227.92/(-6.121 + T/K)$; temp range 373 – $548 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$):

0.3548 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.10 (Hansch & Leo 1979)

4.27 (RP-HPLC- k' correlation, Miyake & Terada 1982)

4.45 (shake flask-GC, Saarikoski & Viluksela 1982)

- 4.12 (shake flask-UV, Beltrame et al. 1984)
- 4.42 (shake flask-HPLC/UV, Schellenberg et al. 1984)
- 4.42, 4.34 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)
- 4.31 (shake flask-GC, Xie & Dyrssen 1984)
- 4.42 (OECD 1981 guidelines, Leuenberger et al. 1985)
- 4.25 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
- 4.42 (shake flask, Shigeoka et al. 1988)
- 4.37 (shake flask/batch equilibration-UV, Beltrame et al. 1988)
- 4.45 (recommended, Sangster 1993)
- 4.24 (shake flask-GC, Kishino & Kobayashi 1994)
- 4.45 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 2.65 (trout, Hattula et al. 1981)
- 2.55–2.69 (estimated, NCASI 1992)
- 3.3, 3.8, 4.4, 4.5 (perch bile to water, Söderström et al. 1994)

Sorption Partition Coefficient, log K_{OC} :

- 4.21 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
- 3.77 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
- 2.94 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
- 4.11 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
- 3.20 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
- 3.82 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
- 3.35 (soil, Seip et al. 1986; quoted, Sabljic 1987a,b)
- 3.32 (soil, calculated-MCI χ , Sabljic 1987a,b)
- 3.90 (calculated, Lagas 1988)
- 2.45, 2.70 (totally dissociated as phenolate-calculated, Lagas 1988)
- 3.35 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.02 (2.35–3.69), 3.06 (2.31–3.81), 3.75(3.69–3.81), 2.28(2.16–2.40) (soils: organic carbon $OC \geq 0.1\%$ and pH 3.4–7.5, $OC \geq 0.5\%$, $OC \geq 0.5\%$ pH ≤ 3.4 undissociated, $OC \geq 0.5\%$ pH ≥ 7.4 dissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: aqueous photolysis $t_{1/2} \sim 1$ –336 h, based on aqueous data for 2,4,5- 2,4,6-trichlorophenols and pentachlorophenol (Howard et al. 1991);
photo-degradation rate constant $k = 21 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 30.6 \text{ min}$ for direct UV radiation aqueous solutions (Benitez et al. 2000).

Photooxidation: atmospheric $t_{1/2} = 364.4$ –3644 h, based on estimated rate constant for reaction with OH radical and aqueous $t_{1/2} = 66.0$ –3480 h, based on reaction rate constants with OH and $RO_2\cdot$ radicals with phenol class (Howard et al. 1991);

photo-oxidation rate constant $k = 9 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 49.5 \text{ min}$ for reaction with Fenton's reagent; and $k = 94 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 10.6 \text{ min}$ at pH 2 and $k = 415 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 1.9 \text{ min}$ at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: decomposition in soil suspensions: $t_{1/2} > 72 \text{ d}$ for complete disappearance (Woodcock 1971; quoted, Verschuere 1983);

aqueous aerobic $t_{1/2} = 672$ –4032 h, based on acclimated aerobic screening test data and aqueous anaerobic $t_{1/2} = 2688$ –16128 h, based on unacclimated aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 364.4\text{--}3644$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 0.88$ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{1/2} = 1\text{--}336$ h, based on estimated aqueous photolysis data for trichlorophenols and PCP (Howard et al. 1991);

photo-oxidation $t_{1/2} = 49.5$ min for reaction with Fenton's reagent; $t_{1/2} = 10.6$ min at pH 2, and $t_{1/2} = 1.9$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

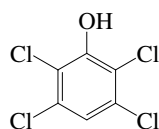
Sediment:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 ± 2 d in Dunkirk silt loam (Alexander & Aleem 1961)

$t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

14.1.2.12 2,3,5,6-Tetrachlorophenol



Common Name: 2,3,5,6-Tetrachlorophenol

Synonym:

Chemical Name: 2,3,5,6-tetrachlorophenol

CAS Registry No: 935-95-5

Molecular Formula: $C_6H_2Cl_4O$, C_6HCl_4OH

Molecular Weight: 231.891

Melting Point ($^{\circ}C$):

115 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

5.30 (Sillen & Martell 1971)

5.03 (Konemann 1981; Ugland et al. 1981)

5.40 (Sangster 1993)

Molar Volume (cm^3/mol):

187.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.131 (mp at $115^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

100 (shake flask-HPLC/UV, pH 5.0, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.90 (Hansch & Leo 1979)

4.42 (calculated-fragment constant, Konemann 1981)

4.88 (HPLC-RT correlation, Butte et al. 1981)

3.88 (shake flask-UV, Beltrame et al. 1984)

4.47 (HPLC-RT correlation, Xie et al. 1984)

3.88 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

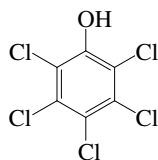
Biodegradation: 100% reduction in concn ($2 \mu M$) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

14.1.2.13 Pentachlorophenol



Common Name: Pentachlorophenol

Synonym: chlorophen, PCP, penchlorol

Chemical Name: pentachlorophenol

CAS Registry No: 87-86-5

Molecular Formula: C_6Cl_5OH

Molecular Weight: 266.336

Melting Point ($^{\circ}C$):

191.0 (Firestone 1977; Weast 198–83)

174 (Lide 2003)

Boiling Point ($^{\circ}C$):

309–310 (dec., Weast 1982–83)

310 (dec., Lide 2003)

Density (g/cm^3):

1.987 (Firestone 1977)

1.978 ($22^{\circ}C$, Weast 1982–83)

Acid Dissociation Constant, pK_a :

4.80 (Blackman et al. 1955; Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)

5.00 (Farquharson et al. 1958; Renner 1990)

4.74 (Drahonovsky & Vacek 1971)

4.71 (spectrophotometric, Cessna & Grover 1978)

5.20 (Renberg 1981; Renner 1990; Larsson et al. 1993)

5.25 (Schellenberg et al. 1984)

4.90 (Xie & Dyrssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)

4.60 (Nendza & Seydel 1988)

Molar Volume (cm^3/mol):

207.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.5 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0350 (mp at $174^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

15.4* (gravimetric method, measured range $0-70^{\circ}C$, Carswell & Nason 1938)

18.0 ($27^{\circ}C$, gravimetric method, Carswell & Nason 1938)

9.59 (shake flask-UV, at pH 5.1, Blackman et al. 1955)

14.0 ($20^{\circ}C$, shake flask-UV, at pH 3.0, Bevenue & Beckman 1967)

10.0 (shake flask-gravimetric, at pH 5.0, Toyota & Kuwahara 1967)

14.0 (gravimetric at pH 5.0, Toyota & Kuwahara 1967)

5–10 (at pH 5–6 in contaminated water, Goerlitz et al. 1985)

14.0 (IUPAC recommended at pH 4.5–5.5, Horvath & Getzen 1985)

8.0 ± 2 (shake flask-UV at pH 2.5, Valsaraj et al. 1991)

32 ± 3 (shake flask-UV at pH 5.0, Valsaraj et al. 1991)

18.4 (shake flask-HPLC/UV, at pH 4.8, Ma et al. 1993)

5.0 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

21.4* ($25.1^{\circ}C$, shake flask-conductimetry, measured range $25.1-46.8^{\circ}C$, Achard et al. 1996)

- 13.0 (shake flask-HPLC/UV, pH 4.55, Huang et al. 2000)
 102* (60.05°C, shake flask-optical method, measured range 333.2–422.3 K, Jaoui et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.0227* (20°C, extrapolated-static method, measured range 100–220°C, Carswell & Nason 1938)
 2666* (192.2°C, summary of literature data, temp range 192.2–309.3°C, Stull 1947)
 0.108* (46.0°C, ebulliometry, measured range 46.0–233.87°C, McDonald et al. 1959)
 0.0147–0.0227 (20°C, Goll 1954; Bevenue & Beckman 1967; Neumüller 1974)
 0.0147 (20°C, Bevenue & Beckman 1967)
 0.100 (extrapolated-Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 16742.6/(T/K)] + 9.150200$; temp range 192.2–309.3°C (Antoine eq., Weast 1972–73)
 0.231 (supercooled liq. extrapolated-Antoine eq., Weast 1976–77; quoted, Bidleman & Renberg 1985)
 0.0213 (Firestone 1977)
 0.0956 (supercooled liquid, GC-RT correlation, Hamilton 1980)
 0.00415 (23°C, OECD, Klöpffer et al. 1982)
 0.1153 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 7.22246 - 2846.009/(230.158 + t/^\circ\text{C})$, temp range 200–253°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 0.115 (capillary GC-RT, supercooled liquid P_L , Bidleman & Renberg 1985)
 0.127 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 8.198 - 3606/(T/K)$, temp range 463–507 K (Antoine eq., Stephenson & Malanowski 1987)
 0.0070* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
 0.0147 (Howard 1991)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 0.284 (calculated-P/C, Mabey et al. 1982)
 0.0025 (calculated-P/C, Hellmann 1987)
 0.0127 (estimated-bond contribution, Hellmann 1987)
 0.277 (calculated-P/C, Howard 1991)
 0.079 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 5.01 (Leo et al. 1971)
 3.81 (Lu & Metcalf 1975)
 5.01, 5.12, 5.86, 3.81 (lit. values, Hansch & Leo 1979)
 5.01 (HPLC-RT correlation, Veith et al. 1979b)
 5.10 (HPLC- k' correlation, Butte et al. 1981)
 4.00 (at pH 4, Renberg 1981)
 5.08 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 5.15 (shake flask-GC, Saarikoski & Viluksela 1982; Saarikoski et al. 1986)
 4.84 (shake flask-GC, apparent value at pH 1.2, Kaiser & Valdmanis 1982)
 1.30 (shake flask-GC, apparent value at pH 10.5, Kaiser & Valdmanis 1982)
 3.69 (Geyer et al. 1982, Schmidt-Bleek et al. 1982)
 3.29 (shake flask average, OECD/EEC Lab. comparison tests, Harnish et al. 1983)
 5.11 ± 0.07 (HPLC-retention volume correlation-ALPM, Garst & Wilson 1984)
 3.69, 3.81 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
 5.24 (shake flask-HPLC/UV, Schellenberg et al. 1984)
 5.04, 5.08 shake flask-GC, HPLC- k' , Xie et al. 1984)
 5.12 (Hansch & Leo 1985)
 5.24 (OECD 1981 guidelines, Leuenberger et al. 1985)
 4.71 (RP-HPLC-RT correlation, Chin et al. 1986)
 2.50 (at pH 4.7, Geyer et al. 1987)
 4.47 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
 5.04 (HPLC-RT correlation, Shigeoka et al. 1988)

- 5.00 (shake flask/batch equilibration-UV, Beltrame et al. 1988)
- 5.18 (recommended, LOGKOW databank, Sangster 1993)
- 5.06, 5.12 (COMPUTOX databank, Kaiser 1993)
- 5.02 (shake flask-GC/ECD, Kishino & Kobayashi 1994)
- 5.12 (recommended, pH 1.4, Hansch et al. 1995)
- 4.74, 4.60, 4.27, 3.69, 3.59 (pH 2.1–3.1, 5.0, 6.1, 7.2, 8.0, shake flask-GC (octanol phase)/HPLC (aqueous phase), measured range pH 2.1–13.3, Nowosielski & Fein 1998)

Bioconcentration Factor, log BCF:

- 3.75 (fish, Statham et al. 1976)
- 3.04 (fish, Körte et al. 1978)
- 2.89 (fathead minnow, Veith et al. 1979)
- 2.89 (fathead minnow, calculated value, Veith et al. 1979b)
- 3.09, 2.64 (algae: exptl., calculated, Geyer et al. 1981)
- 2.00 (trout, Hattula et al. 1981)
- 3.04, 3.10, 3.02 (activated sludge, algae, golden orfe, Freitag et al. 1982)
- 2.54 (mussel *Mytilus edulis*, Geyer et al. 1982)
- 3.69 (calculated- K_{OW} , Mackay 1982)
- 4.20 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.60 (killifish, Trujillo et al. 1982)
- 1.86, 1.72, 1.60 (low-PCP flowing, high-PCP flowing, high-PCP static soft water; Brockway et al. 1984)
- 1.66, 1.62, 1.26 (low-PCP flowing, high-PCP flowing, high-PCP static hard water; Brockway et al. 1984)
- 3.10 (*alga Chlorella fusca* in culture flasks, Geyer et al. 1984; quoted, Brockway et al. 1984)
- 3.10, 2.72 (algae: exptl, calculated- K_{OW} , Geyer et al. 1984)
- 3.10, 3.02, 3.04 (algae, fish, sludge, Klein et al. 1984)
- 3.00 (quoted, LeBlanc 1984)
- 3.04, 3.10, 2.42 (activated sludge, algae, golden ide, Freitag et al. 1985)
- 0.57 (human fat, Geyer et al. 1987)
- 2.99 (zebrafish, Butte et al. 1987; quoted, Devillers et al. 1996)
- 0.46 (15°C, initial concn. 1.0 mg/L uptake by *allolobophora caliginosa* at 24 h, Haque & Ebing 1988)
- 0.38 (15°C, initial concn. 10.0 mg/L uptake by *allolobophora caliginosa* at 24 h, Haque & Ebing 1988)
- 0.80 (whole *allolobophora caliginosa*/soil, uptake from soil after 131 d exposure in outdoor lysimeters, Haque & Ebing 1988)
- 1.35 (whole *lumbricus terrestris*/soil, uptake from soil after 131 d exposure in outdoor lysimeters, Haque & Ebing 1988)
- 2.89 (quoted, Isnard & Lambert 1988)
- 2.80, 2.63 (earthworm *e. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
- 2.80, 2.63 (earthworm *e. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
- 2.66 (daily intake/cow adipose tissue, Travis & Arms 1988; quoted, Hattemer-Frey & Travis 1989)
- 4.38, 4.50, 4.53, 4.90 (earthworm system, collated from literature, Connell & Markwell 1990)
- 4.00, 5.30, 3.40, 8.00 (earthworm system, derived data, Connell & Markwell 1990)
- 2.97, 2.11 (*p. hoyi*, *m. relictus*, Landrum & Dupuis 1990)
- 2.16–2.53 (soft tissue of freshwater mussel, Mäkelä & Oikari 1990)
- 2.33; 3.21 (flagfish: whole fish; fish lipid, Smith et al. 1990)
- 2.78, 2.11, 1.72 (goldfish at pH 7, pH 8, pH 9, Stehly & Hayton 1990)
- 3.0, 3.4, 3.9, 4.0 (perch bile to water, Söderström et al. 1994)
- 2.33; 2.58; 2.89; 2.99; 3.23 (quoted: *Jordanella floridae*; *Oryzias latipes*; *Pimephales promelas*, *Brachydanio rerio*; *Oryzias latipes*; Devillers et al. 1996)
- 3.10 (algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)
- 1.41–1.59, 1.58, 2.01–2.28 (eggshell, yolk sac, embryo of lake salmon *Salmo salar* m. *sebago*, calculated- C_B/C_W , Mäenpää et al. 2004)

Sorption Partition Coefficient, log K_{OC} :

- 2.95 (soil, calculated- K_{OW} , Kenaga & Goring 1980)
- 4.72 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

- 3.11–5.65 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
 3.17–4.54 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
 3.37–3.69 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
 3.00–5.54 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
 2.21–4.49 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
 4.52 (sediment, Schellenberg et al. 1984; quoted, Baker et al. 2000)
 3.73 (quoted average of Kenaga & Goring 1980 & Schellenberg et al. 1984 values, Sabljic 1987a,b)
 3.46 (soil, calculated-MCI χ , Sabljic 1987a,b)
 2.95 (soil, calculated-MCI χ , Bahnick & Doucette 1988)
 4.04 (estimated, HPLC- k' , mobile phase buffered to pH 3, Hodson & Williams 1988)
 4.40 (calculated, Lagas 1988)
 3.10, 3.26 (totally dissociated as phenolate-calculated, Lagas 1988)
 5.27, 5.71 (Bluepoint soil at pH 7.8, pH 7.4, Bellin et al. 1990)
 5.58, 5.52 (Glendale soil at pH 7.3, pH 4.3, Bellin et al. 1990)
 3.49, 3.57 (Norfolk soil at pH 4.3, pH 4.4, Bellin et al. 1990)
 4.32–4.65 (Norfolk + lime soil at pH 6.9, Bellin et al. 1990)
 4.51, 4.54 (neutral form, silt-clay slurries, Jafvert & Weber 1991)
 3.06 (calculated- K_{OW} , Kollig 1993)
 3.73 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.67; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
 3.67, 3.45 (pH 5, 6.5, humic acid from sediments of River Arno, De Paolis & Kukkonen 1997)
 3.64, 3.02 (pH 5, 6.5, HA + FA extracted from sediments of River Arno, De Paolis & Kukkonen 1997)
 3.90, 3.53, 3.29 (pH 5, 6.5, 8, HA extracted from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)
 3.51, 3.26 (pH 5, 6.5, 8, HA + FA from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)
 3.15 (pH 5, HA extracted from water of River Arno, De Paolis & Kukkonen 1997)
 3.40 (pH 5, HA + FA extracted from water of River Arno, De Paolis & Kukkonen 1997)
 3.28, 3.28, 3.15 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH 2.0–> 10, average, Delle Site 2001)
 3.38, 3.51, 2.92 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH 3.4–6.9, average, Delle Site 2001)
 4.48, 4.54, 4.38 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH ≤ 3 undissociated, average, Delle Site 2001)
 2.82, 2.89, 2.63 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH –7.1 dissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization/evaporation: $t_{1/2} = 84$ h from the rate of loss experiment on watch glass for an exposure period of 192 h (Dobbs & Grant 1980);
 stripping loss rate constant $k = 0.0076$ d⁻¹ (Moos et al. 1983);
 $k = 0.028$ d⁻¹ for nondissociated PCP, assuming diffusion coefficient in air to be 7×10^{-6} m²/s and in water 7×10^{-10} m²/s with wind speed 0.1 m above the pond is 2 m/s and the average temperature is 15°C for water depth of 1 m (Crossland & Wolff 1985);
 $k(\text{calc}) = 5 \times 10^{-4}$ d⁻¹ to 1×10^{-7} d⁻¹ for total PCP (Crossland & Wolff 1985).
 Photolysis: photolysis: $t_{1/2}(\text{calc}) = 4.75$ h from observed rate $k = 3.4 \times 10^{-4}$ s⁻¹ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm² between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);
 photolysis $t_{1/2} = 1.5$ d was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);
 exposure of aqueous PCP solutions to either sunlight or laboratory ultraviolet light resulted in rapid degradation at pH 7.3 and slower degradation at pH 3.3 (Wong & Crosby 1981);
 photolytic $t_{1/2} = 10$ –15 d (Brockway et al. 1984); $k = 0.23$ to 0.46 d⁻¹ for direct photo-transformation, is the main loss process for PCP from ponds, with $t_{1/2} = 1.5$ to 3.0 d (Crossland & Wolff 1985);
 photo-transformation rate constants $k = 0.6$ h⁻¹ with $t_{1/2} = 1$ h for distilled water in summer (mean temperature 25°C) and $k = 0.37$ h⁻¹ with $t_{1/2} = 2$ h in winter (mean temperature 11°C); $k = 0.37$ h⁻¹ with $t_{1/2} = 2$ h for

- both poisoned estuarine water and estuarine water in summer and $k = 0.27 \text{ h}^{-1}$ with $t_{1/2} = 3 \text{ h}$ in winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);
- photo-mineralization rate constants $k = 0.11 \text{ h}^{-1}$ with $t_{1/2} = 6 \text{ d}$ for distilled water in summer (mean temperature 25°C) and $k = 0.049 \text{ h}^{-1}$ with $t_{1/2} = 14 \text{ d}$ in winter (mean temperature 11°C); $k = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 6 \text{ d}$ for poisoned estuarine water in summer and $t_{1/2} = 0.07 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ in winter; $k = 0.25 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ for estuarine water in summer and $k = 0.10 \text{ h}^{-1}$ with $t_{1/2} = 7 \text{ d}$ for winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);
- photochemical transformation $t_{1/2} = 0.75 \text{ h}$ in Xenotest 1200 (Svenson & Björndal 1988);
- aqueous $t_{1/2} = 1\text{--}110 \text{ h}$ (Hwang et al. 1986; Sugiura et al. 1984; selected, Howard et al. 1991)
- $t_{1/2} = 7.43 \text{ d}$, assuming a linear rate of photolysis during 96-h period, (Smith et al. 1987)
- photodegradation $k = 0.60 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 1.0 \text{ h}$ (summer), $k = 0.37 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 2 \text{ h}$ (winter) in distilled water; and $t_{1/2} = 0.37 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 2 \text{ h}$ (summer), 0.27 h^{-1} corresponding to a $t_{1/2} = 3.0 \text{ h}$ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).
- Oxidation: aqueous oxidation rate constant $k < 7 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);
- $k \gg 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ with 3 mM AcOH as scavenger for the reaction with ozone in water at pH 2.0 (Hoigné & Bader 1983b);
- photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reported reaction rate constants for reaction of OH and RO_2 radicals with phenol class in aqueous solution (Mill & Mabey 1985; Güesten et al. 1981; quoted, Howard et al. 1991);
- photooxidation $t_{1/2} = 139.2\text{--}1392 \text{ h}$, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- rate constant $k = 4.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in air (Bunce et al. 1991)
- rate constant $k = (0.2 \pm 5.5) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991);
- atmospheric $t_{1/2} < 24 \text{ h}$ at noon in mid-summer to $t_{1/2} = 216 \text{ h}$ in January at latitude of 41.79°N for reaction with OH radical (Bunce et al. 1991).
- Hydrolysis: is not expected to occur (Crossland & Wolff 1985).
- Biodegradation: first order microbial degradation rate constant $k = 7.4 \times 10^{-4} \text{ h}^{-1}$ in sediment and water (Yoshida & Kojima 1978, quoted, Addison et al. 1983);
- $t_{1/2} = 1800\text{--}2160 \text{ h}$ and $480\text{--}\infty \text{ h}$ to obtain 75% degradation in mineral medium and seawater, respectively (de Kreuk & Hanstveit 1981);
- $k = 0.10 \text{ d}^{-1}$ with a $t_{1/2} = 7 \text{ d}$ in unadapted Nutrient Broth and $k = 1.0 \text{ d}^{-1}$ with a $t_{1/2} = 0.7 \text{ d}$ in adapted Nutrient Broth under aerobic conditions (Mills et al. 1982);
- aqueous aerobic $t_{1/2} = 552\text{--}4272 \text{ h}$, based on unacclimated and acclimated aerobic sediment grab sample data (Delaune et al. 1983; Baker & Mayfield 1980; quoted, Howard et al. 1991);
- aqueous anaerobic $t_{1/2} = 1008\text{--}36480 \text{ h}$, based on unacclimated anaerobic grab sample data for soil and ground water (Ide et al. 1972; Baker & Mayfield 1980; quoted, Howard et al. 1991);
- aerobic degradation rate constant $k = 0.0017 \text{ L } \mu\text{g}^{-1} \cdot \text{d}^{-1}$ (Moos et al. 1983);
- microbial degradation negligible in darkness (Hwang et al. 1986);
- 100% reduction in concn ($2 \mu\text{M}$) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)
- degradation rate constant $k = 0.12 \pm 0.01 \text{ h}^{-1}$ in the absence of light (Minero et al. 1993).
- $t_{1/2}(\text{aerobic}) = 23 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 42 \text{ d}$ in natural waters (Capel & Larson 1995)
- Biotransformation: first order fish metabolism $k = 1.5 \times 10^{-5} \text{ h}^{-1}$ (Sanborn et al. 1975, quoted, Addison et al. 1983);
- bacterial transformation $k = 3 \times 10^9 \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982);
- degradation rate $k = 3 \times 10^{-14} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).
- Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:
- $k_1 = 18.3 \text{ h}^{-1}$, 19 h^{-1} (at 1 mM buffer concn.), 18.5 h^{-1} (at 10 mM buffer concn.) at pH 8 (guppy *p. reticulata*, Saarikoski et al. 1986)
- $k_1 = 222 \text{ d}^{-1}$, 1677 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)
- $k_2 = 1.03 \text{ d}^{-1}$, 1.03 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

$k_2 = 1.03 \text{ d}^{-1}$, 0.95 d^{-1} (flagfish: BCF based, toxicity based, Smith et al. 1990)
 $k_2 = 0.00195 \pm 0.00063 \text{ h}^{-1}$ (*m. relictus*, Landrum & Dupuis 1990)
 $k_2 = 0.00330 \pm 0.00140 \text{ h}^{-1}$ (*p. hoyi*, Landrum & Dupuis 1990)
 $k_1 = 662.4 \text{ d}^{-1}$, $k_2 = 0.502 \text{ d}^{-1}$ (algae *Chlorella fusca*, Wang et al. 1996)
 $k_1 = 0.733 \text{ d}^{-1}$, $k_2 = 0.020 \text{ d}^{-1}$ (eggshell of dissected parts of lake salmon, Mäenpää et al. 2004)
 $k_1 = 0.680 \text{ d}^{-1}$, $k_2 = 0.000 \text{ d}^{-1}$ (yolk sac of dissected parts of lake salmon, Mäenpää et al. 2004)
 $k_1 = 2.828 \text{ d}^{-1}$, $k_2 = 0.015 \text{ d}^{-1}$ (embryo of dissected parts of lake salmon, Mäenpää et al. 2004)

Half-Lives in the Environment:

- Air: tropospheric lifetime of 4 d for reaction with OH radical on March 21 at 43°N (Bunce et al. 1991);
 $t_{1/2} = 139.2\text{--}1392 \text{ h}$, based on an estimated rate constant for the vapor phase reaction with hydroxyl radicals in air; photolysis $t_{1/2} = 6.5 \text{ h}$ in noonday summer sunshine (Howard 1991);
 atmospheric transformation lifetime was estimated to be $> 5 \text{ d}$ (Kelly et al. 1994).
- Surface water: calculated photolysis $t_{1/2} = 4.75 \text{ h}$ from a determined rate $k = 3.4 \times 10^{-4} \text{ s}^{-1}$ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm² between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);
 photolysis $t_{1/2} = 1.5 \text{ d}$ was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);
 photolytic $t_{1/2} = 10\text{--}15 \text{ d}$ (Brockway et al. 1984);
 rate constant $k \gg 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 2.0 (Hoigné & Bader 1983);
 estimated direct photolysis midday $t_{1/2} = 20 \text{ min}$ from experimentally determined rate constant $k = 2.1 \text{ h}^{-1}$ (quoted unpublished result, Zepp et al. 1984);
 $t_{1/2} = 1.5 \text{ to } 3.0 \text{ d}$ for direct photo-transformation from outdoor ponds (Crossland & Wolff 1985);
 $t_{1/2} = 1 \text{ h}$ (summer), $t_{1/2} = 2 \text{ h}$ (winter) for distilled water; $t_{1/2} = 2 \text{ h}$ (summer), $t_{1/2} = 3 \text{ h}$ (winter) for estuarine water; $t_{1/2} = 2 \text{ h}$ (summer), $t_{1/2} = 3 \text{ h}$ (winter) for poisoned estuarine water, based on photo-transformation rate constants (Hwang et al. 1986); $t_{1/2} = 6 \text{ d}$ (summer), $t_{1/2} = 14 \text{ d}$ (winter) for distilled water; $t_{1/2} = 3 \text{ d}$ (summer), $t_{1/2} = 7 \text{ d}$ (winter) for estuarine water; $t_{1/2} = 6 \text{ d}$ (summer), $t_{1/2} = 10 \text{ d}$ (winter) for poisoned estuarine water, based on photo-mineralization rate constants (Hwang et al. 1986);
 $t_{1/2} = 0.75 \text{ h}$ and 0.96 h , based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);
 $t_{1/2} = 1\text{--}110 \text{ h}$, based on aqueous photolysis half-life (Howard et al. 1991);
 photodegradation half-lives ranging from hours to days, more rapid at the surface (Howard 1991);
 photodegradation $t_{1/2} = 1.0 \text{ h}$ (summer), $t_{1/2} = 2.0 \text{ h}$ (winter) in distilled water and $t_{1/2} = 2.0 \text{ h}$ (summer), $t_{1/2} = 3.0 \text{ h}$ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).
 $t_{1/2}(\text{aerobic}) = 23 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 42 \text{ d}$ in natural waters (Capel & Larson 1995)
- Ground water: $t_{1/2} = 1104\text{--}36480 \text{ h}$, based on estimated unacclimated aqueous aerobic sediment grab sample data (Delaune et al. 1983; selected, Howard et al. 1991) and unacclimated anaerobic grab sample data for ground water (Baker & Mayfield 1980; selected, Howard et al. 1991).
- Sediment: first order microbial degradation rate constant $k = 7.4 \times 10^{-4} \text{ h}^{-1}$ in sediment and water (Yoshida & Kojima 1978, quoted, Addison et al. 1983).
- Soil: Days for complete disappearance by microbial decomposition in soil suspension: $72 + \text{d}$ in Dunkirk silt loam (Alexander & Aleem 1961)
 disappearance $t_{1/2} = 23.2 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 47.9 \text{ d}$ from Holten soil with earthworm *e. fetida andrei* and $t_{1/2} = 27.4 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 31.8 \text{ d}$ from Holten soil with earthworm *I. rubellus* (van Gestel & Ma 1988);
 $t_{1/2} = 552\text{--}4272 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
 $t_{1/2} = 2.0 \text{ d}$ in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 6.7 \text{ d}$ in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).
- Biota: biological $t_{1/2} = 30 \text{ d}$ in guppy *lebistes reticulatus* (Landner et al. 1977);
 elimination $t_{1/2} = 23, 9.3, 6.9$, and 6.2 h for fat, liver muscle, and blood, respectively (rainbow trout, Call et al. 1980);
 estimated $t_{1/2} = 7.0 \text{ d}$ in trout (Niimi & Cho 1983; quoted, Niimi & Palazzo 1985);
 clearance from flagfish: $t_{1/2} = 0.68 \text{ d}$ from whole fish and $t_{1/2} = 0.68 \text{ d}$ from fish lipid (Smith et al. 1990).

TABLE 14.1.2.13.1
Reported aqueous solubilities of pentachlorophenol at various temperatures

Carswell & Nason 1938		Achard et al. 1996		Jaoui et al. 1999	
shake flask		shake flask-conductivity		static visual method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
0	5	25.1	21.4	333.2	102
27	18	34.5	57.8	342.7	118.4
50	35	46.8	86.2	353.2	140.6
62	58			361.2	156.8
70	85			372.0	173.1
				386.0	195.3
				402.0	211.6
				407.0	232.3
				422.3	253.0

Note: PCP data in Table I incorrect, correction made
Figure 3 in ref
based on Figure 3 in ref.

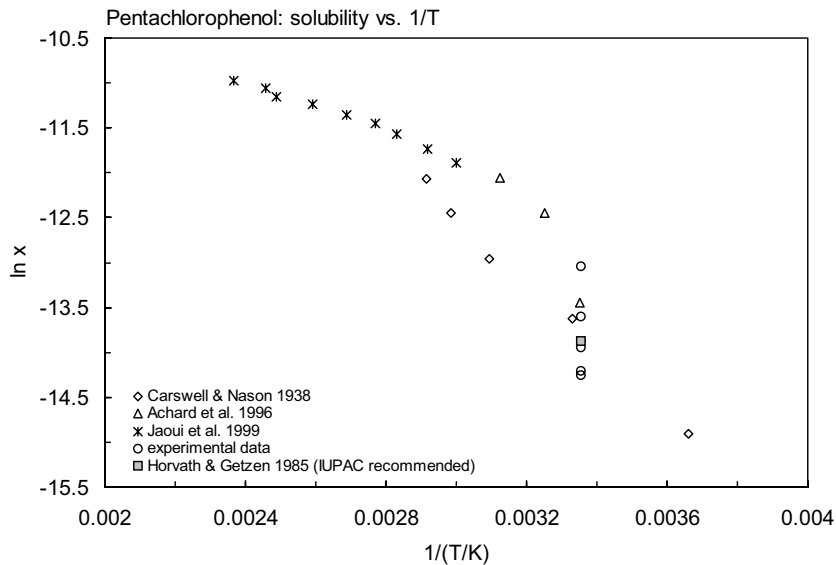


FIGURE 14.1.2.13.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for pentachlorophenol.

TABLE 14.1.2.13.2

Reported vapor pressures of pentachlorophenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P= A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Carswell & Nason 1938		Stull 1947		McDonald et al. 1959		Rordorf 1989	
static method		summary of literature data		ebulliometry		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	0.00227*	192.2	2666	46.0	0.108	25	0.0070
20	0.0227*	211.2	5333	60.0	0.1853	50	0.110
50	0.4133*	223.4	7999	70.0	0.2573	75	1.20
75	3.200*	239.6	13332	71.8	0.3960	100	9.50
100	18.67	261.8	26664	80.0	0.9746	125	57.0
120	63.99	285.0	53329	93.6	3.3597		
140	200.0	309.3	101325	106.5	8.5460		for solid
160	573.3			119.5	23.60	eq. 1	P _s /Pa
180	1453	mp/°C	188.5	200.6	4133	A	13.413
200	3413			215.51	6759	B	4640.9
220	7493			233.87	12279		
240	14705*						for liquid
260	30358*			eq. 2	P/mmHg	eq. 1	P _L /Pa
280	56622*			A	9.073	A	11.47085
300	101112*			B	3606.0	B	3750.68
300.6	101325			C	273.15		
measured range 100–220°C				mp/°C	189.65		
*extrapolated from graph							

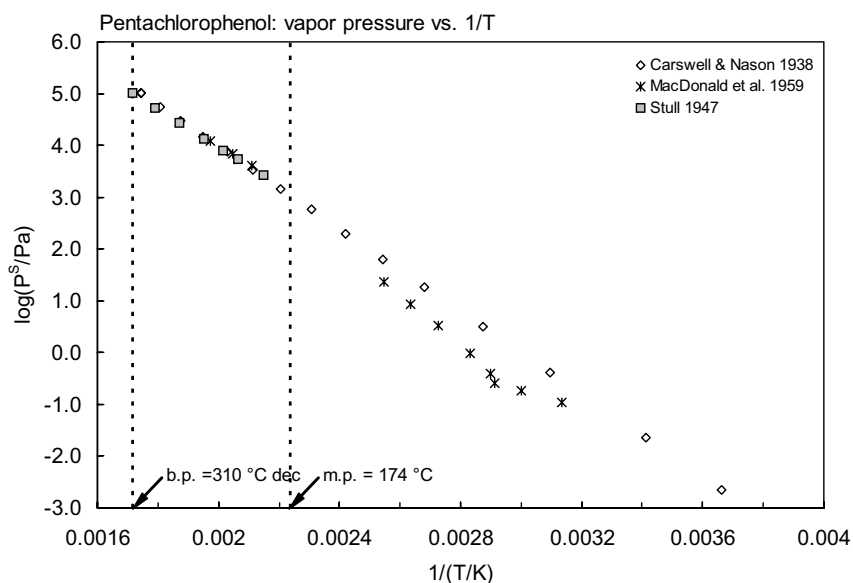
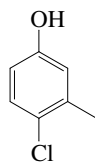


FIGURE 14.1.2.13.2 Logarithm of vapor pressure versus reciprocal temperature for pentachlorophenol.

14.1.2.14 4-Chloro-*m*-cresol

Common Name: 4-Chloro-*m*-cresol

Synonym: *p*-chloro-*m*-cresol, 2-chloro-5-hydroxytoluene, 4-chloro-3-methylphenol

Chemical Name: 4-chloro-*m*-cresol, 4-chloro-3-methylphenol

CAS Registry No: 59-50-7

Molecular Formula: C_7H_7ClO , $CH_3(Cl)C_6H_3OH$

Molecular Weight: 142.583

Melting Point ($^{\circ}C$):

67 (Lide 2003)

Boiling Point ($^{\circ}C$):

235.0 (Weast 1977; Callahan et al. 1979; Dean 1985; Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

146.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, $F: 0.387$ (mp at $67^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3990 (shake flask-UV with buffer at pH 5.1, Blackman et al. 1955)

3990 (IUPAC selected, Horvath & Getzen 1985)

3650 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

6.67 (Mabey et al. 1982)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

0.253 ($20^{\circ}C$, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.18 (Hansch & Leo 1979)

2.95 (calculated as per Tute 1971, Callahan et al. 1979)

3.10 (HPLC-RT correlation, Veith et al. 1979)

3.10 (recommended, Sangster 1993)

3.10 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.60 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{oc}$:

2.78 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

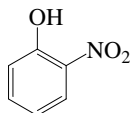
Oxidation: rate constants $k < 7 \times 10^5 M^{-1} h^{-1}$ for singlet oxygen and $k = 1 \times 10^7 M^{-1} h^{-1}$ for peroxy radical (Mabey et al. 1982).

Biotransformation: bacterial transformation $k = 3 \times 10^{-9} mL cell^{-1} h^{-1}$ in water (Mabey et al. 1982).

Half-Lives in the Environment:

14.1.3 NITROPHENOLS

14.1.3.1 2-Nitrophenol



Common Name: 2-Nitrophenol

Synonym: *o*-nitrophenol, 2-hydroxynitrobenzene

Chemical Name: 2-nitrophenol

CAS Registry No: 88-75-5

Molecular Formula: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$

Molecular Weight: 139.109

Melting Point ($^{\circ}C$):

44.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

216.0 (Weast 1982-83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.485, 1.2942 (14, $40^{\circ}C$, Weast 1982-83)

131.9 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

7.21 (Pearce & Simkins 1968)

7.23 (Serjeant & Dempsey 1979)

8.28 (Mabey et al. 1982)

7.22 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.57 (Tsonopoulos & Prausnitz 1971)

17.44 (Beneš & Dohnal 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

55.23 (Tsonopoulos & Prausnitz 1971)

48.95, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.630 (mp at $44.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3210* ($38.4^{\circ}C$, shake flask-residue volume method, measured range 34.8 – $196^{\circ}C$, critical solution temp above $200^{\circ}C$, Sidgwick et al. 1915)

1390, 1095 ($20^{\circ}C$, shake flask-UV, calculated, Hashimoto et al. 1984)

1080* ($20 \pm 0.5^{\circ}C$, shake flask-UV with buffer at pH 1.5, measured range 5 – $30^{\circ}C$, Schwarzenbach et al. 1985)

2100 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

1697* ($24.8^{\circ}C$, shake flask-conductimetry, measured range 15.6 – $34.7^{\circ}C$, Achard et al. 1996)

1350* ($20^{\circ}C$, shake flask-UV spectrophotometry, measured range 10 – $40^{\circ}C$, Beneš & Dohnal 1999)

1169* ($17.35^{\circ}C$, shake flask-optical method, measured range 290.5 – $322.7\ K$, Jaoui et al. 2002)

$\ln [S/(mol\ kg^{-1})] = 16.237 - 4672.3/(T/K)$; temp range 288 – $308\ K$ (eq. derived using reported exptl. data, Jaoui et al. 2002)

$\ln [S/(mol\ kg^{-1})] = 6.9022 - 1784.4/(T/K)$; temp range 308 – $332\ K$ (eq. derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

29.10* (extrapolated-regression of tabulated data, temp range 49.3 – $214.5^{\circ}C$, Stull 1947)

$\log (P/mmHg) = [-0.2185 \times 12497.3/(T/K)] + 8.497320$; temp range 49.3 – $214.5^{\circ}C$ (Antoine eq., Weast 1972-73)

- 24.43 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 487.905/(T/K)] \times 10^4 \{0.885400 - 6.30106 \times 10^{-4} \cdot (T/K) + 6.42867 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 322.5–487.7 K (Cox eq., Chao et al. 1983)
 12.4 \pm 0.2 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
 17.25 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 7.8446 - 2864.6/(T/K)$, temp range 273–292 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.04963 - 1571.7/(-101.17 + T/K)$, temp range 366–490 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 18.86 (supercooled liquid P_L at 20°C, GC-RT correlation, Schwarzenbach et al. 1988)
 10.61 (20°C, solid P_s , converted from P_L with ΔS_{fus} and mp, Schwarzenbach et al. 1988)
 $\log (P/\text{atm}) = 5.735 - 2776/(T/K)$ (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.766 (calculated-P/C, Mabey et al. 1982)
 0.355 (Leuenberger et al. 1985)
 1.367 (20°C, calculated-P/C, Schwarzenbach et al. 1988)
 1.25* (gas stripping-UV, measured range 5–40°C, Müller & Heal 2001)
 $\ln [H/(M \text{ atm}^{-1})] = 6290/(T/K) - 16.6$; temp range 278–303 K (gas stripping-UV, Müller & Heal 2001)
 1.178* (gas stripping-UV, measured range 284–302 K, Harrison et al. 2002)
 $\ln [H/(M \text{ atm}^{-1})] = 6270/(T/K) - 16.6$; temp range 284–302 K, Harrison et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

- 1.79 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971)
 2.00 (shake flask, Umeyama et al. 1971)
 1.25, 1.18 (calculated-fragment const., calculated- π const., Rekker 1977)
 1.79 (shake flask, Korenman et al. 1977)
 1.68 (shake flask at pH 7, Unger et al. 1978)
 1.35 (HPLC-RT correlation, Veith et al. 1979)
 1.91 (HPLC-RT correlation, Miyake et al. 1986)
 1.89 ($21.5 \pm 0.5^\circ\text{C}$, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)
 1.76 (shake flask-UV, Kramer & Henze 1990)
 1.68 (CPC-RV at pH 7.4, El Tayar et al. 1991)
 2.24 (HPLC-RT correlation, Saito et al. 1993)
 1.77 (recommended, Sangster 1993)
 1.85, 1.79 (COMPUTOX databank, Kaiser 1993)
 1.79, 1.68 (recommended, value at pH 7.4; Hansch et al. 1995)
 2.03 (solid-phase microextraction, Dean et al. 1996)
 1.63, 1.99, 2.28, 1.90 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, $\log \text{BCF}$:

- 2.10 (bluegill sunfish, Veith et al. 1980)
 1.23 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)
 1.15 (calculated- K_{ow} , Howard 1989)

Sorption Partition Coefficient, $\log K_{\text{oc}}$:

- 1.43 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)
 1.81 (soil, calculated-S, quoted, Howard 1989)
 2.17; 2.50 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
 2.424, 1.507, 1.852, 1.763, 2.336 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
 2.043, 1.758, 1.854, 1.708, 2.283 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)

2.043, 1.758, 1.854, 1.708, 2.283 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} = 296$ h from a model river was estimated using Henry's law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind (Howard 1989)

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

rate constant $k < 2 \times 10^5 \text{ M}^{-1}\cdot\text{h}^{-1}$ for singlet oxygen, and $k = 2 \times 10^6 \text{ M}^{-1}\cdot\text{h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

$k_{OH} = 0.922 \times 10^{-12} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ at 296 K (Becker et al. 1984; quoted, Carrier et al. 1986);

$k_{OH}(\text{exptl}) = 0.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{OH}(\text{exptl}) = 0.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 4.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1987)

$k_{OH} = 0.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (Atkinson 1989)

photooxidation $t_{1/2} = 7\text{--}71$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Howard et al. 1991)

$k_{O_3} = 2.0 \times 10^{-23} \text{ cm}^3\cdot\text{molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–323 K (quoted, Atkinson & Carter 1984)

$k_{OH} = (2.34 \pm 0.33) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(24.6 \pm 0.4)^\circ\text{C}$ (Edney et al. 1986)

$k_{OH} = 2.34 \times 10^{-12} \text{ cm}^3\cdot\text{molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{NO_3} = 9.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{NO_3} < 0.02 \times 10^{-12} \text{ cm}^3\cdot\text{molecule}^{-1} \text{ s}^{-1}$ at 296 K and $k_{OH} = 0.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

aqueous photooxidation $t_{1/2} = 480$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992)

photo-transformation decay rate constant $k = 0.27 \text{ min}^{-1}$ on 0.2 g/L of TiO_2 solution (Minero et al. 1993).

Hydrolysis: resistant to hydrolysis (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $14.0 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

time necessary for complete degradation of 16 mg/L in 3–5 d by wastewater and 7–14 d by soil (Haller 1978);

aqueous aerobic $t_{1/2} = 168\text{--}672$ h, based on unacclimated aerobic screening test data (Sasaki 1978; Gerike & Fischer 1979; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 168\text{--}672$ h, based on anaerobic soil grab sample data (Sudhakar-Barik & Sethunathan 1978; selected, Howard et al. 1991).

Biotransformation: estimated bacterial transformation rate constant of $2 \times 10^{-9} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 14$ h for the gas phase reaction with hydroxyl radical (GEMS 1986; quoted, Howard 1989)

photooxidation $t_{1/2} = 7\text{--}71$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: $t_{1/2} = 168\text{--}672$ h, based on aerobic river die-away test data (Ludzack et al. 1958; selected value, Howard et al. 1991);

volatilization $t_{1/2} = 12$ d from a model river was estimated using Henry's law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind and $t_{1/2} = 1\text{--}8$ d in freshwater (Howard 1989);

calculated $t_{1/2} = 390$ h for a body of water with 1 m in depth (Schmidt-Bleek et al. 1982; quoted, Howard 1989);

photooxidation $t_{1/2} = 480$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

Groundwater: $t_{1/2} = 336\text{--}672$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 10$ d in flooded soil (Howard 1989);

$t_{1/2}$ = 168–672 h, based on estimated aqueous aerobic biodegradation half-life and anaerobic soil grab sample data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991).

Biota:

TABLE 14.1.3.1.1

Reported aqueous solubilities of 2-nitrophenol at various temperatures

Sidgwick et al. 1915		Schwarzenbach et al. 1988		Beneš & Dohnal 1999		Jaoui et al. 2002	
shake flask-synthetic method		shake flask-UV spec.		shake flask-UV spec		shake flask-optical method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
solid							
38.4	3210	0	747	10	895	17.35	1169
42.8	3460	10	898	20	1350	31.35	2434
47.5	3760	20	1080	30	2000	36.85	3144
59.4	4550	30	1457	40	2840	49.55	3951
65.7	5130	for supercooled liquid		17.35		1169	
72.8	5890	0	2058	mp/K	317.95	30.05	2281
80.3	6900	10	1920	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 17.44$		37.55	3186
88.9	8330	20	2011	Enthalpies of solution*:		49.55	3951
109.9	13430	30	1877	$\Delta H_{\text{sol}}(\text{solid}) = 28.7 \text{ kJ mol}^{-1}$		17.35	1169
151.8	30300			$\Delta H_{\text{sol}}(\text{liq.}) = 11.2 \text{ kJ mol}^{-1}$		31.25	2434
169.5	50400					36.85	3144
196.5	99000					49.55	3951
...	...	Achard et al. 1996					
196.5	906800	shake flask-conductimetry					
163.4	951400	t/°C	S/g·m ⁻³				
91.7	984800						
82.9	987300	15.6	1076				
59.3	992400	24.8	1697				
43.6	995100	34.7	2935				
44.9	1000000						
critical solution temp >200°							
triple point 43.5°C							

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

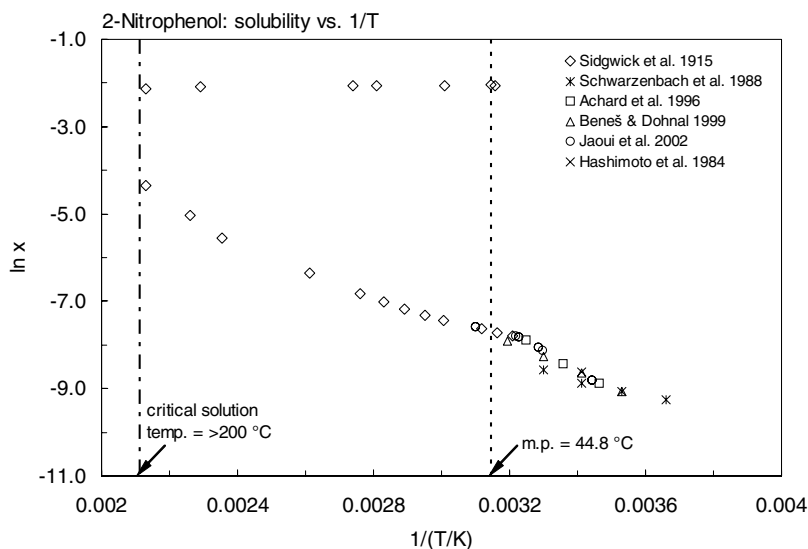


FIGURE 14.1.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-nitrophenol.

TABLE 14.1.3.1.2

Reported vapor pressures and Henry's law constants of 2-nitrophenol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Vapor pressure		Henry's law constant			
Stull 1947		Müller & Heal 2001		Harrison et al. 2002	
summary of literature data		gas stripping-UV spec.		gas stripping-UV	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$	T/K	$H/(\text{Pa m}^3/\text{mol})$
non-equilibrium					
49.3	133	5	0.274	281	0.362
76.8	666.6	10	0.442	284.5	0.396
90.4	1333	15	0.600	289.5	0.607
105.8	2666	20	0.641	293.5	0.930
122.1	5333	25	1.267	298	1.178
132.6	7999	30	1.689	302	1.559
146.4	13332	equilibrium			
167.6	26664	5	0.242	eq. 4	$H=/(M \text{ atm}^{-1})$
191.0	53329	10	0.409	A	-16.6
214.5	101325	15	0.569	B	-6270
		20	0.714		
mp/ $^{\circ}\text{C}$	45	25	1.251		
		30	1.608		
		eq.4	$H=/(M \text{ atm}^{-1})$		
		A	-16.6		
		B	-6290		
For gas-to-liquid transfer					
$\Delta H^{\circ}/(\text{kJ mol}^{-1}) = -52.3 \pm 8.1$					
$\Delta S^{\circ}/(\text{J mol}^{-1}\text{K}^{-1}) = -138 \pm 28$					

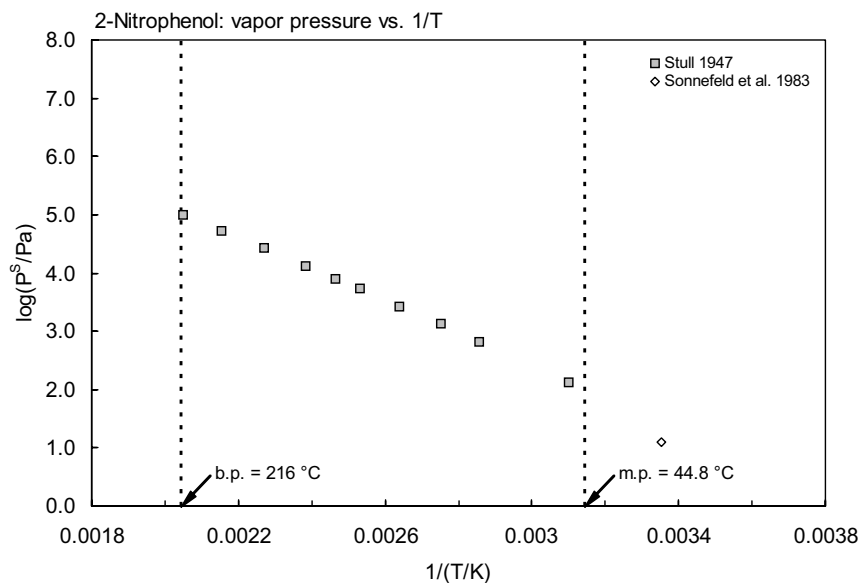


FIGURE 14.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for 2-nitrophenol.

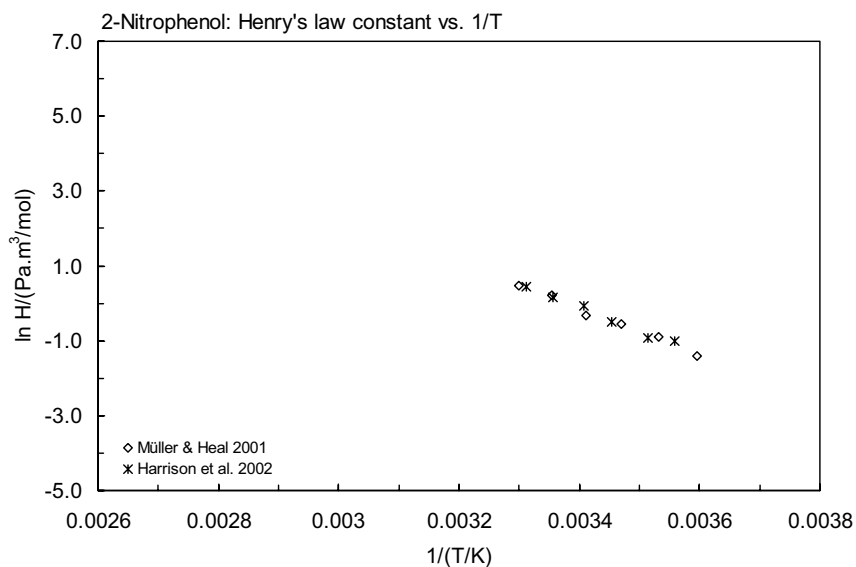
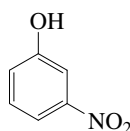


FIGURE 14.1.3.1.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-nitrophenol.

14.1.3.2 3-Nitrophenol



Common Name: 3-Nitrophenol

Synonym: *m*-nitrophenol

Chemical Name: 3-nitrophenol

CAS Registry No: 554-84-7

Molecular Formula: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$

Molecular Weight: 139.109

Melting Point (°C):

96.8 (Lide 2003)

Boiling Point (°C):

194.0 (at 70 mm Hg, Weast 1982–83)

Density (g/cm³ at 20°C):

1.2797 (10°C, Verschueren 1983)

Molar Volume (cm³/mol):

108.7 (100°C, Stephenson & Malanowski 1987)

131.9 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a:

8.00 (Fieser & Fieser 1958)

8.36 (Serjeant & Dempsey 1979; Dean 1985; Howard 1989; Haderlein & Schwarzenbach 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.34 (Tsonopoulos & Prausnitz 1971)

19.20 (Beneš & Dohnal 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

57.74 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.197 (mp at 96.8°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

30300* (40.4°C, shake flask-residue volume method, measured range 40.4–98.7°C, critical solution temp 98.7°C, Sidgwick et al. 1915)

13000 (shake flask-UV spectrophotometry, Roberts et al. 1977)

11546 (20°C, shake flask-UV, Hashimoto et al. 1984)

10800* (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

3.83×10^{-2} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 8.93697 - 3981.386/(T/\text{K})$, temp range 305–334 K (solid, Antoine eq., Stephenson & Malanowski 1987)

99.98 (Weber et al. 1981)

Henry's Law Constant (Pa·m³/mol at 25°C):

2.203×10^{-4} (quoted, Gaffney et al. 1987)

1.033 (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

2.00 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971)

2.00 (shake flask-UV at pH 5.6, Umeyama et al. 1971)

2.00 (20°C, shake flask, Korenman et al. 1976)

2.02	(Scherrer & Howard 1979)
1.74	(HPLC-RT correlation, Butte et al. 1981)
2.05	(Beltrame et al. 1988, 1989)
2.01, 2.03	(shake flask, HPLC-RT correlation, Wang et al. 1989)
1.88	(shake flask-UV, Kramer & Henze 1990)
1.74	(centrifugal partition chromatography CPC-RV at pH 7.4, El Tayar et al. 1991)
2.00	(recommended, Sangster 1993)
1.92, 1.51	(COMPUTOX databank, Kaiser 1993)
2.00	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.40	(goldfish, ratio of rate constant k_1/k_2 , Nagel & Urich 1980)
1.40	(<i>Brachydanio rerio</i> , Butte et al. 1987)
1.28	(estimated- K_{ow} , Howard 1989)

Sorption Partition Coefficient, log K_{OC} :

1.72	(Brookton clay loam, Boyd 1982)
1.36	(soil, estimated-S, Howard 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} = 4.2$ d from a model river was estimated using Henry's law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind (Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{1/2} \sim 14$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard 1989);

phototransformation decay rate $k = 0.18 \text{ min}^{-1}$ in 0.2 g/L of TiO_2 solution (Minero et al. 1993).

Hydrolysis: resistant to hydrolysis (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);

decomposition by a soil microflora in 4 d (Alexander & Lustigman 1966; quoted, Verschuereen 1983)

complete degradation of 16 mg/L in 3–5 d by wastewater, and 3–5 d by soil (Haller 1978);

average rate of biodegradation $17.5 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2} = 6.3$ d or less in flooded soil under anaerobic conditions (Howard 1989)

$t_{1/2}(\text{aerobic}) = 0.76$ d, $t_{1/2}(\text{anaerobic}) = 6.8$ d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 1.54 \text{ h}^{-1}$; $k_2 = 0.00 \text{ h}^{-1}$ (goldfish, Nagel & Urich 1980)

Half-Lives in the Environment:

Air: $t_{1/2} = 14$ h for reaction with hydroxyl radical in vapor phase (Howard 1989).

Surface water: $t_{1/2} = 4.2$ d in a model river (Howard 1989)

$t_{1/2}(\text{aerobic}) = 0.76$ d, $t_{1/2}(\text{anaerobic}) = 6.8$ d in natural waters (Capel & Larson 1995).

Groundwater:

Sediment:

Soil: $t_{1/2} = 6.3$ d in flooded soil under anaerobic conditions (Howard 1989).

Biota: elimination from goldfish within 4 h (Nagel & Urich 1980).

TABLE 14.1.3.2.1
Reported aqueous solubilities of 3-nitrophenol at various temperatures

Sidgwick et al. 1915						Beneš & Dohnal 1999	
shake flask-synthetic method						shake flask-UV spec	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
40.4	30300	98.5	291000	72.7	673800	10	7200
49.5	36500	98.5	351300	55.8	715600	20	10800
61.1	46600	98.6	388400	42.3	758900	30	16700
67.1	54200	98.7	409400	43.9	793200	40	19000
79.1	76400	98.5	431200	62.0	899000		
85.1	94700	97.9	481200	95.1	1000000	mp/K	369.95
88.5	109400	94.5	539500			$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 19.20$	
93.2	139200	91.9	571900	critical solution temp 98.7°C		Enthalpies of solution*:	
97.1	188500	87.3	607400	triple point 41.5°C		$\Delta H_{\text{sol}}(\text{solid}) = 29.3 \text{ kJ mol}^{-1}$	
98.0	215500	82.6	634700			$\Delta H_{\text{sol}}(\text{liq.}) = 16.1 \text{ kJ mol}^{-1}$	

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

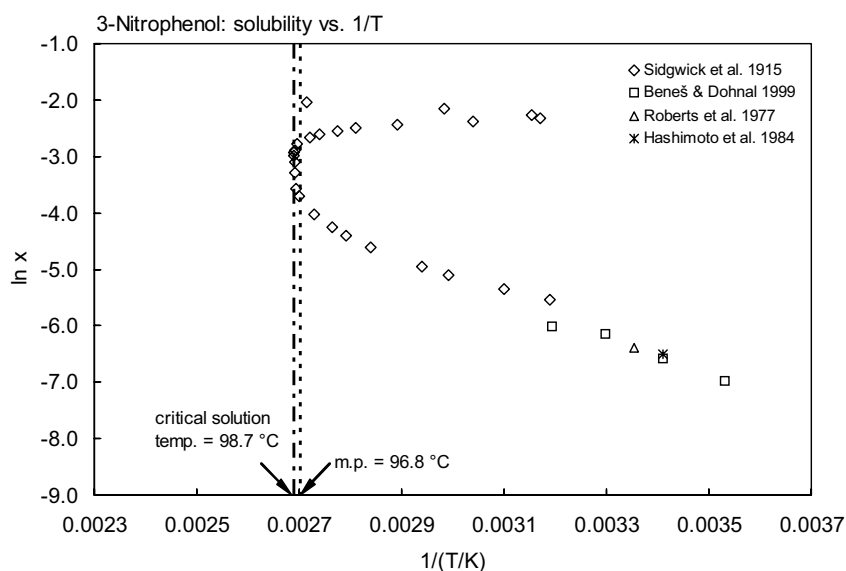
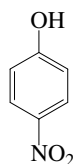


FIGURE 14.1.3.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-nitrophenol.

14.1.3.3 4-Nitrophenol



Common Name: 4-Nitrophenol

Synonym: *p*-nitrophenol, 4-hydroxynitrobenzene

Chemical Name: 4-nitrophenol

CAS Registry No: 100-02-7

Molecular Formula: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$

Molecular Weight: 139.109

113.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

279.0 (decomposes, Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.479 (Weast 1982–83)

Molar Volume (cm^3/mol):

131.9 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

7.08 (21.5 $^{\circ}C$, UV, Schwarzenbach et al. 1988)

7.17 (Fieser & Fieser 1958)

7.16 (Serjeant & Dempsey 1979; Howard 1989; Haderlein & Schwarzenbach 1993)

7.15 (Dean 1985; Miyake et al. 1987; Brecken-Folse et al. 1994; Howe et al. 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.90 (Tsonopoulos & Prausnitz 1971)

18.25 (Beneš & Dohnal 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

41.09 (Tsonopoulos & Prausnitz 1971)

62.76, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.135 (mp at $113.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

29100* (34.8 $^{\circ}C$, shake flask-residue volume method, measured range 34.8–92.8 $^{\circ}C$, critical solution temp 92.8 $^{\circ}C$, Sidgwick et al. 1915)

14000 (shake flask-spectrophotometry, Roberts et al. 1977)

9950, 14800 (15, 25 $^{\circ}C$, shake flask, average values of 6 laboratories, OECD 1981)

13490, 11140 (20 $^{\circ}C$, shake flask-UV, calculated, Hashimoto et al. 1984)

11570 (20 \pm 0.5 $^{\circ}C$, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)

16000 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

15599* (shake flask-conductimetry, measured range 15.3–34.9 $^{\circ}C$, Achard et al. 1996)

12200* (20 $^{\circ}C$, shake flask-UV spectrophotometry, measured range 10–38 $^{\circ}C$, Beneš & Dohnal 1999)

15052* (23.65 $^{\circ}C$, shake flask-optical method, measured range 285.9–313.8 K, Jaoui et al. 2002)

$\ln [S/(mol\ kg^{-1})] = 17.110 - 4273.4/(T/K)$; temp range 288–314 K (eq. derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0054 (20 $^{\circ}C$, Schmidt-Bleek et al. 1982)

0.0012 (selected, Yoshida et al. 1983)

0.0044 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 11.9529 - 5159.7/(T/K)$, temp range 304–352 K (solid, Antoine eq., Stephenson & Malanowski 1987)

- 0.111 (supercooled liquid P_L at 20°C, GC-RT correlation, Schwarzenbach et al. 1988)
 0.0131 (20°C, solid P_S , converted from P_L with ΔS_{fus} and mp, Schwarzenbach et al. 1988)
 $\log(P/\text{mmHg}) = 8.305 - 4180/(T/K)$ (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)
 0.133 (Howard 1989)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 4.21×10^{-5} (exptl., Hine & Mookerjee 1975)
 5.55×10^{-4} , 9.87×10^{-3} (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 1.04×10^{-5} (calculated-P/C, Yoshida et al. 1983)
 0.00335 (20°C, calculated-P/C, Schwarzenbach et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 1.91 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)
 1.18, 1.27 (calculated- π const., calculated-fragment const., Rekker 1977)
 1.68 ± 0.01 (RP-HPLC- k' correlation, Unger et al. 1978)
 2.07 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 1.86 (HPLC-ref. substances extrapolated, Harnish et al. 1983)
 1.88 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
 1.96 ± 0.08 (HPLC-RV correlation.-ALPM, Garst 1984; Garst & Wilson 1984)
 1.85, 1.92 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
 0.70 (calculated- γ from UNIFAC, Campbell & Luthy 1985)
 1.90 (HPLC-RV correlation, Brooke et al. 1986)
 2.10 (HPLC- k' correlation, Miyake et al. 1987)
 1.93 (shake flask/batch equilibration-UV, Beltrame et al. 1988, 1989)
 2.04 ($21.5 \pm 1.5^\circ\text{C}$, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)
 1.77 (CPC-RV at pH 7.4, El Tayar et al. 1991)
 1.85, 1.91 (COMPUTOX databank, Kaiser 1993)
 1.91 (recommended, Sangster 1993)
 1.90 ± 0.14 , 1.09 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
 1.91 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

- 2.10 (fathead minnow, Veith et al. 1980)
 2.56 (mean whole body ^{14}C in fathead minnow, Call et al. 1980)
 1.90, 2.34 (total ^{14}C in fathead minnow: observed, calculated, mean exposure level $0.0041 \mu\text{g}\cdot\text{mL}^{-1}$, Call et al. 1980)
 2.44, 2.65 (total ^{14}C in fathead minnow: observed, calculated, mean exposure level $0.0441 \mu\text{g}\cdot\text{mL}^{-1}$, Call et al. 1980)
 1.76; 1.04 (golden orfe; green algae, Freitag et al. 1982)
 1.48 (activated sludge, Freitag et al. 1982)
 1.43 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)
 0.301 (calculated- K_{ow} , Yoshida et al. 1983)
 1.48, 1.45 (alga *Chlorella fusca*, wet wt. basis, calculated- K_{ow} , Geyer et al. 1984)
 1.60, 1.48, 1.48 (golden ide, algae, activated sludge, Freitag et al. 1985)
 1.90 (fathead minnow, quoted, Howard 1989)

Sorption Partition Coefficient, $\log K_{oc}$:

- 1.65 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)
 2.41 (soil, calculated- K_{ow} , Yoshida et al. 1983)
 1.74 (Brookston clay loam, Boyd 1982)
 2.18 (HPLC- k' correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
 1.32 (soil, calculated-S, Howard 1989)
 2.37 (soil, quoted exptl., Meylan et al. 1992)
 2.49 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

- 2.16, 2.07 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 2.05; 2.49 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
 2.03, 1.94 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, and $pH \leq 5.4$, average, Delle Site 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric photolysis $t_{1/2} = 3.1\text{--}329$ h, based on sunlight photolysis at pH 9 and pH 4 (Hustert et al. 1981; Lemaire et al. 1985; selected, Howard et al. 1991);
 rate constant $k = 3.96 \times 10^{-3} \text{ h}^{-1}$ for the direct photolysis in water (Yoshida et al. 1983);
 photolysis $t_{1/2}$ range from hours to a week or more in atmosphere and $t_{1/2} = 2\text{--}14$ d in clear surface waters (Howard 1989).

Oxidation: oxidation rate constant $k < 2 \times 10^5 \text{ M}^{-1}\cdot\text{h}^{-1}$ for singlet oxygen, $k = 2 \times 10^6 \text{ M}^{-1}\cdot\text{h}^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 21$ d to 5.6 y in water, based on rate constants for reaction in water with hydroxyl radical (Dorfman & Adams 1973; Scully & Hoigné 1987; selected, Howard et al. 1991);

rate constant $k < 50 \text{ M}^{-1}\cdot\text{s}^{-1}$ for 0.01–14 mM to react with ozone in water using PrOH as scavenger at pH 1.7 and 20–23°C in water (Hoigné & Bader 1983a,b);

rate constant $k = 8.3 \times 10^{-12} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ for the gas-phase reaction with OH radical at 296 K in the atmosphere (Becker et al. 1984; quoted, Carlier et al. 1986);

photooxidation $t_{1/2} = 14.5\text{--}145$ h in air, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

aqueous photooxidation $t_{1/2} = 440$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992);

phototransformation decay $k = 0.15 \text{ min}^{-1}$ on 0.20 g/L of TiO_2 solution (Minero et al. 1993).

Hydrolysis:

Biodegradation: 95% degradation in 3–6 d in mixture bacteria cultures (Tabak et al. 1964);

decomposition by a soil microflora in 16 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate of biodegradation $17.5 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

time necessary for complete degradation of 16 mg/L in 3–5 d by wastewater and 7–14 d by soil (Haller 1978);

aqueous aerobic $t_{1/2} = 18.2\text{--}168$ h, based on pond die-away test data (Paris et al. 1983; Bourquin 1984; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 163\text{--}235$ h, based on anaerobic die-away data in two different flooded soils (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991);

was not biodegraded with activated sludge at a concn. of 94 mg/L but completely degraded with a decreased concn. of 19 mg/L in 28 d expt. (Kool 1984).

Biotransformation: estimated bacterial transformation rate constant of $1.00 \times 10^{-7} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982);

rate constant of $(3.80 \pm 1.40) \times 10^{-11} \text{ L}\cdot\text{organism}^{-1}\cdot\text{h}^{-1}$ (Paris et al. 1983; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 14.5\text{--}145$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1–5 to > 5 d (Kelly et al. 1994).

Surface water: photodegradation $t_{1/2} = 5.7$ d at pH 5, $t_{1/2} = 6.7$ d at pH 7 and $t_{1/2} = 13.7$ d at pH 9 in water (Hustert et al. 1981);

$t_{1/2} = 1\text{--}8$ d in freshwater, $t_{1/2} = 1\text{--}3$ yr in marine systems but decreased to 13–20 d with the presence of sediment, the mean $t_{1/2} = 7.7$ d estimated by a nonsteady-state equilibrium model, and photolysis $t_{1/2} = 2\text{--}14$ d in clear surface waters (Howard 1989);

$t_{1/2} = 18.2\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 440$ min for photolysis in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

Groundwater: $t_{1/2}$ = 36.4–235 h, based on pond die-away test data and anaerobic die-away data in two different flooded soils (Paris et al. 1983; Sudhakar-Barik & Sethunnathan 1978; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ ~ 1 d in agricultural topsoil and $t_{1/2}$ = 10 d in flooded soil, $t_{1/2}$ > 40 d in subsoil under aerobic conditions and longer still under anaerobic conditions (Howard 1989);

$t_{1/2}$ = 17–29 h, based on aerobic soil die-away test data (Loekke 1985; selected, Howard et al. 1998).

$t_{1/2}$ = 75 d in a coarse sandy soil, $t_{1/2}$ = 145 d in sandy loam (Kjeldsen et al. 1990)

Biota: depuration $t_{1/2}(\text{obs.})$ = 72 h, $t_{1/2}(\text{calc.})$ = 37 h for mean exposure level of $0.0041 \mu\text{g}\cdot\text{mL}^{-1}$ and $t_{1/2}(\text{obs.})$ = 228 h, $t_{1/2}(\text{calc.})$ = 206 h for mean exposure level of $0.041 \mu\text{g}\cdot\text{mL}^{-1}$ (Call et al. 1980).

TABLE 14.1.3.3.1

Reported aqueous solubilities of 4-nitrophenol at various temperatures

Sidgwick et al. 1915		Achard et al. 1996		Beneš & Dohnal 1999		Jaoui et al. 2002	
shake flask-synthetic method		shake flask-conductimetry		shake flask-UV spec.		shake flask-optical method	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
34.8	29100	15.3	10162	10	8050	12.75	8694
37.2	31100	25.0	15599	20	12000	18.15	11477
40.4	33400	30.3	29600	30	17800	23.65	15052
47.7	39300	34.9	28845	38	23900	34.55	25082
51.2	43000					41.05	33428
59.1	53300			mp/K	386.95	14.65	9599
67.8	69900			$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.25$		19.65	12367
72.6	82800			Enthalpies of solution*:		25.35	16345
79.3	106100	OECD 1981		$\Delta H_{\text{sol}}(\text{solid}) = 28.9 \text{ kJ mol}^{-1}$		33.55	23969
84.4	137000	shake flask (6 laboratories)		$\Delta H_{\text{sol}}(\text{liq.}) = 16.9 \text{ kJ mol}^{-1}$		39.25	30896
87.9	175300	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$			11.15	7999
90.2	215800	15	9950 [†]			15.85	10211
91.3	261600	25	14800 [‡]			23.15	14690
92.3	304100					34.55	25082
92.8	331900	[†] mean, 8880–10900 $\text{g}\cdot\text{m}^{-3}$				40.65	32844
...	...	[‡] mean, 13800–15900 $\text{g}\cdot\text{m}^{-3}$					
critical solution temp 92.8°C							
triple point 39.6°C							

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

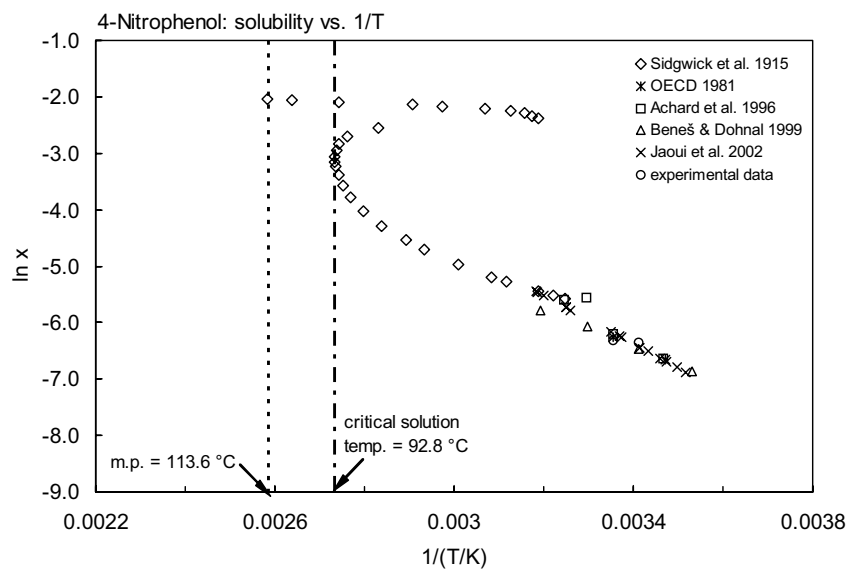
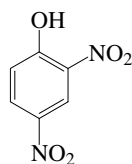


FIGURE 14.1.3.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 4-nitrophenol.

14.1.3.4 2,4-Dinitrophenol



Common Name: 2,4-Dinitrophenol

Synonym: 2,4-hydroxynitrobenzene, Aldifen, 2,4-DNP

Chemical Name: 2,4-dinitrophenol

CAS Registry No: 57-28-5

Molecular Formula: $C_6H_4N_2O_5$, $C_6H_3(NO_2)_2OH$

Molecular Weight: 184.106

Melting Point ($^{\circ}C$):

114.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.684 ($24^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

160.4 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

4.09 (Pearce & Simkins 1968)

3.94 (Schwarzenbach et al. 1988; Haderlein & Schwarzenbach 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F : 0.132 (mp at $114.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6000 (Morrison & Boyd 1959, Howard 1989)

5600 ($18^{\circ}C$, Verschueren 1977)

335* ($20 \pm 0.5^{\circ}C$, shake flask-UV at pH 1.5, Schwarzenbach et al. 1988)

2787 ($20 \pm 0.5^{\circ}C$, supercooled liquid S_L , Schwarzenbach et al. 1988)

5000 (selected, Brecken-Folse et al. 1994; Howe et al. 1994)

560 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

691* (shake flask-conductimetry, measured range 15.1 – $35^{\circ}C$, Achard et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.52×10^{-3} (Knudsen effusion method, Hoyer & Peperle 1958)

$\log(P/mmHg) = 13.95 - 5466/(T/K)$, temp range 20 – $60^{\circ}C$ (Knudsen effusion method, Hoyer & Peperle 1958)

1.987×10^{-3} ($18^{\circ}C$, Mabey et al. 1982)

5.520×10^{-3} (Interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_S/kPa) = 13.075 - 5466/(T/K)$, temp range 291 – $333 K$ (solid, Antoine eq., Stephenson & Malanowski 1987)

0.111 ($20^{\circ}C$: supercooled liquid P_L , GC-RT correlation, Schwarzenbach et al. 1988)

0.0207 ($20^{\circ}C$: solid P_S , converted from P_L with ΔS_{fus} and mp, Schwarzenbach et al. 1988)

$\log(P_L/atm) = 7.392 - 3680/(T/K)$ (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.54×10^{-5} ($18^{\circ}C$, calculated-P/C, Mabey et al. 1982)

0.00335 ($20^{\circ}C$, calculated-P/C, Schwarzenbach et al. 1988)

8.880×10^{-5} (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, log K_{OW} :

1.53	(Leo et al. 1971)
1.50	(shake flask-UV, Stockdale & Selwyn 1971)
1.54	(shake flask-GC, Kurihara et al. 1973)
1.56	(shake flask-UV, Korenman et al. 1977)
1.52	(QSAR, Scherrer & Howard 1979)
1.55	(shake flask-UV, Terada et al. 1981)
1.79 \pm 0.06	(HPLC-RV correlation-ALPM, Garst 1984)
1.51	(shake flask, Log P Database, Hansch & Leo 1987)
1.67	(21 \pm 1.5°C, shake flask-UV, both phases, Schwarzenbach et al. 1988)
1.54	(recommended, Sangster 1993)
1.53	(22°C, shake flask, Brecken-Folse et al. 1994)
-0.23	(shake flask, pH 7.5, Howe et al. 1994)
1.67	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.19	(microorganism-water, calculated- K_{OW} , Mabey et al. 1982)
< 1.0	(calculated, Howard 1989)

Sorption Partition Coefficient, log K_{OC} :

1.22	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)
1.56, 2.14	(calculated-S, K_{OW} , Howard 1989)
-0.09	(calculated- K_{OW} , Kollig 1993)
3.09	(activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: aqueous oxidation rate constants $k = 3 \times 10^4 \text{ M}^{-1}\cdot\text{h}^{-1}$ for singlet oxygen, and $k = 5 \times 10^5 \text{ M}^{-1}\cdot\text{h}^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$ in water, based on reported reaction rate constants for RO_2 with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 111\text{--}1114 \text{ h}$ in air, based on the estimated reaction rate constant $k = 1.7 \times 10^{-11} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ with an ambient hydroxyl radical concentration of $8 \times 10^5 \text{ molecules}\cdot\text{cm}^{-3}$ for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

aqueous photooxidation $t_{1/2} = 200 \text{ min}$ in the presence of hydrogen peroxide irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

Hydrolysis:

Biodegradation: 95% degradation in 7–10 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $6.0 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

first-order rate constant $k = 0.2 \text{ d}^{-1}$ corresponding to a $t_{1/2} = 3.6 \text{ d}$ in adapted activated sludge under aerobic conditions (Mills et al. 1982);

aqueous aerobic $t_{1/2} = 1622\text{--}6312 \text{ h}$, based on data from aerobic soil column studies (Kincannon & Lin 1985; selected, Howard et al. 1991) and aerobic soil die-away test data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)

aqueous anaerobic $t_{1/2} = 68\text{--}170 \text{ h}$, based on anaerobic flooded soil die-away tests (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 68 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2.8 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: bacterial transformation rate constant $k = 3 \times 10^{-9} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated vapor-phase $t_{1/2} = 14 \text{ h}$ for reaction with photochemically generated OH radical (Howard 1989)

photooxidation $t_{1/2} = 111\text{--}1114$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: calculated $t_{1/2} = 58$ d for reaction with alkylperoxy radical in water (Howard 1989);

$t_{1/2} = 77\text{--}3840$ h, based on reported reaction rate constants for RO_2 radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 200$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992)

$t_{1/2}(\text{aerobic}) = 69$ d, $t_{1/2}(\text{anaerobic}) = 2.8$ d in natural waters (Capel & Larson 1995)

Groundwater: $t_{1/2} = 68\text{--}14624$ h, based on estimated aqueous aerobic biodegradation half-life and estimated aqueous anaerobic biodegradation half-life (quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 1622\text{--}6312$ h, based on data from aerobic soil column studies (Kincannon & Lin 1985) and aerobic soil die-away test data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991);

a Class C compounds with a $t_{1/2} > 50$ d in soil (Ryan et al. 1988).

$t_{1/2} = 145$ d in sandy loam (Kjeldsen et al. 1990)

Biota:

TABLE 14.1.3.4.1

Reported aqueous solubilities of 2,4-dinitrophenol at various temperatures

Schwarzenbach et al. 1988				Achard et al. 1996	
shake flask-UV spec.				shake flask-conductimetry	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
	solid		supercooled liquid		
5	171.8	0	2019	15.1	415
10	206.6	10	2213	25.0	691
20	335.0	20	2852	35.0	975
30	473.2	30	3199		

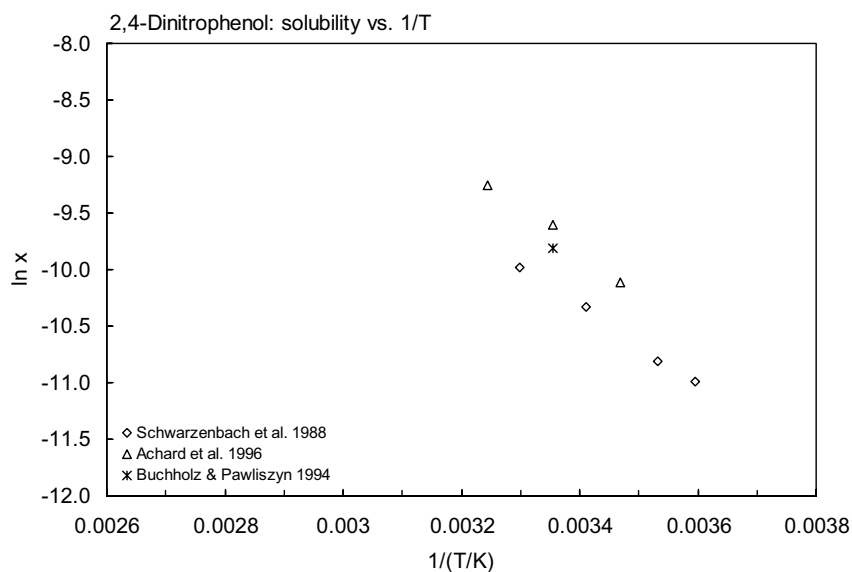
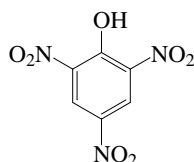


FIGURE 14.1.3.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,4-dinitrophenol.

14.1.3.5 2,4,6-Trinitrophenol (Picric acid)



Common Name: 2,4,6-Trinitrophenol

Synonym: Picric acid

Chemical Name: 2,4,6-trinitrophenol

CAS Registry No: 88-89-1

Molecular Formula: $C_6H_3N_3O_7$, $C_6H_2(NO_2)_3OH$

Molecular Weight: 229.104

Melting Point ($^{\circ}C$):

122.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

> 300 (explodes, Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.763 (Weast 1982–83; Dean 1985)

Acid Dissociation Constant, pK_a :

0.78 (Schwarzenbach et al. 1988)

Molar Volume (cm^3/mol):

188.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.50 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

49.37 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.111 (mp at $122.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

14000 (Morrison & Boyd 1959)

13750 (selected, Tsonopoulos & Prausnitz 1971)

14000 ($20^{\circ}C$, Verschueren 1983)

13000 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.68×10^{-5} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 11.319 - 5560/(T/K)$, temp range 468–598 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

7.66×10^{-7} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.44 (shake flask-GC, Korenman et al. 1977)

1.34 (Scherrer & Howard 1979)

1.46 (HPLC-RV correlation, Garst 1984)

–0.97, 0.87 (shake flask, Log P database: pH 2.7, pH 1, Hansch & Leo 1987)

2.03 (shake flask, Log P Database, Hansch Leo 1987)

1.33 (recommended, Sangster 1993)

1.82 (COMPUTOX databank, Kaiser 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 677\text{--}4320$ h, based on estimated reaction rates with OH and NO₃ radicals in air (Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);

aqueous aerobic $t_{1/2} = 672\text{--}8640$ h, based on aerobic biodegradation screening test (Howard et al. 1991);
aqueous anaerobic $t_{1/2} = 48\text{--}300$ h, based on aqueous anaerobic natural water die-away test data (Howard et al. 1991)

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: $t_{1/2} = 672\text{--}4320$ h, based on estimated photooxidation half-lives in air (Howard et al. 1991).

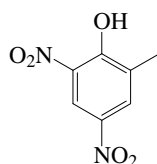
Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}8640$ h, based on estimated both aqueous aerobic and aqueous anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated photooxidation aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biota:

14.1.3.6 4,6-Dinitro-*o*-cresol

Common Name: 4,6-Dinitro-*o*-cresol

Synonym: 2,4-dinitro-6-methylphenol, DNOC, 2-methyl-4,6-dinitrophenol, 6-methyl-2,4-dinitrophenol

Chemical Name: 4,6-dinitro-*o*-cresol, 2,4-dinitro-6-methylphenol

CAS Registry No: 534-52-1

Molecular Formula: $C_7H_6N_2O_5$, $CH_3C_6H_2(NO_2)_2OH$

Molecular Weight: 198.133

Melting Point ($^{\circ}C$):

86.5 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

312 (Howard 1991)

Density (g/cm^3 at $20^{\circ}C$):

Acid Dissociation Constant, pK_a :

4.35 (Pearce & Simkins 1968; Callahan et al. 1979; Westall et al. 1985)

4.31 (Schwarzenbach et al. 1988; Howard 1991)

4.46 (Jafvert 1990; quoted, Bintein & Devillers 1994)

Molar Volume (cm^3/mol):

182.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.249$ (mp at $86.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

258, 250 (Günther et al. 1968)

290 (calculated- K_{ow} , Mabey et al. 1982)

198 ($20^{\circ}C$, neutral species at pH 1.5 of buffer solution HCl/NaH_2PO_4 , shake flask-UV, Schwarzenbach et al. 1988)

150 ($20^{\circ}C$, quoted, Howard 1991)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.048 ($35^{\circ}C$, Knudsen effusion method, Hamaker & Kerlinger 1969)

6.670 ($20^{\circ}C$, estimated, Mabey et al. 1982)

0.0142 (interpolated-Antoine eq., solid, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 13.265 - 5400/(T/K)$; temp range 290–324 K (Antoine eq., solid, Stephenson & Malanowski 1987)

0.240 ($20^{\circ}C$, GC-RT correlation, supercooled liquid value P_L , Schwarzenbach et al. 1988)

0.0432 ($20^{\circ}C$, solid P_s , Schwarzenbach et al. 1988)

0.0111 ($20^{\circ}C$, quoted, Howard 1991)

Henry's Law Constant ($Pa \cdot m^3/mol$):

4.050 (calculated- P/C , Mabey et al. 1982)

43.22 ($20^{\circ}C$, calculated- P/C , Schwarzenbach et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ or as indicated:

2.70 (calculated-fragment const., Mabey et al. 1982)

2.12 ($21.5^{\circ}C$, neutral species, shake flask-UV, Schwarzenbach et al. 1988)

−0.81 ($21.5^{\circ}C$, ionic species at pH 12, Schwarzenbach et al. 1988)

2.12 (Howard 1991)

- 2.12 (Sangster 1993)
 2.56, 1.98 (COMPUTOX databank, Kaiser 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 2.10 (microorganism-water, calculated- K_{OW} , Mabey et al. 1982)
 1.38, 1.57 (calculated-S, K_{OW} regression equations., Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.38 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 3.57 ± 0.130 (natural sediment, Jafvert 1990)
 2.44, 2.0–2.53 (calculated-S, K_{OW} regression eq., Howard 1991)
 2.41, 2.78 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 3.28 (activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: nonvolatile from water, based on low Henry's law constant value (Howard 1991).

Photolysis:

Oxidation: aqueous oxidation rate constant $k = 3 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 5 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);
 photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$ in water, based on reported reaction rate constants for RO_2 radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
 photooxidation $t_{1/2} = 310\text{--}3098 \text{ h}$ in air, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 168\text{--}504 \text{ h}$, based on data from a soil die-away study (Kincannon & Lin 1985; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 68\text{--}170 \text{ h}$, based on flooded soil die-away tests for 2,4-dinitrophenol (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)
 $t_{1/2}(\text{aerobic}) = 7 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: estimated bacterial transformation rate constant $k = 3 \times 10^9 \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 310\text{--}3098 \text{ h}$ in air, based on estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);
 $t_{1/2} = 77 \text{ d}$ for the vapor-phase reaction with OH radical (concn. of $5 \times 10^5 \text{ molecule}\cdot\text{cm}^{-3}$) (Howard 1991);
 atmospheric transformation lifetime was estimated to be $> 5 \text{ d}$ (Kelly et al. 1994).

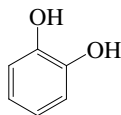
Surface water: photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$ in water, based on reported reaction rate constants for RO_2 radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
 $t_{1/2} \sim 58 \text{ d}$, estimated for photooxidation via peroxy radicals and $t_{1/2} = 2600 \text{ yr}$ for reaction with singlet oxygen in water (Howard 1991)
 $t_{1/2}(\text{aerobic}) = 7 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2.8 \text{ d}$ in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 68\text{--}1008 \text{ h}$, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}504 \text{ h}$, based on data from a soil die-away study (Kincannon & Lin 1985; selected, Howard et al. 1991).

Biota:

14.1.4 DIHYDROXYBENZENES, METHOXYPHENOLS AND CHLOROGUAIACOLS**14.1.4.1 Catechol (1,2-Dihydroxybenzene)**

Common Name: Catechol

Synonym: 1,2-dihydroxybenzene, 1,2-benzenediol, pyrocatechol

Chemical Name: 1,2-dihydroxybenzene

CAS Registry No: 120-80-9

Molecular Formula: $C_6H_4(OH)_2$

Molecular Weight: 110.111

Melting Point ($^{\circ}C$):

104.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

245 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

1.1493 (22 $^{\circ}C$, Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.40 (Fieser & Fieser 1958)

9.50 (McLeese et al. 1979)

Molar Volume (cm^3/mol):

110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.76 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

60.25 (Tsonopoulos & Prausnitz 1971)

60.21 (Yalkowsky & Valvani 1980)

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.166 (mp at 104.6 $^{\circ}C$)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated):

71166 (30 $^{\circ}C$, synthetic method, Walker et al. 1931)

45000 (Fieser & Fieser 1958; Morrison & Boyd 1959)

636190 (quoted, Tsonopoulos & Prausnitz 1971)

35630 (calculated- K_{OW} , Yalkowsky & Morozowich 1980)

42724, 38610 (calculated- ΔS_{fus} and mp, estimated, Yalkowsky & Valvani 1980)

43000 (Dean 1985)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* (104 $^{\circ}C$, summary of literature data, temp range 104–245.5 $^{\circ}C$, Stull 1947)

1333* (118.5 $^{\circ}C$, ebulliometry, measured range 118.5–245.5 $^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 13779.7/(T/K)] + 8.694319$; temp range 104–245.5 $^{\circ}C$ (Antoine eq., Weast 1972–73)

1.34 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log(P/mmHg) = 7.57299 - 2024.422/(186.533 + t/^{\circ}C)$; temp range 118.5–245.5 $^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log(P/mmHg) = [1 - 517.477/(T/K)] \times 10^{0.902426 - 6.04783 \times 10^{-4} \cdot (T/K) + 6.58278 \times 10^{-7} \cdot (T/K)^2}$; temp range: 377.15–518.65 K, (Cox eq., Chao et al. 1983)

5.44 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.9896 - 3144.241/(281.825 + t/^{\circ}C)$; temp range 118.5–245.5 $^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.03(extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.577 - 2054/(187.0 + t/^{\circ}\text{C})$; temp range 118–246°C (Antoine eq., Dean 1985, 1992)

1.06(P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.61028 - 1954.6/(-94.25 + T/\text{K})$; temp range 395–519y K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.022 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.86 (shake flask-UV, Fujita et al. 1964)
 0.95 (Leo et al. 1971)
 0.85 (shake flask-UV, pH 5.6, Umeyama et al. 1971)
 0.84 (shake flask, Korenman 1972)
 0.86 (shake flask at pH 7, Unger et al. 1978)
 0.88, 1.01, 0.85, 0.84 (literature values, Hansch & Leo 1979)
 0.95 (GC-RT correlation, Veith et al. 1979)
 1.10 (HPLC-RT correlation, Butte et al. 1981)
 0.53 (HPLC- k' correlation, Haky & Young 1984)
 1.10 (HPLC-RT correlation, Webster et al. 1985)
 0.88 (recommended, LOGKOW databank, Sangster 1993)
 0.88 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

2.03 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 1.42; 1.74, 2.25, 2.01, 1.98, 1.82 (soil: calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 2.6\text{--}26 \text{ h}$ in air, based on vapor-phase reaction rate constant with OH radical in atmosphere (Howard et al. 1991);

aqueous photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$, based on reaction rate constant for RO_2^- radical in aqueous solution (Mill & Mabey 1985; selected, Howard et al. 1991).

Hydrolysis:

Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $k = 55.5 \text{ mg COD g}^{-1} \cdot \text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

2 mM catechol rapidly degraded by strain Cat $_{1/2}$ in batch culture in 9 d (Schnell et al. 1989);

aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on aerobic biological screening test data (Heukelekian & Rand 1955; Okey & Bogan 1965; Pitter 1976; Urushigawa et al. 1983; Gerike & Fischer 1979; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated photooxidation half-lives in air (Atkinson 1987; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biota:

TABLE 14.1.4.1.1

Reported vapor pressures of catechol (1,2-dihydroxybenzene) at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
104.0	666.6	118.5	1333
118.3	1333	139.3	3333
134.0	2666	157.0	6666
150.6	5333	168.0	9999
161.7	7999	176.2	13332
176.0	13332	188.2	19998
197.7	26664	198.0	26664
221.5	53329	204.0	33330
245.5	101325	210.9	39997
		213.3	43330
mp/ $^{\circ}\text{C}$	105	215.8	46663
		220.0	53329
		224.6	59995
		228.2	66661
		231.4	73327
		235.0	79993
		237.8	86659
		241.0	93325
		245.5	101327
		bp/ $^{\circ}\text{C}$	243.823

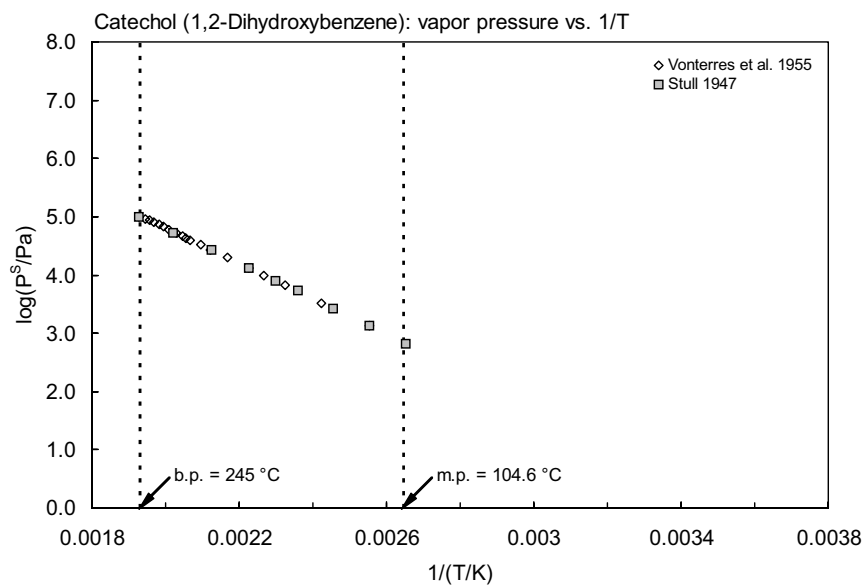
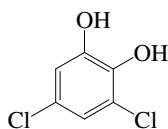


FIGURE 14.1.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for catechol.

14.1.4.2 3,5-Dichlorocatechol



Common Name: 3,5-Dichlorocatechol

Synonym:

Chemical Name: 3,5-dichlorocatechol

CAS Registry No: 13673-92-2

Molecular Formula: $C_6H_4Cl_2O_2$, $C_6H_2Cl_2(OH)_2$

Molecular Weight: 179.001

Melting Point ($^{\circ}C$):

83–84 (Varhanířková 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constants, pK_a :

7.78 (Varhanířková 1995)

Molar Volume (cm^3/mol):

152.6 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

7910 (at pH 4.70. shake flask-HPLC/UV, Varhanířková 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

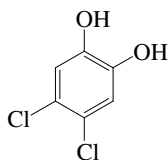
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.3 4,5-Dichlorocatechol

Common Name: 4,5-Dichlorocatechol

Synonym:

Chemical Name: 4,5-dichlorocatechol

CAS Registry No: 3428-24-8

Molecular Formula: $C_6H_4Cl_2O_2$, $C_6H_2Cl_2(OH)_2$

Molecular Weight: 179.001

Melting Point ($^{\circ}C$):

116–117 (Varhanířková 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

8.17 (Varhanířková 1995)

Molar Volume (cm^3/mol):

152.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

12000 (at pH 3.20, shake flask-HPLC/UV, Varhanířková 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations

0.408 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3680/(T/K) - 11.95$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.00078 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.51–2.93 (NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

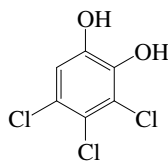
1.18–1.51 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.4 3,4,5-Trichlorocatechol



Common Name: 3,4,5-Trichlorocatechol

Synonym: 3,4,5-trichloro-1,2-benzenediol

Chemical Name: 3,4,5-trichlorocatechol

CAS Registry No: 56961-20-7

Molecular Formula: $C_6H_3Cl_3O_2$, $C_6HCl_2(OH)_2$

Molecular Weight: 213.446

Melting Point ($^{\circ}C$):

130 (Varhaníčková 1995)

134 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a : 6.95 (Varhaníčková 1995)

Molar Volume (cm^3/mol):

173.5 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

79.3 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.085 (mp at $134^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

511 (at pH 4.05, shake flask-HPLC/UV, Varhaníčková 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.106 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4135/(T/K) - 12.89$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.79, 3.71 (shake flask-GC, HPLC-RT correlation, Xie et al. 1984)

3.89, 3.17 (calculated- π constant, fragment constant, Xie et al. 1984)

3.71 (HPLC-RT correlation, Xie et al. 1984; quoted, Sangster 1993)

3.75 (quoted, NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.16 (estimated- K_{OW} , NCASI 1992)

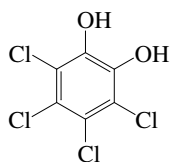
Sorption Partition Coefficient, $\log K_{OC}$:

4.35 (sediment, $K_p = 22 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.5 Tetrachlorocatechol



Common Name: Tetrachlorocatechol

Synonym: 3,4,5,6-tetrachloro-1,2-benzenediol

Chemical Name: tetrachlorocatechol

CAS Registry No: 1198-55-6

Molecular Formula: $C_6H_2Cl_4O_2$, $C_6Cl_4(OH)_2$

Molecular Weight: 247.891

Melting Point ($^{\circ}C$):

194 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

5.83 (Varhaníčková 1995)

Molar Volume (cm^3/mol):

194.4 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.9 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.022 (mp at $194^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

70.5 (at pH 5.13, shake flask-HPLC/UV, Varhaníčková 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.068 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4070/(T/K) - 12.48$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.035 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.29 (shake flask-GC, Fujita et al. 1964)

4.27 (HPLC-RT correlation, Saarikoski & Viluksela 1982)

4.19, 4.27 (shake flask-GC, HPLC-RT correlation, Xie et al. 1984)

4.29 (recommended, Sangster 1993)

4.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.54 (estimated- K_{ow} , NCASI 1992)

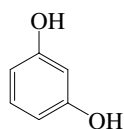
Sorption Partition Coefficient, $\log K_{OC}$:

4.56 (sediment, $K_p = 36.1 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.6 Resorcinol (1,3-Dihydroxybenzene)



Common Name: Resorcinol

Synonym: 1,3-benzenediol, *m*-dihydroxybenzene, *m*-hydroxyphenol, resorcin

Chemical Name: 1,3-dihydroxybenzene

CAS Registry No: 108-46-3

Molecular Formula: $C_6H_6O_2$, $C_6H_4(OH)_2$

Molecular Weight: 110.111

Melting Point ($^{\circ}C$):

109.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

276.5 (Lide 2003)

Density (g/cm^3):

1.2717 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.40 (Fieser & Fieser 1958; McLeese et al. 1979)

Molar Volume (cm^3/mol):

110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.30 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

55.65 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.149 (mp at $109.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2188900 ($33.6^{\circ}C$, synthetic method, Walker et al. 1931)

1230000 (Fieser & Fieser 1958; Morrison & Boyd 1959)

1309000 (Tsonopoulos & Prausnitz 1971)

840000, 2290000 (0, $30^{\circ}C$, Verschueren 1983)

110000 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.3300* (extrapolated-regression of tabulated data, temp range 108.4 – $276.5^{\circ}C$, Stull 1947)

1333* ($151.5^{\circ}C$, ebulliometry, measured range 151.5 – $276.5^{\circ}C$, Vonterres et al. 1955)

0.0118 (Knudsen method, calculated-Antoine eq., Hoyer & Peperle 1958)

$\log (P/mmHg) = [-0.2185 \times 16400.8/(T/K)] + 9.413304$; temp range 108.4 – $276.5^{\circ}C$ (Antoine eq., Weast 1972–73)

0.0280* (gas saturation, extrapolated-Antoine eq., measured range 55 – $106^{\circ}C$, Bender et al. 1983)

$\log (P/mmHg) = [1 - 549.041/(T/K)] \times 10^{0.958295 - 5.78954 \times 10^{-4} \cdot (T/K) + 6.46841 \times 10^{-7} \cdot (T/K)^2}$; temp range 381.55 – $549.65\ K$ (Cox eq., Chao et al. 1983)

0.0515 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 7.16673 - 2359.273/(180.962 + t/^{\circ}C)$; temp range 151.5 – $216.5^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.0300 (extrapolated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 7.889 - 2231/(169.0 + t/^{\circ}C)$, temp range 151 – $276^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.0118 (P_s , interpolated-Antoine eq.-I, temp range 10 – $50^{\circ}C$, Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 11.425 - 4876/(T/K)$; temp range 283 – $323\ K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.52635 - 1918.1/(-128.65 + T/\text{K})$; temp range 419–550 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.1041 - 1745.2/(-133.81 + T/\text{K})$; temp range 392–463 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$):

4.0×10^{-8} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.80 (shake flask-UV, Fujita et al. 1964; Leo et al. 1969)

0.78 (20°C, shake flask-UV, Korenman 1972)

0.80, 0.77, 0.78 (Hansch & Leo 1979)

0.77 (shake flask-UV, Beezer et al. 1980)

0.88 (shake flask-HPLC both phases, Nahum & Horvath 1980)

0.36 (HPLC-RT correlation, Butte et al. 1981)

0.77 (shake flask, Log P Database, Hansch & Leo 1987)

0.82 (HPLC-RT correlation, Minnick et al. 1988)

0.79 (shake flask-UV, pH 2-8, Wang et al. 1989)

0.80 (COMPUTOX, Kaiser 1993)

0.80 (recommended, Sangster 1993)

0.72 ± 0.15 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)

0.80 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: measured pseudo-first-order reaction rate constant $k = 0.014 \text{ min}^{-1}$ for direct photolysis in aqueous solutions with $t_{1/2} = 50.7 \text{ min}$. (Peijnenburg et al. 1992).

Photooxidation: rate constant $k > 3 \times 10^5 \text{ M}^{-1}\cdot\text{s}^{-1}$ for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C in water (Hoigné & Bader 1983a,b).

Hydrolysis:

Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $k = 57.5 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

2 mM resorcinol solution degraded by strain Re10 within 4 d (Schnell et al. 1989).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air:

Surface water: $t_{1/2} = (50.7 \pm 1.0) \text{ min}$ for directly photolysis in aqueous solutions (Peijnenburg et al. 1992).

Ground water:

Sediment:

Soil:

Biota:

TABLE 14.1.4.6.1

Reported vapor pressures of resorcinol (1,3-dihydroxybenzene) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)			
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Vonterres et al. 1955		Bender et al. 1983	
summary of literature data		ebulliometry		gas saturation-IR	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
					solid
108.4	133.3	151.5	1333	55.35	0.86
138.0	666.6	175.0	3333	66.35	2.73
152.1	1333	190.3	6666	76.45	6.94
168.0	2666	201.7	9999	85.45	14.4
185.3	5333	210.0	13332	92.65	29.2
195.8	7999	221.7	19998	100.05	50.8
209.8	13332	230.1	26664	105.95	81.3
230.8	26664	237.0	33330		
253.4	53329	240.2	39997		
276.5	101325	246.0	43330	eq. 1a	P ^s /Pa
		248.0	46663	A	33.807
mp/°C	110.7	252.0	53329	B	11147
		257.0	59995		
		261.0	66661		
		264.0	73327		
		267.0	79993		
		270.0	86659		
		273.0	93325		
		276.5	101325		
		bp/°C	276.205		

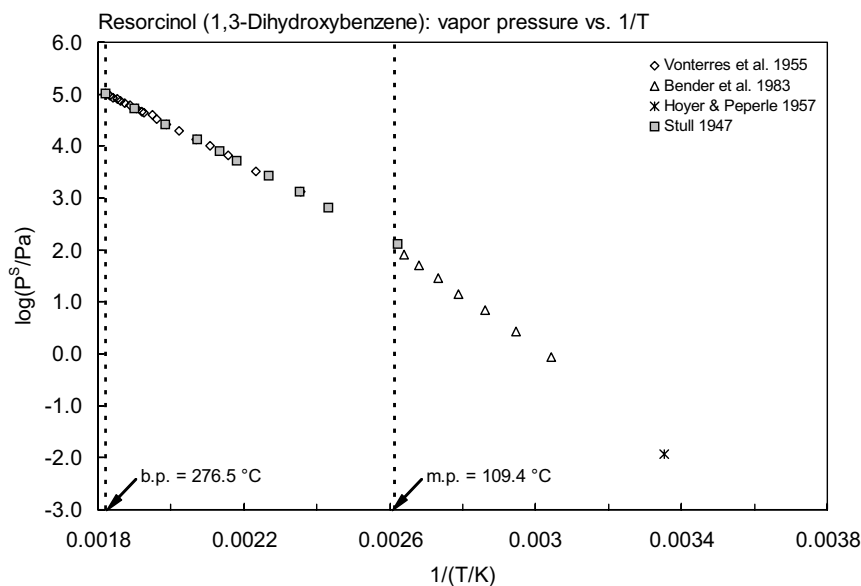
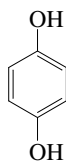


FIGURE 14.1.4.6.1 Logarithm of vapor pressure versus reciprocal temperature for resorcinol.

14.1.4.7 Hydroquinone (1,4-Dihydroxybenzene)



Common Name: Hydroquinone

Synonym: 1,4-benzenediol, *p*-dihydroxybenzene, *p*-hydroxyphenol, quinol, hydroquinol

Chemical Name: 1,4-dihydroxybenzene

CAS Registry No: 123-31-9

Molecular Formula: $C_6H_4(OH)_2$

Molecular Weight: 110.111

Melting Point ($^{\circ}C$):

172.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.328 (15 $^{\circ}C$, Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.90 (McLeese et al. 1979)

Molar Volume (cm^3/mol):

110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.11 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

60.67 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.036 (mp at 172.4 $^{\circ}C$)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

73700 (synthetic method, Walker et al. 1931)
 80140 (shake flask-interferometry, Korman & La Mer 1936)
 80000 (Fieser & Fieser 1958; Morrison & Boyd 1959)
 80750 (selected, Tsonopoulos & Prausnitz 1971)
 70000 (20–25 $^{\circ}C$, Geyer et al. 1981)
 70000 (Rott et al. 1982; Verschuere 1983; Dean 1985)
 86450 (Windholz 1983)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (132.4 $^{\circ}C$, summary of literature data, temp range 132.4–286.2 $^{\circ}C$, Stull 1947)

$\log (P/mmHg) = [-0.2185 \times 18734.0/(T/K)] + 10.309301$; temp range 132.4–286.2 $^{\circ}C$ (Antoine eq., Weast 1972–73)

0.00276* (gas saturation, extrapolated - Antoine eq., measured range 68–126 $^{\circ}C$, Bender et al. 1983)

$\log (P/mmHg) = [1 - 558.031/(T/K)] \times 10^4 \{0.941185 - 5.32724 \times 10^{-4} \cdot (T/K) + 5.41185 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 432.25–559.15 K, (Cox eq., Chao et al. 1983)

0.03940 (extrapolated - liquid, Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 7.41617 - 2397.626/(194.743 + t/^{\circ}C)$; temp range 159.1–286 $^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.00255 (P_s , interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.585 - 5420/(T/K)$; temp range 298–346 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 7.00575 - 2321.92/(-95.235 + T/K)$; temp range 448–559 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 3.89×10^{-6} (quoted, Meylan & Howard 1991)
- 5.91×10^{-6} (estimated-bond contribution, Meylan & Howard 1991)
- 4.00×10^{-6} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.59 (Leo et al. 1971)
- 0.495 (shake flask-UV at pH 5.62, Umeyama et al. 1971)
- 0.59 (shake flask-GC, Kurihara et al. 1973)
- 0.61 (20°C , shake flask, Korenman 1974)
- 0.55, 0.59 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
- 0.61 (HPLC-RT correlation, Nahum & Horvath 1980)
- 0.54 (shake flask-HPLC, Nahum & Horvath 1980)
- 0.99 (HPLC-RT correlation, Fujisawa & Masuhara 1981)
- 0.50 (shake flask, Log P Database, Hansch & Leo 1987)
- 0.50 (centrifugal partition chromatography CPC, Berthod et al. 1988)
- 0.59 (shake flask, Wang et al. 1989)
- 0.59 (recommended, Sangster 1993)
- 0.59 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.81 (green algae, *Chlorella*, exposure to $50 \mu\text{g/L}$ for 24 h, Geyer et al. 1981)
- 0.95 (calculated-S, Geyer et al. 1981)
- 1.60, 2.72 (golden orfe, activated sludge, Freitag et al. 1982)
- 1.60, 1.60 (algae, fish, Freitag et al. 1984)
- 1.54 (algae, wet weight basis after 1 d, Geyer et al. 1984)
- 0.602 (calculated- K_{OW} , Geyer et al. 1984)
- 2.93 (activated sludge, Freitag et al. 1987)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $k = 1 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 12 \text{ min}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

aqueous photooxidation $t_{1/2} = 0.39\text{--}19.3 \text{ h}$ in surface water, based on measured rate data for the reaction with alkyl peroxy radical in aqueous solution (Mill 1982; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 6\text{--}26.1 \text{ h}$ in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991);

72.1 mg/L of total organic carbon (TOC) degraded to 98% TOC after 5 h of illumination with a 250 W tungsten lamp by photo-Fenton reaction (Ruppert et al. 1993).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $54.2 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on aqueous screening test data (Ludzack & Ettinger 1960; Belly & Goodhue 1976; Gerike & Fischer 1979; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: photooxidation $t_{1/2} = 6\text{--}26.1$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: aqueous photooxidation $t_{1/2} = 0.39\text{--}19.3$ h, based on measured rate data for the reaction with alkylperoxyl radical in aqueous solution (Mill 1982; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 14.1.4.7.1

Reported vapor pressures of hydroquinone (1,4-dihydroxybenzene) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)			
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Vonderres et al. 1955		Bender et al. 1983	
summary of literature data		ebulliometry		gas saturation-IR	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
					solid
132.4	133.3*	159.1	1333	67.85	0.46
153.3	666.6*	181.0	3333	79.95	1.70
163.5	1333*	199.1	6666	90.75	4.79
174.6	2666	210.0	9999	100.75	11.2
192.0	5333	218.5	13332	111.25	26.9
203.0	7999	230.1	19998	116.05	40.2
216.5	13332	239.2	26664	121.15	61.1
238.0	26664	246.1	33330	126.45	92.3
262.5	53329	252.0	39997		
286.2	101325	254.8	43330	eq. 1a	P ^s /Pa
		257.2	46663	A	35.137
	*solid	259.0	53329	B	12233
mp/ $^{\circ}\text{C}$	170.3	266.1	59995		
		269.5	66661		
		273.0	73327		
		276.7	79993		
		278.8	86659		
		282.0	93325		
		286.0	101325		
		bp/ $^{\circ}\text{C}$	276.17		

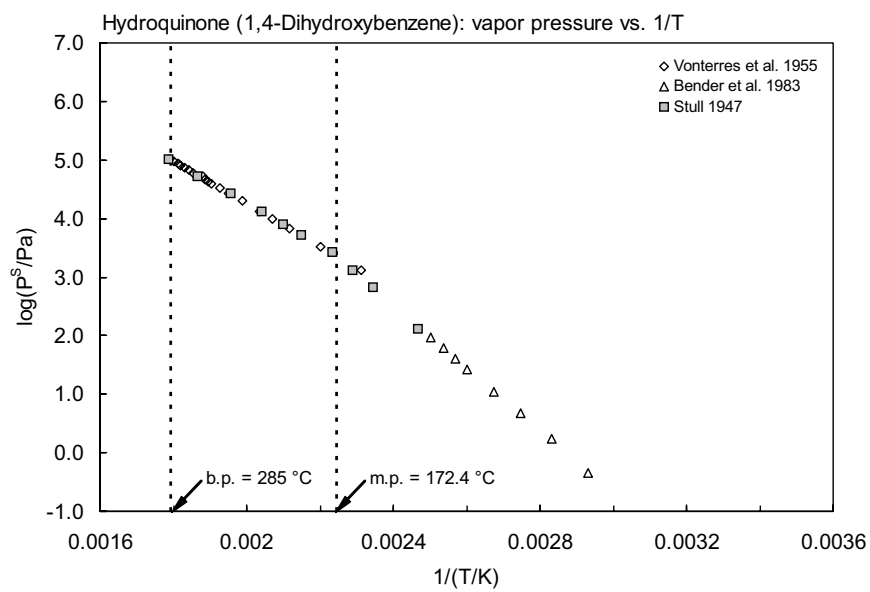
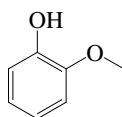


FIGURE 14.1.4.7.1 Logarithm of vapor pressure versus reciprocal temperature for hydroquinone.

14.1.4.8 2-Methoxyphenol (Guaiacol)



Common Name: Guaiacol

Synonym: 2-methoxyphenol, methylcatechol, *o*-hydroxyanisole, 1-hydroxy-2-methoxybenzene, pyrocatechol mono-methylether

Chemical Name: *o*-methoxyphenol

CAS Registry No: 90-05-1

Molecular Formula: $C_7H_8O_2$, $C_6H_4(OCH_3)OH$

Molecular Weight: 124.138

Melting Point ($^{\circ}C$):

32 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$): 204–206

205 (Lide 2003)

Density (g/cm^3):

1.129 (crystal)

1.112 (liquid, solidified at $28^{\circ}C$)

Acid Dissociation Constant, pK :

Molar Volume (cm^3/mol):

134.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 5 J/mol K$), F : 0.854 (mp at $32^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

143000–16700 (Windholz 1983)

16000 ($15^{\circ}C$, Verschueren 1983)

15000 (room temp., Dean 1985)

18700, 1316 ($15^{\circ}C$, $37^{\circ}C$, Yalkowsky et al. 1987)

24800 ($25^{\circ}C$, shake flask-HPLC/UV, Tam et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($52.4^{\circ}C$, summary of literature data, temp range 52.4 – $205^{\circ}C$, Stull 1947)

1333* ($82.0^{\circ}C$, ebulliometry, measured range 82.0 – $205.0^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 13425.8/(T/K)] + 9.027299$; temp range 52.4 – $205^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [1 - 477.010/(T/K)] \times 10^4 \{0.858892 - 4.47192 \times 10^{-4} \cdot (T/K) + 3.228549 \times 10^{-7} \cdot (T/K)^2\}$; temp range 355.15 – $478.15 K$ (Cox eq., Chao et al. 1983)

13.73 (Verschueren 1983)

8.88 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.40415 - 1121.391/(125.407 + t/^{\circ}C)$; temp range 82 – $205^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6.79 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.161 - 1051/(116.0 + t/^{\circ}C)$; temp range 82 – $205^{\circ}C$ (Antoine eq., Dean 1985, 1992)

24.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.44572 - 1786.15/(-76.43 + T/K)$; temp range 378 – $479 K$ (Antoine eq., Stephenson & Malanowski 1987)

21.00 (quoted, Sagebiel & Seiber 1993)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.30 (calculated- P/C , Sagebiel et al. 1992)

- 0.13, 0.11 (gas stripping-UV, headspace-GC, Sagebiel et al. 1992)
 0.132 (bubble chamber, Sagebiel & Seiber 1993)
 0.049 (calculated-group contribution, Lee et al. 2000)
 0.0724 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 6.198 - 3144/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.33 (shake flask-UV, Umeyama et al. 1971)
 1.35 (shake flask-UV, Korenman 1973)
 1.33 (shake flask-UV, Norrington et al. 1975)
 1.58 (Hansch & Leo 1979)
 1.25 (HPLC-RT correlation, Butte et al. 1981)
 1.32 (shake flask, Log P Database, Hansch & Leo 1987)
 1.32 (recommended, LOGKOW databank, Sangster 1993)
 1.32 (recommended, Hansch et al. 1995;)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.56 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.4.8.1
Reported vapor pressures of 2-methoxyphenol (guaiacol) at various temperatures

Stull 1947		Vonderres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
52.4	133.3	82.0	1333
79.1	666.6	102.0	3333
92.0	1333	119.0	6666
106.0	2666	129.5	9999
121.6	5333	136.0	13332
131.0	7999	149.0	19998
144.0	13332	155.5	26664
162.7	26664	164.8	33330
184.1	53329	169.0	39997
205.0	101325	173.0	43330
		175.9	46663
mp/°C	28.5	179.0	53329
		184.7	59995
		187.0	66661
		191.0	73327
		194.0	79993
		198.0	86659
		201.0	93325
		205.0	101325
		bp/°C	204.566

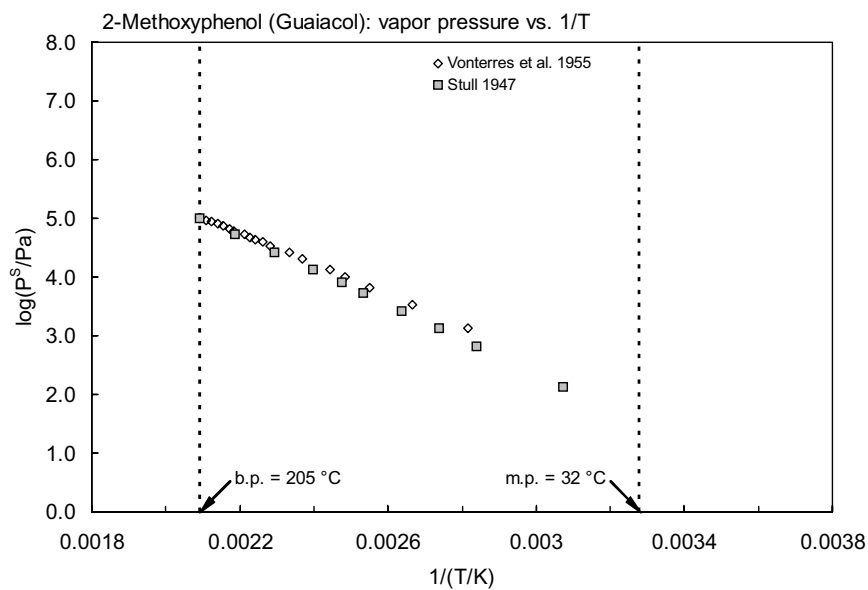
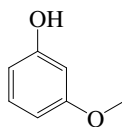


FIGURE 14.1.4.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methoxyphenol (guaiacol).

14.1.4.9 3-Methoxyphenol



Common Name: 3-Methoxyphenol

Synonym: *m*-methoxyphenol, *m*-hydroxyanisole, resorcinol monomethylether

Chemical Name: 3-methoxyphenol

CAS Registry No: 150-19-6

Molecular Formula: $\text{CH}_3\text{OC}_6\text{H}_4\text{OH}$

Molecular Weight: 124.138

Melting Point ($^{\circ}\text{C}$):

< -17 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

244 (Stephenson & Malanowski 1987)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

134.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

67800 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.262 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.12536 - 1572.51/(-136.16 + T/\text{K})$; temp range 413–518 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.10 (estimated as per Sagebiel et al. 1992 data on 2-methoxyphenol)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.58 (Leo et al. 1969; Hansch & Leo 1979)

1.47 (HPLC- k' correlation, Minick et al. 1988)

1.58 (COMPUTOX databank, Kaiser 1993)

1.58 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

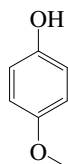
Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.10 4-Methoxyphenol



Common Name: 4-Methoxyphenol

Synonym: *p*-methoxyphenol, *p*-hydroxyanisole, hydroquinone monomethylether

Chemical Name: 4-methoxyphenol

CAS Registry No: 150-76-5

Molecular Formula: $\text{CH}_3\text{OC}_6\text{H}_4\text{OH}$

Molecular Weight: 124.138

Melting Point ($^{\circ}\text{C}$):

57 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

243 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

134.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F: 0.485 (mp at 57°C))

Water Solubility (g/m^3 or mg/L at 25°C):

40000 (Verschueren 1977, 1983)

19500 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.033 (extrapolated-Antoine eq., Boublik et al. 1984)

0.556 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_g/\text{kPa}) = 12.27865 - 4631.266/(T/\text{K})$; temp range 278–300 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.8462 - 2111.03/(-81.56 + T/\text{K})$; temp range 418–518 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

0.979 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/\text{Pa}) = -3664/(T/\text{K}) + 12.28$ (GC-RT correlation, Lei et al. 1999)

1.05 (supercooled liquid P_L , calculated-group contribution, Lee et al. 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

1.34 (shake flask-UV, Fujita et al. 1964)

1.37 (shake flask-UV at pH 7.45, Umeyama et al. 1971)

1.34, 1.33, 1.37 (lit. values, Hansch & Leo 1979)

1.47 (shake flask, Korenman et al. 1980)

1.62 (HPLC- k' correlation, Miyake & Terada 1982)

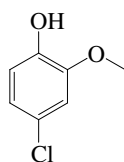
1.24 (HPLC- k correlation, Minick et al. 1988)

1.34 (recommended, LOGKOW databank, Sangster 1993)

1.34 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{oc}}$:

14.1.4.11 4-Chloroguaiacol

Common Name: 4-Chloroguaiacol

Synonym: 4-chloromethoxyphenol

Chemical Name: 4-chloroguaiacol, 4-chloromethoxyphenol

CAS Registry No: 16766-30-6

Molecular Formula: $C_7H_7ClO_2$

Molecular Weight: 158.582

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

155.6(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol \cdot K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5140 (shake flask-HPLC/UV, pH 2.8, Tam et al. 1994)

5604 (shake flask-GC/ECD, pH 2.8, Tam et al. 1994)

5370 (selected, Tam et al. 1994)

4856* ($19^{\circ}C$, shake flask-HPLC/UV, measured range 10 – $50^{\circ}C$, Larachi et al. 2000)

5132; 13200, 10500 (quoted exptl.; calculated-group contribution, calculated-AQUAFAC, Lee et al. 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.15 (calculated-fragment const., Niimi et al. 1990)

2.11–2.52 (literature range, NCASI 1992)

Bioconcentration Factor, $\log BCF$:

0.0 (trout, 1–21 d exposure, $BCF < 1$, Niimi et al. 1990)

0.86–1.19 (quoted, NCASI 1992)

Sorption Partition Coefficient, $\log K_{oc}$:

TABLE 14.1.4.11.1

Reported aqueous solubilities of 4-chloroguaiacol at various temperatures

Larachi et al. 2000

shake flask-HPLC/UV	
t/°C	S/g·m ⁻³
10.0	4395
11.0	4467
15.0	4548
19.0	4856
36.3	5406
41.0	6658
50.0	6213
54.5	7054
66.0	7040
70.5	8639
78.0	9171
85.6	9540
90.0	10255

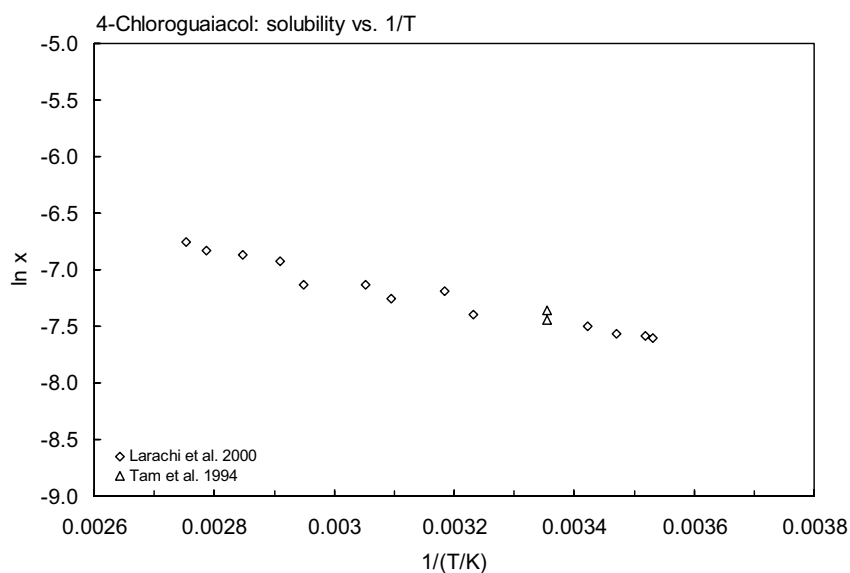
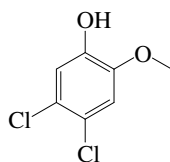


FIGURE 14.1.4.11.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-chloroguaiacol.

14.1.4.12 4,5-Dichloroguaiacol



Common Name: 4,5-Dichloroguaiacol

Synonym: 4,5-dichloro-2-methoxyphenol

Chemical Name: 4,5-dichloroguaiacol

CAS Registry No: 2460-49-3

Molecular Formula: $C_7H_6Cl_2O_2$

Molecular Weight: 193.028

Melting Point ($^{\circ}C$): 69–70

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

8.26, 8.52 (20 $^{\circ}C$, regressions, Xie & Dyrssen 1984)

Molar Volume (cm^3/mol):

176.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

584 (shake flask-HPLC/UV, pH 5.6, Tam et al. 1994)

565 (shake flask-GC/ECD, pH 5.6, Tam et al. 1994)

3130, 1086 (supercooled liquid values: calculated-group contribution, calculated- AQUAFAC, Lee et al. 2000)

Vapor Pressure (Pa at 25 $^{\circ}C$):

1.54 (supercooled liquid P_L , correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant ($Pa\cdot m^3/mol$ at 25 $^{\circ}C$):

0.44 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.04 (calculated-fragment const., Rekker 1977)

3.28 (Hansch & Leo 1979)

3.26 (shake flask-UV, Saarikoski & Viluksela 1982)

3.18 (shake flask-GC, Xie et al. 1984)

3.28 (HPLC- k' correlation, Xie et al. 1984)

3.20, 3.19, 3.19 (shake flask-GC, regressions, Xie & Dryssen 1984)

3.26 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.74–2.05, 2.03 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)

1.18–1.51, 1.75 (quoted, estimated, NCASI 1992)

2.03 (*Oncorhynchus mykiss*, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

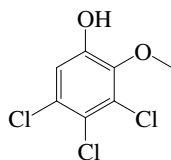
Biodegradation: 5% reduction in concn (5 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d (Neilson et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

14.1.4.13 3,4,5-Trichloroguaiacol



Common Name: 3,4,5-Trichloroguaiacol

Synonym: 3,4,5-trichloro-2-methoxyphenol

Chemical Name: 3,4,5-trichloroguaiacol

CAS Registry No: 57057-83-7

Molecular Formula: $C_7H_3Cl_3O_2$

Molecular Weight: 227.473

Melting Point ($^{\circ}C$): 85–86

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.55 (Könemann 1981)

7.43, 7.52, 7.56 ($20^{\circ}C$, regressions, Xie & Dyrssen 1984)

7.90 (Leuenberger et al. 1985)

7.56 (Xie et al. 1986)

Molar Volume (cm^3/mol):

197.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

305 (shake flask-HPLC/UV, pH 5.9, Tam et al. 1994)

313 (shake flask-GC/ECD, pH 5.9, Tam et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

0.64 (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.12 (calculated-P/C, Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.77 (shake flask-UV, Saarikoski & Viluksela 1982)

4.11 (shake flask-GC, Xie et al. 1984)

4.18 (HPLC- k' correlation, Xie et al. 1984)

4.14 (shake flask-GC, Xie & Dyrssen 1984)

3.77 (recommended, Sangster 1993)

3.77 (COMPUTOX databank, Kaiser 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.60 (rainbow trout, Oikari et al. 1985)

2.06–2.51, 2.41 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)

1.78–1.95 (field studies, bile of rainbow trout, Niimi et al. 1990)

2.47 (estimated, NCASI 1992)

2.20 (*Oncorhynchus mykiss*, Devillers et al. 1996)

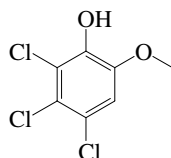
Sorption coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 1\text{--}2$ d in bleak and $t_{1/2} = 2$ d in trout (Niimi et al. 1990).

14.1.4.14 4,5,6-Trichloroguaiacol



Common Name: 4,5,6-Trichloroguaiacol

Synonym: 2,3,4-trichloro-6-methoxyphenol

Chemical Name: 4,5,6-trichloroguaiacol

CAS Registry No: 2668-24-8

Molecular Formula: $C_7H_5Cl_3O_2$

Molecular Weight: 227.473

Melting Point ($^{\circ}C$): 112–115

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.07 (Leuenberger et al. 1985)

7.20 ($20^{\circ}C$, regressions, Xie & Dyrssen 1984)

Molar Volume (cm^3/mol):

197.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

57.0 (shake flask-HPLC/UV, pH 5.8, Tam et al. 1994)

50.0 (shake flask-GC/ECD, pH 5.8, Tam et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

0.249 (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

8.82 (calculated-P/C)

0.14 (calculated-P/C, Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.74 (shake flask-GC, Xie et al. 1984)

3.92, 3.91, 3.78 (HPLC- k' correlation, calculated- π const., calculated-f const., Xie et al. 1984)

3.73, 3.74, 3.72 (shake flask-GC, regressions, Xie & Dyrssen 1984)

3.57 (calculated-fragment const., Niimi et al. 1990)

3.72, 3.92 (literature values, Sangster 1993)

3.82 (COMPUTOX databank, Kaiser 1993)

3.72, 3.92 (literature values, Hansch et al. 1995)

3.19 (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.60 (bleaks, Renberg et al. 1980)

1.90–2.11 (rainbow trout, Oikari et al. 1985)

2.59 (bleaks, Walden et al. 1986)

- 1.88–2.05, 1.97 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
 1.78–1.95 (field studies, bile of trout, Niimi et al. 1990)
 4.81 (fourhorn sculpin *myoxocephalus quadricornis*, bile BCF in brackish water, during 6–20 d exposure under continuous water-flow conditions, Wachtmeister et al. 1991)
 2.22 (estimated, NCASI 1992)
 1.97 (*Oncorhynchus mykiss*, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{oc} :

- 3.11 (sediment, $K_p = 1.3 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986, quoted, Neilson et al. 1991)
 2.80, 2.94 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 2.80 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 1.35 (sediment, $K_p = 22 \text{ ml kg of organic C}^{-1}$, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: 16% reduction in concn (5 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

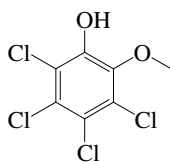
Biotransformation:

Bioconcentration, Uptake(k_1) and Elimination (k_2) Rate Constants Rates:

Half-Lives in the Environment:

Biota: $t_{1/2} = 1$ to 2 d in bleak (Niimi et al. 1990).

14.1.4.15 3,4,5,6-Tetrachloroguaiacol



Common Name: 3,4,5,6-Tetrachloroguaiacol

Synonym: 2,3,4,5-tetrachloro-6-methoxyphenol

Chemical Name: 3,4,5,6-tetrachloroguaiacol

CAS Registry No: 2539-17-5

Molecular Formula: $C_7H_4Cl_4O_2$

Molecular Weight: 261.918

Melting Point ($^{\circ}C$): 121–122

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.26 (Leuenberger et al. 1985)

6.19, 6.12, 6.26 ($20^{\circ}C$, regressions, Xie & Dyrssen 1984)

Molar Volume (cm^3/mol):

218.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

27.0 (shake flask-HPLC/UV, pH 4.2, Tam et al. 1994)

25.0 (shake flask-GC/ECD, pH 4.2, Tam et al. 1994)

165, 28 (supercooled liquid values: calculated-group contribution, calculated-AQAUFAC, Lee et al. 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

0.138 (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.013 (Leuenberger et al. 1985; quoted, Barton 1987)

0.15 (calculated-P/C, Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.29 (Saarikoski & Viluksela 1982)

4.45 (shake flask-GC, Xie et al. 1984)

4.76, 5.01, 4.52 (HPLC- k' correlation, calculated- π const., calculated-fragment const., Xie et al. 1984)

4.41, 4.43, 4.42 (shake flask, regressions, Xie & Dyrssen 1984)

4.53 (Leuenberger et al. 1985)

4.28 (calculated-fragment, Niimi et al. 1990)

4.59 (COMPUTOX databank, Kaiser 1993)

4.42, 4.76 (literature values, Sangster 1993)

4.42 (selected, Hansch et al. 1995)

3.83 (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.60 (bleaks, after 2 weeks exposure, Renberg et al. 1980)

1.60–2.18 (rainbow trout, Oikari et al. 1985)

- 1.78–1.95 (bile of rainbow trout, field studies, Niimi et al. 1990)
2.04–2.38, 2.26 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
3.20 (roach, Niimi et al. 1990, quoted, NCASI 1992)
2.84 (estimated, NCASI 1992)
2.26 (*Oncorhynchus mykiss*, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC} :

- 2.85 (soil, Seip et al. 1986)
3.15 (sediment, $K_p = 1.5 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986)
2.30 (soil, calculated-MCI χ , Bahnick & Doucette 1988)
2.85, 3.17 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.85 (soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: 100% reduction in concn (5 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

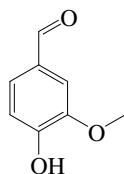
Biotransformation:

Bioconcentration, Uptake(k_1) and Elimination (k_2) Rate Constants Rates:

Half-Lives in the Environment:

Biota: $t_{1/2} < 10$ d in trout liver (Niimi et al. 1990); $t_{1/2} = 1\text{--}2$ d in bleak (Niimi et al. 1990).

14.1.4.16 Vanillin (4-Hydroxy-3-methoxybenzaldehyde)



Common Name: Vanillin

Synonym: 4-hydroxy-3-methoxybenzaldehyde, vanillic aldehyde, methylprotocatechuic aldehyde

Chemical Name: 4-hydroxy-3-methoxybenzaldehyde

CAS Registry No: 121-33-5

Molecular Formula: $C_8H_8O_3$, $C_6H_3OHCHO(OCH_3)$

Molecular Weight: 152.148

Melting Point ($^{\circ}C$):

81.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Weast 1982–83; Lide 2003)

284 (decomposes, Stephenson & Malanowski 1987)

Density (g/cm^3):

1.056 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

7.40 (Sangster 1993)

7.62 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

156.9 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.279 (mp at $81.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2480 (at pH 4.50, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

133.3 ($107^{\circ}C$, summary of literature data, temp range 107 – $285^{\circ}C$, Stull 1947)

$\log(P_S/kPa) = 10.997 - 4623/(T/K)$; temp range 288 – 333 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_S/kPa) = 10.93562 - 4535.023/(T/K)$; temp range 297 – 328 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.01734 - 3198.18/(-17.047 + T/K)$; temp range 380 – 558 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -25.583 - 4.086 \times 10^3/(T/K) + 17.515 \cdot \log(T/K) - 2.8177 \times 10^{-2} \cdot (T/K) + 1.0912 \times 10^{-5} \cdot (T/K)^2$; temp range 355 – 777 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.31 (shake flask-UV, Korenman & Sotnikova 1975)

1.21 (shake flask-UV, Holmes & Lough 1976)

1.21 (shake flask-HPLC, Bazaco & Coca 1989)

1.21 (recommended, Sangster 1993)

1.21 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

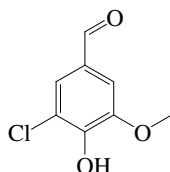
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.17 5-Chlorovanillin



Common Name: 5-Chlorovanillin

Synonym:

Chemical Name: 5-chlorovanillin

CAS Registry No: 19463-48-0

Molecular Formula: $C_8H_7ClO_3$, $C_6H_2ClCHO(OCH_3)$

Molecular Weight: 185.593

Melting Point ($^{\circ}C$):

165 (Weast 1982–83; Lide 2003)

169 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a

6.80 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

177.8 (Le Bas method -calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.042 (mp at $165^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

932 (at pH 4.55, shake flask-HPLC/UV, Varhaníčková et al 1995)

249* ($24^{\circ}C$, shake flask-HPLC/UV, measured range 7.5 – $85.9^{\circ}C$, Larachi et al. 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.76 (NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

0.59 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.4.17.1

Reported aqueous solubilities of 5-chlorovanillin at various temperatures

Larachi et al. 2000

shake flask-HPLC/UV

t/°C	S/g·m ⁻³
7.5	171
12.0	171
16.8	184
19.8	168
24.0	249
30.0	286
36.5	505
46.0	629
50.0	760
59.0	932
65.0	1139
70.0	1267
80.0	1767
85.9	2314

$$\Delta S_{\text{fus}}/(\text{kJ mol}^{-1}) = 89.1$$

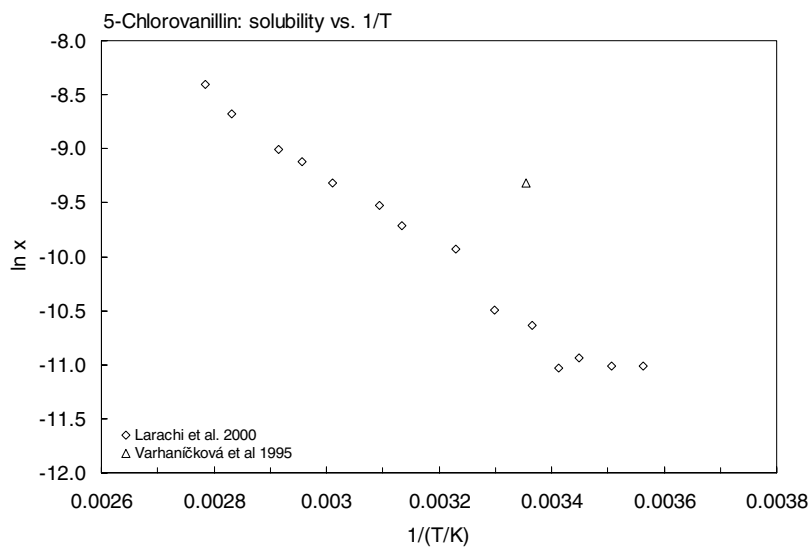
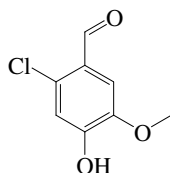


FIGURE 14.1.4.17.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 5-chlorovanillin.

14.1.4.18 6-Chlorovanillin



Common Name: 6-Chlorovanillin

Synonym:

Chemical Name: 6-chlorovanillin

CAS Registry No: 18268-76-3

Molecular Formula: $C_8H_7ClO_3$, $C_6H_2ClCHO(OCH_3)$

Molecular Weight: 185.593

Melting Point ($^{\circ}C$):

171–172 (Varhanířková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.11 (Varhanířková et al 1995)

Molar Volume (cm^3/mol):

177.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

132 (at pH 5.35, shake flask-HPLC/UV, Varhanířková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.76 (NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{oa}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

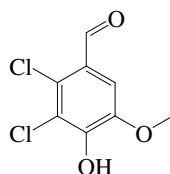
0.59 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.19 5,6-Dichlorovanillin



Common Name: 5,6-Dichlorovanillin

Synonym:

Chemical Name: 5,6-dichlorovanillin

CAS Registry No: 18268-69-4

Molecular Formula: $C_8H_6Cl_2O_3$, $C_6HCl_2CHO(OCH_3)$

Molecular Weight: 221.038

Melting Point ($^{\circ}C$):

198–199 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

5.28 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

198.7 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

23.0 (at pH 4.0, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.47 (NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

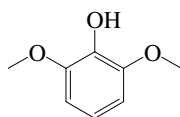
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.76 (estimated, K_{OW} , NCASI 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.20 Syringol (2,6-Dimethoxyphenol)

Common Name: Syringol

Synonym: 2,6-dimethoxyphenol

Chemical Name: 2,6-dimethoxyphenol

CAS Registry No: 91-10-1

Molecular Formula: C₈H₁₀O₃, C₆H₃OH(OCH₃)₂

Molecular Weight: 154.163

Melting Point (°C):

53–56 (Aldrich catalog 1998–1999)

56.5 (Lide 2003)

Boiling Point (°C):

261 (Aldrich catalog 1998–1999; Lide 2003)

Density (g/cm³):

Acid Dissociation Constant, pK_a:

Molar Volume (cm³/mol):

166.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

18200 (shake flask-UV spectroscopy, Sagebiel & Seiber 1993)

Vapor Pressure (Pa at 25°C):

0.45 (GC-RT correlation, Sagebiel & Seiber 1993)

Henry's Law Constant (Pa m³/mol at 25°C):

0.00271 (gas stripping-GC, Sagebiel & Seiber 1993)

Octanol/Water Partition Coefficient, log K_{ow}:

1.15 (shake flask-UV, Fujita et al. 1964)

1.15 (recommended, Sangster 1993)

1.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa}:

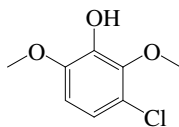
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

14.1.4.21 3-Chlorosyringol



Common Name: 3-Chlorosyringol

Synonym: 3-chloro-2,6-dimethoxyphenol

Chemical Name: 3-chlorosyringol

CAS Registry No: 18113-22-9

Molecular Formula: $C_8H_9ClO_3$, $C_6H_2(OH)Cl(OCH_3)_2$

Molecular Weight: 188.608

Melting Point ($^{\circ}C$):

35-36 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

9.09 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

186.9 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

68.6 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5170 (at pH 4.30, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.825 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3580/(T/K) - 11.93$ (GC-RT correlation, Lei et al. 2001)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.011 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

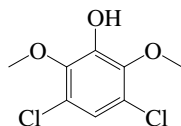
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.22 3,5-Dichlorosyringol



Common Name: 3,5-Dichlorosyringol

Synonym: 3,5-dichloro-2,6-dimethoxyphenol

Chemical Name: 3,5-dichlorosyringol

CAS Registry No: 78782-46-4

Molecular Formula: $C_8H_8Cl_2O_2$, $C_6H(OH)Cl_2(OCH_3)_2$

Molecular Weight: 223.054

Melting Point ($^{\circ}C$):

105–106 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constants, pK_a :

7.27 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

207.8 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.4 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

244 (at pH 5.80, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.465 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3679/(T/K) - 12.01$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.069 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

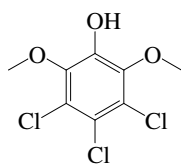
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.23 Trichlorosyringol



Common Name: Trichlorosyringol

Synonym: 3,4,5-trichloro-2,6-dimethoxyphenol

Chemical Name: 3,4,5-trichloro-2,6-dimethoxyphenol

CAS Registry No: 2539-26-6

Molecular Formula: $C_8H_7Cl_3O_3$, $C_6(OH)Cl_3(OCH_3)_2$

Molecular Weight: 257.499

Melting Point ($^{\circ}C$):

122–123 (Varhanířková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.73 (Varhanířková et al 1995)

Molar Volume (cm^3/mol):

228.7 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.4 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

100 (at pH 3.90, shake flask-HPLC/UV, Varhanířková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.077 (supercooled liquid P_L , GC-RT correlation; Lei et al. 1999)

$\log(P_L/Pa) = -4014/(T/K) - 12.44$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.022 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.74 (shake flask-GC, Saarikoski & Viluksela 1982)

4.20 (quoted, NCASI 1992)

3.74 (recommended, Sangster 1993)

3.74 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

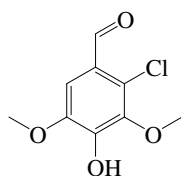
1.19 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.24 2-Chlorosyringaldehyde



Common Name: 2-Chlorosyringaldehyde

Synonym:

Chemical Name: 2-chlorosyringaldehyde

CAS Registry No: 76341-69-0

Molecular Formula: $C_9H_9ClO_4$, $C_6H(OH)Cl(CHO)(OCH_3)_2$

Molecular Weight: 216.619

Melting Point ($^{\circ}C$):

196–197 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.80 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

209.1 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.7 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

33 (at pH 5.30, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.079 (supercooled liquid P_L , GC-RT correlation; Lei et al. 1999)

$\log(P_L/Pa) = -4058/(T/K) - 12.51$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.069 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.81 (quoted, NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

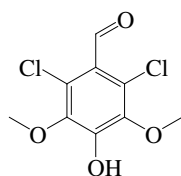
0.62 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.25 2,6-Dichlorosyringaldehyde



Common Name: 2,6-Dichlorosyringaldehyde

Synonym:

Chemical Name:

CAS Registry No: 76330-06-8

Molecular Formula: $C_9H_8Cl_2O_4$, $C_6(OH)Cl_2(CHO)(OCH_3)_2$

Molecular Weight: 251.064

Melting Point ($^{\circ}C$):

195.6 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

230.0 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

82.2 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

26.0 (at pH 4.60, shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

0.025 (supercooled liquid P_L , GC-RT correlation; Lei et al. 1999)

$\log(P_L/Pa) = -4293/(T/K) - 12.79$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

0.0037 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.52 (quoted, NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.19 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 14.2.1

Summary of physical properties of phenolic compounds

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol		pK _a
							MW/ ρ at 20°C	Le Bas	
Alkylphenols and other substituted phenols:									
Phenol	108-95-2	C ₆ H ₅ OH	94.111	40.89	181.87	0.698	88.99	103.4	9.89
<i>o</i> -Cresol (2-Methylphenol)	95-48-7	C ₆ H ₄ (CH ₃)OH	108.138	31.03	191.04	0.873	105.26	125.6	10.26
<i>m</i> -Cresol (3-Methylphenol)	108-39-4	C ₆ H ₄ (CH ₃)OH	108.138	12.24	202.27	1	104.62	125.6	10
<i>p</i> -Cresol (4-Methylphenol)	106-44-5	C ₆ H ₄ (CH ₃)OH	108.138	34.77	201.98	0.802	106.25	125.6	10.26
2,6-Di- <i>t</i> -butyl-4-methylphenol	128-37-0	C ₁₅ H ₂₄ O	220.351	71	265	0.354		303.2	
2,3-Dimethylphenol	526-75-0	C ₈ H ₁₀ O	122.164	72.5	216.9	0.342		147.8	
2,4-Dimethylphenol	105-67-9	C ₈ H ₁₀ O	122.164	24.5	210.98	1		147.8	10.6
2,5-Dimethylphenol	98-87-4	C ₈ H ₁₀ O	122.164	74.8	211.1	0.325		147.8	10.3
2,6-Dimethylphenol	576-26-1	C ₈ H ₁₀ O	122.164	45.8	201.07	0.625		147.8	10.6
3,4-Dimethylphenol	95-65-8	C ₈ H ₁₀ O	122.164	65.1	227	0.404	124.28	147.8	10.4
3,5-Dimethylphenol	108-68-9	C ₈ H ₁₀ O	122.164	63.4	221.74	0.420		147.8	10.2
2,3,5-Trimethylphenol	697-82-5	C ₉ H ₁₂ O	136.190	94.5	233	0.208		170.0	10.6
2,3,6-Trimethylphenol	2416-94-6	C ₉ H ₁₂ O	136.190	63		0.424		170.0	
2,4,5-Trimethylphenol	496-78-6	C ₉ H ₁₂ O	136.190	72	232	0.346		170.0	
2,4,6-Trimethylphenol	527-60-6	C ₉ H ₁₂ O	136.190	73	220	0.338		170.0	10.9
3,4,5-Trimethylphenol	527-54-8	C ₉ H ₁₂ O	136.190	108	248.5	0.153		170.0	
3-Methyl-5-ethylphenol		C ₉ H ₁₂ O	136.190					170.0	10.1
<i>o</i> -Ethylphenol	90-00-6	C ₈ H ₁₀ O	122.164	18	204.5	1		147.8	
<i>m</i> -Ethylphenol	620-17-7	C ₈ H ₁₀ O	122.164	−4	218.4	1		147.8	
<i>p</i> -Ethylphenol	123-07-9	C ₈ H ₁₀ O	122.164	45	217.9	0.636		147.8	
2-Propylphenol	644-35-9	C ₉ H ₁₂ O	136.190	7	220	1		170.0	
4-Propylphenol	645-56-7	C ₉ H ₁₂ O	136.190	22	232.6	1	134.98	170.0	10.3
2-Isopropylpheonol	88-69-7	C ₉ H ₁₂ O	136.190	15.5	213.5	1		170.0	
4-Isopropylphenol	99–89–8	C ₉ H ₁₂ O	136.190	62.3	230	0.431		170.0	10.3
4-Butylphenol	1638-22-8	C ₁₀ H ₁₄ O	150.217	22	248	1		192.2	10.3
2- <i>sec</i> -Butylphenol	89–72–5	C ₁₀ H ₁₄ O	150.217	16	228	1		192.2	
2- <i>tert</i> -Butylphenol	88-18-6	C ₁₀ H ₁₄ O	150.217	B6.8	223	1		192.2	

(Continued)

TABLE 14.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol		pK _a
							MW/ ρ at 20°C	Le Bas	
3- <i>tert</i> -Butylphenol	585-34-2	C ₁₀ H ₁₄ O	150.217	42.3	240	0.676		192.2	10.1
4- <i>sec</i> -Butylphenol	99-71-8	C ₁₀ H ₁₄ O	150.217	61.5	241	0.438		192.2	
4- <i>tert</i> -Butylphenol	98-54-4	C ₁₀ H ₁₄ O	150.217	98	237	0.192		192.2	9.9
2-Methyl-5- <i>tert</i> -butylphenol		C ₁₁ H ₁₆ O	164.244					214.4	
2,6-Di- <i>sec</i> -butylphenol	128-39-2	C ₁₄ H ₂₂ O	206.324	39		0.729		281.0	
3,5-Di- <i>tert</i> -butylphenol	1138-52-9	C ₁₄ H ₂₂ O	206.323	88		0.241		281.0	
3-Pentylphenol		C ₁₁ H ₁₆ O	164.244					214.4	
4-Hexylphenol	2446-69-7	C ₁₂ H ₁₈ O	178.270	32		0.854		236.6	
2-Heptylphenol		C ₁₃ H ₂₀ O	192.297					258.8	
4-Heptylphenol	1987-50-4	C ₁₃ H ₂₀ O	192.297					258.8	
4-Octylphenol	1806-26-4	C ₁₄ H ₂₂ O	206.324	43		0.666		281.0	
4- <i>tert</i> -Octylphenol	140-66-9	C ₁₄ H ₂₂ O	206.324	85.8	279	0.253		281.0	
4-Nonylphenol	104-40-5	C ₁₅ H ₂₄ O	220.351	42	approx. 295	0.681		303.2	
1-Naphthol	90-15-3	C ₁₀ H ₈ O	144.170	95	288	0.206		155.0	
2-Naphthol	135-19-3	C ₁₀ H ₈ O	144.170	121.5	285	0.113	112.63	155.0	
2-Phenylphenol (2-Hydroxybiphenyl)	90-43-7	C ₁₂ H ₁₀ O	170.206	57.5	286	0.480		192.0	
3-Phenylphenol (3-Hydroxybiphenyl)	588-51-8	C ₁₂ H ₁₀ O	170.206	78	>300	0.302		192.0	
4-Phenylphenol (4-Hydroxybiphenyl)	92-69-3	C ₁₂ H ₁₀ O	170.206	166	305	0.0414		192.0	
2-Allylphenol	1745-81-9	C ₉ H ₁₀ O	134.174	B6	220	1		162.6	
Chlorophenols:									
2-Chlorophenol	95-57-8	C ₆ H ₄ OHCl	128.556	9.4	174.9	1	101.75	124.3	8.49
3-Chlorophenol	108-43-0	C ₆ H ₄ OHCl	128.556	32.6	214	0.842		124.3	8.85
4-Chlorophenol	106-48-9	C ₆ H ₄ OHCl	128.556	42.8	220	0.669	101.62	124.3	9.18
2,3-Dichlorophenol	576-24-9	C ₆ H ₄ Cl ₂ O	163.001	58	206	0.474		145.2	6.44
2,4-Dichlorophenol	120-83-2	C ₆ H ₄ Cl ₂ O	163.001	45	210	0.636		145.2	7.68
2,5-Dichlorophenol	583-78-8	C ₆ H ₄ Cl ₂ O	163.001	59	211	0.464		145.2	6.45
2,6-Dichlorophenol	87-65-0	C ₆ H ₄ Cl ₂ O	163.001	68.5	220	0.374		145.2	6.8
3,4-Dichlorophenol	95-77-2	C ₆ H ₄ Cl ₂ O	163.001	68	253	0.379		145.2	7.39
3,5-Dichlorophenol	591-35-5	C ₆ H ₄ Cl ₂ O	163.001	68	233	0.379		145.2	6.92
2,3,4-Trichlorophenol	15950-66-0	C ₆ H ₃ Cl ₃ O	197.446	83.5	sublim	0.267		166.1	7.66
2,3,5-Trichlorophenol	933-78-8	C ₆ H ₃ Cl ₃ O	197.446	62		0.433		166.1	7.37
2,3,6-Trichlorophenol	933-75-5	C ₆ H ₃ Cl ₃ O	197.446	58		0.474		166.1	7.13
2,4,5-Trichlorophenol	95-95-4	C ₆ H ₃ Cl ₃ O	197.446	69	247	0.370		166.1	7.43

2,4,6-Trichlorophenol	88-06-2	C ₆ H ₃ Cl ₃ O	197.446	69	246	0.370	166.1	7.42
3,4,5-Trichlorophenol	609-19-8	C ₆ H ₃ Cl ₃ O	197.446	101	275	0.180	166.1	7.74
2,3,4,5-Tetrachlorophenol	4901-51-3	C ₆ H ₂ Cl ₄ O	231.891	116.5	sublim	0.127	187.0	6.96
2,3,4,6-Tetrachlorophenol	58-90-3	C ₆ H ₂ Cl ₄ O	231.891	70		0.362	187.0	5.38
2,3,5,6-Tetrachlorophenol	935-95-5	C ₆ H ₂ Cl ₄ O	231.891	115		0.131	187.0	5.48
Pentachlorophenol	87-86-5	C ₆ HCl ₅ O	266.336	174	310 dec	0.0345	207.9	4.92
4-Chloro- <i>m</i> -cresol	59-50-7	C ₇ H ₇ ClO	142.583	67	235	0.387	146.5	
Nitrophenols:								
2-Nitrophenol	88-75-5	C ₆ H ₄ OHNO ₂	139.109	44.8	216	0.639	131.9	7.23
3-Nitrophenol	554-84-7	C ₆ H ₄ OHNO ₂	139.109	96.8		0.197	131.9	8.36
4-Nitrophenol	100-02-7	C ₆ H ₄ OHNO ₂	139.109	113.6	279	0.135	131.9	7.08
2,4-Dinitrophenol	51-28-5	C ₆ H ₄ N ₂ O ₅	184.106	114.8	sublim	0.132	160.4	4.09
2,6-Dinitrophenol	329-71-5	C ₆ H ₄ N ₂ O ₅	184.106	108		0.153	160.4	
2,4,6-Trinitrophenol (Picric acid)	88-89-1	C ₆ H ₃ N ₃ O ₇	229.104	122.5	300 exp	0.111	188.9	0.8
4,6-Dinitro- <i>o</i> -cresol	534-52-1	C ₇ H ₆ N ₂ O ₅	198.133	86.5		0.249	182.6	4.35
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:								
Catechol (1,2-Dihydroxybenzene)	120-80-9	C ₆ H ₄ (OH) ₂	110.111	104.6	245	0.166	110.8	9.5
3,5-Dichlorocatechol	13673-9-2	C ₆ H ₂ Cl ₂ (OH) ₂	179.001	83-84		0.267	152.6	7.78
4,5-Dichlorocatechol	3428-24-8	C ₆ H ₂ Cl ₂ (OH) ₂	179.001	116-117		0.127	152.6	
3,4,5-Trichlorocatechol	56961-20-7	C ₆ HCl ₃ (OH) ₂	213.446	134		0.0850	173.5	6.95
Tetrachlorocatechol	1198-55-6	C ₆ Cl ₄ (OH) ₂	247.891	194		0.0220	194.4	5.83
Resorcinol (1,3-Dihydroxybenzene)	108-46-3	C ₆ H ₄ (OH) ₂	110.111	109.4	276.5	0.149	110.8	9.4
Hydroquinone (1,4-Dihydroxybenzene)	123-31-9	C ₆ H ₄ (OH) ₂	110.111	172.4	285	0.0358	110.8	
2-Methoxyphenol (Guaiacol)	90-05-1	C ₇ H ₈ O ₂	124.138	32	205	0.854	134.7	
3-Methoxyphenol	150-19-6	C ₇ H ₈ O ₂	124.138	< B17	244	1	134.7	
4-Methoxyphenol	150-76-5	C ₇ H ₈ O ₂	124.138	57	243	0.485	134.7	
4-Chloroguaiacol	16766-30-6	C ₇ H ₇ ClO ₂	158.582	liquid		1	155.6	
5-Chloroguaiacol	3753-23-5	C ₇ H ₇ ClO ₂	158.582	34-35		0.807	155.6	
4,5-Dichloroguaiacol	2460-49-3	C ₇ H ₆ Cl ₂ O ₂	193.028	69-79		0.331	176.5	8.52
4,6-Dichloroguaiacol	2460-49-3	C ₇ H ₆ Cl ₂ O ₂	193.028	63-64		0.419	176.5	
3,4,5-Trichloroguaiacol	57057-83-7	C ₇ H ₃ Cl ₃ O ₂	227.473	85-86		0.255	197.4	7.56
4,5,6-Trichloroguaiacol	2668-24-8	C ₇ H ₃ Cl ₃ O ₂	227.473	112-115		0.137	197.4	7.2
Tetrachloroguaiacol	2539-17-5	C ₇ H ₄ Cl ₄ O ₂	261.918	121-122		0.113	218.3	6.26
Vanillin	121-33-5	C ₈ H ₈ O ₃	152.148	81.5	285	0.279	156.9	7.42
5-Chlorovanillin	19463-48-0	C ₈ H ₇ ClO ₃	185.593	165		0.0423	177.8	6.80
6-Chlorovanillin	18268-69-4	C ₈ H ₇ ClO ₃	185.593	171-172		0.0365	177.8	6.11

(Continued)

TABLE 14.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm ³ /mol		pK _a
							MW/ ρ at 20°C	Le Bas	
5,6-Dichlorovanillin	18113-22-9	C ₈ H ₆ Cl ₂ O ₃	221.038	198-199		0.0198		198.7	5.28
Syringol (2,6-Dimethoxyphenol)	91-10-1	C ₈ H ₁₀ O ₃	154.163	56.5	261	0.491		166.0	
3-Chlorosyringol	18113-22-9	C ₈ H ₉ ClO ₃	188.608	35-36		0.789		186.9	9.09
3,5-Dichlorosyringol	78782-46-4	C ₈ H ₈ Cl ₂ O ₃	223.054	105-106		0.162		207.8	7.27
Trichlorosyringol	2539-26-6	C ₈ H ₇ Cl ₃ O ₃	257.499	122-123		0.111		228.7	7.73
2-Chlorosyringaldehyde	76341-69-0	C ₉ H ₉ ClO ₄	216.619	196-197		0.0208		209.1	6.80
2,6-Dichlorosyringaldehyde	76330-06-8	C ₉ H ₈ Cl ₂ O ₄	251.064	195.6		0.0212		230.0	

* Assuming $\Delta S_{fus} = 56$ J/mol K.

TABLE 14.2.2

Summary of selected physical-chemical properties of phenolic compounds at 25°C

Compound	Selected properties					log K _{OW}	Henry's law constant H/(Pa·m ³ /mol) calculated P/C
	Vapor pressure		Solubility				
	P _S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		
Alkylphenols and other substituted phenols:							
Phenol	47	67.66	88360	938.9	1345	1.46	0.0500
<i>o</i> -Cresol (2-Methylphenol)		41	26000	240.4	237.32	1.98	0.1489
<i>m</i> -Cresol (3-Methylphenol)		16	22000	203.4	203.4	1.98	0.0786
<i>p</i> -Cresol (4-Methylphenol)		13	20000	184.9	230.6	1.96	0.0564
2,3-Dimethylphenol		8.05	6000	49.11	143.6		0.0560
2,4-Dimethylphenol		13.02	8795	71.99	71.99	2.35	0.1808
2,5-Dimethylphenol		10.68	3176	26.00	80.00		0.1335
2,6-Dimethylphenol		32.82	6230	51.00	81.60	2.36	0.4022
3,4-Dimethylphenol		2.241	5100	41.75	103.3	2.23	0.0217
3,5-Dimethylphenol		3.76	5500	45.02	107.2	2.35	0.0351
2,3,5-Trimethylphenol		2.43	800	5.874	28.24		0.0860
2,4,5-Trimethylphenol		7.73				2.67	
2,4,6-Trimethylphenol		19.58	1200	8.81	26.07	2.73	0.7511
3,4,5-Trimethylphenol		2.144	1540	11.31	73.91		0.0290
3-Methyl-5-ethylphenol		1.18	2314	16.99			
<i>o</i> -Ethylphenol		20.4	14042	114.9	114.9	2.47	0.1775
<i>m</i> -Ethylphenol		6.7				2.5	
<i>p</i> -Ethylphenol		5	7980	65.32	102.7	2.5	0.0487
2-Propylphenol		11.2				2.93	
4-Propylphenol		7.3	1728	12.69	12.69	3.2	0.5753
2-Isopropylphenol		12.45	4423	32.48	32.48	2.88	0.3834
4-Isopropylphenol			3263	23.96	55.59		
4-Butylphenol			617	4.107	4.107	3.65	
2- <i>sec</i> -Butylphenol		5				2.8	
2- <i>tert</i> -Butylphenol						2.7	
3- <i>tert</i> -Butylphenol			2070	13.78	20.38	2.6	
4- <i>sec</i> -Butylphenol		4	960	6.391	14.59	2.1	0.2741
4- <i>tert</i> -Butylphenol		1.24	580	3.861	20.11	3.04	0.0617
2-Methyl-5- <i>tert</i> -butylphenol		3.688	410	2.496			
2,6-Di- <i>sec</i> -butylphenol						4.4	

(Continued)

TABLE 14.2.2 (Continued)

Compound	Selected properties					log K _{OW}	Henry's law constant H/(Pa·m ³ /mol) calculated P/C
	Vapor pressure		Solubility				
	P _s /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		
3,5-Di- <i>tert</i> -butylphenol			14	0.0678	0.2816		
2,6-Di- <i>tert</i> -butyl-4-methylphenol		0.0338				4.17	
3-Pentylphenol						3.13	
4-Hexylphenol			391	2.193	2.568	3.6	
2-Heptylphenol						4.45	
4-Heptylphenol						4.15	
4-Octylphenol		0.071	12.6	0.0611	0.0917	4.12	0.7743
4- <i>tert</i> -Octylphenol						3.7	
2-Nonylphenol						5.76	
3-Nonylphenol						5.61	
4-Nonylphenol		0.1	5.43	0.0246	0.0362	4.48	2.764
1-Naphthol		0.5	438	3.038	14.75	2.84	0.0339
2-Naphthol		0.4	740	5.133	45.42	2.7	8.81×10 ^{B3}
2-Phenylphenol		30	700	4.113	8.568	3.09	3.501
4-Phenylphenol		8.7	9.8	0.0576	1.391	3.2	6.256
2-Allylphenol						2.64	
Chlorophenols:							
2-Chlorophenol	132	132	24650	191.7	191.7	2.17	0.6884
3-Chlorophenol	35	41.57	22000	171.1	203.2	2.5	0.2045
4-Chlorophenol	20	29.90	27000	210.0	313.9	2.4	0.0952
2,3-Dichlorophenol			8215	50.40	106.3	3.15	
2,4-Dichlorophenol	12	18.87	4500	27.61	43.41	3.2	0.4347
2,5-Dichlorophenol						3.2	
2,6-Dichlorophenol	12	32.09	2625	16.10	43.06	2.86	0.7451
3,4-Dichlorophenol			9256	56.79	149.8	3.37	
3,5-Dichlorophenol			7394	45.36	119.7	3.2	
2,3,4-Trichlorophenol	1	3.74	500	2.532	9.484	3.8	0.3949
2,3,5-Trichlorophenol	1	2.31	500	2.532	5.848	3.69	0.3949
2,3,6-Trichlorophenol			450	2.279	4.808	3.8	
2,4,5-Trichlorophenol	2.5	6.76	948	4.801	12.98	3.72	0.5207
2,4,6-Trichlorophenol	1.25	3.44	434	2.198	5.941	3.69	0.5687
3,4,5-Trichlorophenol						4.3	

(Continued)

2,3,4,5-Tetrachlorophenol	0.1	0.79	166	0.7158	5.637	4.8	0.1397
2,3,4,6-Tetrachlorophenol	0.28	0.78	183	0.7892	2.180	4.45	0.3548
2,3,5,6-Tetrachlorophenol	0.1	0.78	100	0.4312	3.292	4.9	0.2319
Pentachlorophenol	4.15×10 ^{B3}	0.12	14	0.0526	1.524	5.05	0.0789
Nitrophenols:							
2-Nitrophenol		20	1080	7.764	12.15	1.8	1.646
3-Nitrophenol			11550	83.03	421.5	2	
4-Nitrophenol			13500	97.05	718.9	1.91	
2,4-Dinitrophenol			335	1.820	13.78	1.67	
2,4,6-Trinitrophenol (Picric acid)			13750	60.02	540.7	1.33	
4,6-Dinitro- <i>o</i> -cresol			222	1.120	4.500	2.12	
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:							
Catechol (1,2-Dihydroxybenzene)		1.34	45000	408.7	2462	0.88	5.44×10 ^{B4}
Resorcinol (1,3-Dihydroxybenzene)	0.0118	0.079	110000	999.0	6705	0.80	1.18×10 ^{B5}
Hydroquinone (1,4-Dihydroxybenzene)	2.55×10 ^{B3}	0.071	70000	635.7	17758	0.59	4.01×10 ^{B6}
2-Methoxyphenol (Guaiacol)	20.825	24.4	24800	199.8	233.9	1.33	0.1042
3-Methoxyphenol			67800	546.2	546.2	1.58	
4-Methoxyphenol			19500	157.1	323.9	1.34	
4-Chloroguaiacol			5370	33.86	33.86	2.15	
5-Chloroguaiacol			3960	24.97	30.94		
4,5-Dichloroguaiacol	0.570	1.72	575	2.98	9.000	3.26	0.1913
4,6-Dichloroguaiacol			708	3.668	8.754	2.86	
3,4,5-Trichloroguaiacol	0.163	0.64	310	1.363	5.344	3.77	0.1996
4,5,6-Trichloroguaiacol	0.032	0.23	54	0.2374	1.733	3.74	0.1348
Tetrachloroguaiacol	0.016	0.14	26	0.0993	0.8785	4.45	0.1612

TABLE 14.2.3

Suggested half-life classes for phenolic compounds in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Alkylphenols and other substituted phenols:				
Phenol	2	3	4	5
<i>o</i> -Cresol	1	2	3	4
<i>p</i> -Cresol	1	2	3	4
2,4-Dimethylphenol	2	3	4	5
Chlorophenols:				
2,4-Dichlorophenol	3	3	5	6
2,4,5-Trichlorophenol	4	4	6	7
2,4,6-Trichlorophenol	4	4	6	7
2,3,4,6-Tetrachlorophenol	5	5	6	7
Pentachlorophenol	5	5	6	7
Nitrophenols:				
2-Nitrophenol	3	3	5	6
4-Nitrophenol	3	3	5	6
2,4-Dinitrophenol	4	4	6	7
2,4,6-Trinitrophenol				
4,6-Dinitro- <i>o</i> -cresol	4	4	6	7
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:				
Catechol	2	3	4	5
2-Methoxyphenol (Guaiacol)	2	3	4	5
Tetrachloroguaiacol	4	4	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

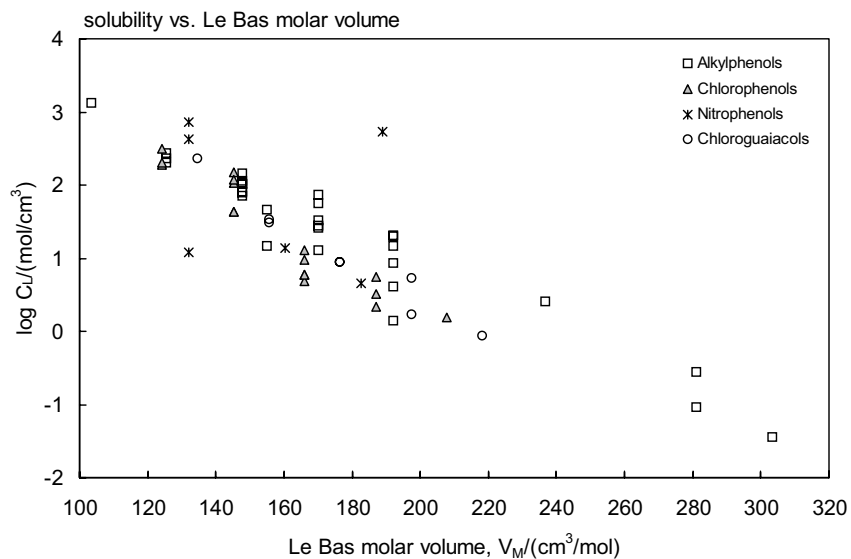


FIGURE 14.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for phenolic compounds.

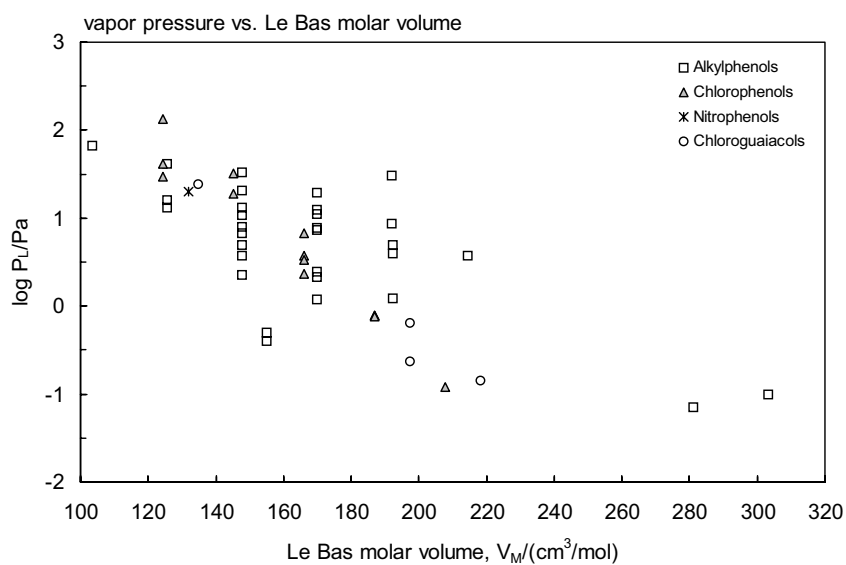


FIGURE 14.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for phenolic compounds.

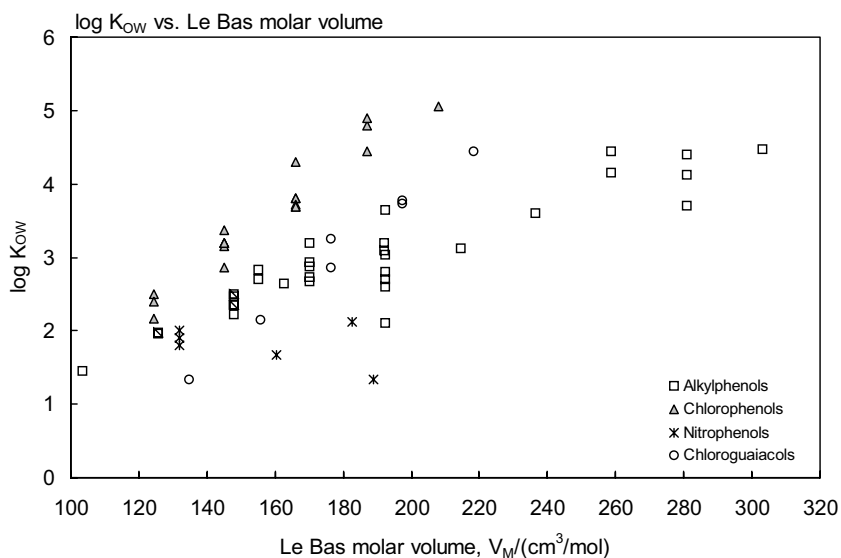


FIGURE 14.2.3 Octanol-water partition coefficient versus Le Bas molar volume for phenolic compounds.

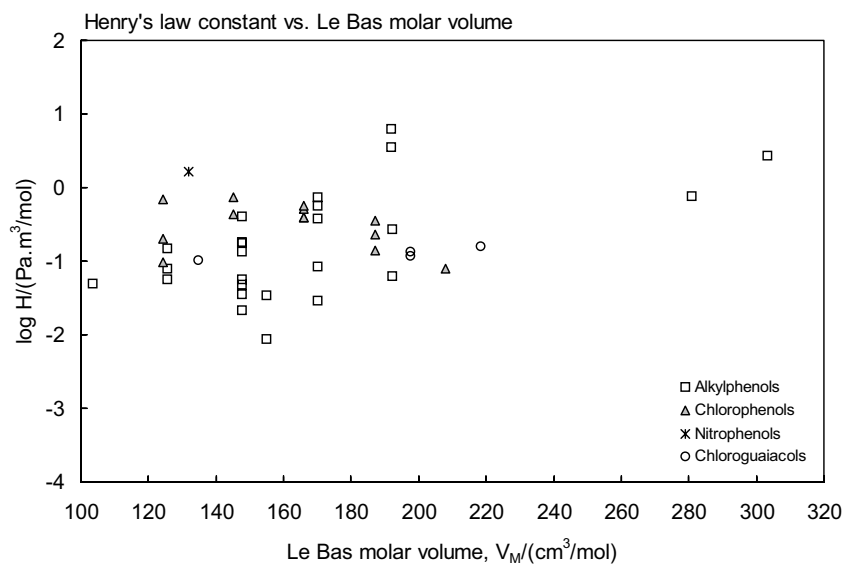


FIGURE 14.2.4 Henry's law constant versus Le Bas molar volume for phenolic compounds.

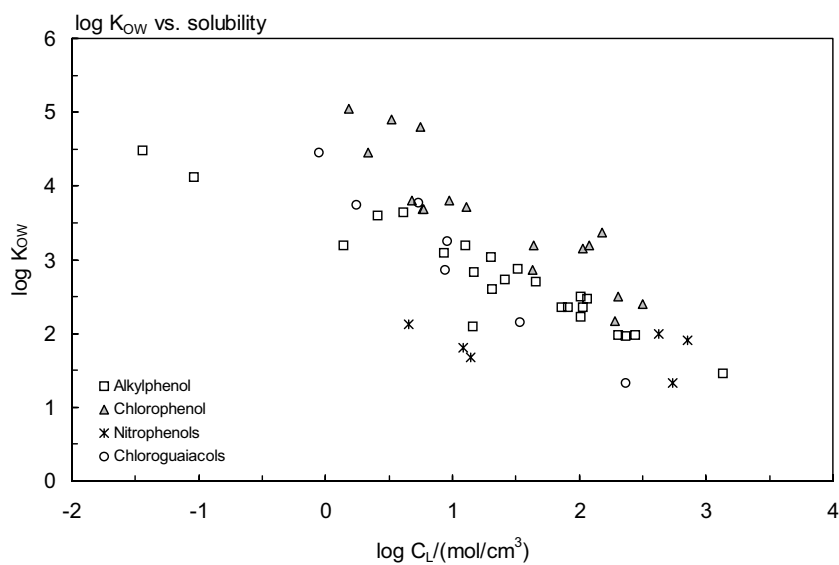


FIGURE 14.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for phenolic compounds.

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15 Esters

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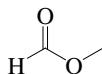
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15.1 LIST OF CHEMICALS AND DATA COMPILATIONS

15.1.1 ALIPHATIC ESTERS

15.1.1.1 Methyl formate



Common Name: Methyl formate

Synonym: formic acid methyl ester, methyl methanoate

Chemical Name: methyl formate

CAS Registry No: 107-31-3

Molecular Formula: $C_2H_4O_2$, $HCOOCH_3$

Molecular Weight: 60.052

Melting Point ($^{\circ}C$):

-99.0 (Weast 1982–83; Dean 1985; Lide 2003)

Boiling Point ($^{\circ}C$):

31.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9742 (Weast 1982–83)

0.9742, 0.9664 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

62.8 (exptl. at normal bp, Lee et al. 1972)

61.6 ($20^{\circ}C$, calculated-density)

62.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

30.59; 29.72 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.75 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

230000 (USEPA 1975; quoted, Howard 1993)

304000 ($20^{\circ}C$, Verschueren 1983)

230000 (Dean 1985; Riddick et al. 1986)

23800 (solubility data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

83260* (isoteniscope method, measured range 21 – $31.7^{\circ}C$, Nelson 1928)

$\log(P/mmHg) = 7.2202 - 1320.8/(T/K)$; temp range 21 – $31.7^{\circ}C$, Nelson 1928)

53329* ($16^{\circ}C$, summary of literature data, temp range -74.2 to $213^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 7027.8/(T/K)] + 7.852144$; temp range -74.2 to $213^{\circ}C$ (Antoine eq., Weast 1972–73)

63980, 93310 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

80840 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 2.11093 - 1.573/(-17.263 + t/^{\circ}C)$, temp range: 21 – $31.7^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

83440 (calculated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 3.207 - 3.02/(-11.9 + t/^{\circ}C)$, temp range: 21 – $32^{\circ}C$ (Antoine eq., Dean 1985, 1992)

78060 (selected lit., Riddick et al. 1986)

$\log(P/kPa) = 6.29529 - 1125.2/(174.2 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

78600 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.225693 - 1088.955/(-46.675 + T/\text{K})$; temp range 279–305 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.39684 - 1196.323/(-32.629 + T/\text{K})$; temp range 305–443 K (Antoine eq.-II, Stephenson & Malanowski 1987)

78070 (Daubert & Danner 1989)

$\log (P/\text{mmHg}) = 28.9576 - 2.3582 \times 10^3/(T/\text{K}) - 7.4848 \cdot \log(T/\text{K}) + 7.4384 \times 10^{-10} \cdot (T/\text{K}) + 2.7013 \times 10^{-6} \cdot (T/\text{K})^2$, temp range 174–487 K (vapor pressure eq., Yaws 1994)

114881 (35°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

22.61 (exptl., Hine & Mookerjee 1975)

20.15, 17.96 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

15.64 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

26.02 (calculated-P/C, Hoff et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

−0.010 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)

−0.264 (estimated, Howard 1993)

0.03 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

1.75 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

−0.222 (estimated-S, Lyman et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

0.699 (soil, estimated-S, Lyman et al. 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on Henry's law constant, $t_{1/2} \sim 5.3$ h from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius equation see reference:

$k_{OH} = (2.27 \pm 0.34) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a, quoted, Atkinson 1989)

$k_{OH}(\text{calc}) = 0.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: aqueous base-catalyzed hydrolysis $k = 36.6 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C corresponds to $t_{1/2} = 21.9$ d, 2.19 d, 9.1 h and 0.91 h at respective pHs of 6, 7, 8, and 9 (Mabey & Mill 1978; quoted, Howard 1993)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 74$ d, based on experimental reaction rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere at 23°C (Atkinson 1989; quoted, Howard 1993).

TABLE 15.1.1.1.1
Reported vapor pressures of methyl formate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
Nelson 1928		Stull 1947	
isoteniscope		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
21.0	80101	−74.2	133.3
25.0	83260	−57.0	666.6
26.6	86286	−48.6	1333
26.8	87286	−39.2	2666
27.1	88392	−28.7	5333
28.3	90406	−21.9	7999
28.9	94845	−12.9	13332
30.1	96378	0.80	26664
31.4	101431	16.0	53329
31.7	102351	32.0	101325
bp/°C	31.6	mp/°C	−99.8
eq. 1	P/mmHg		
A	7.2203		
B	1329.8		

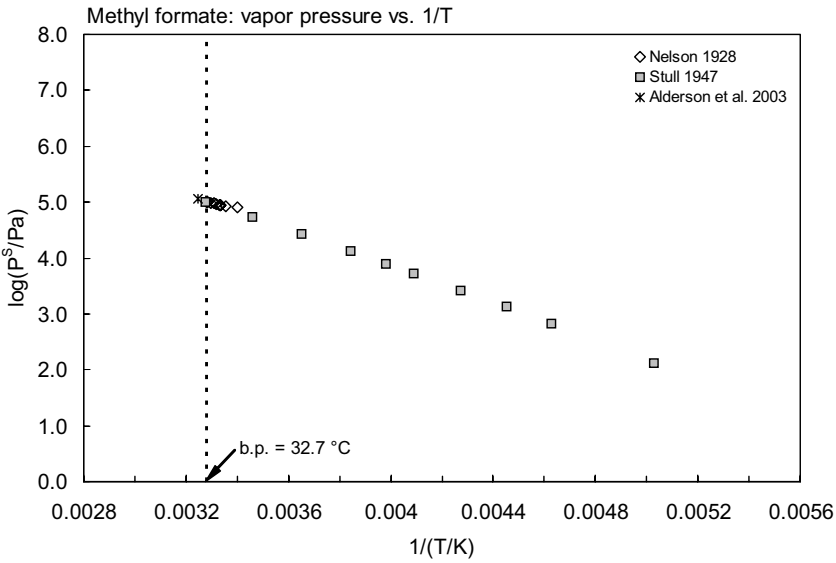
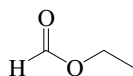


FIGURE 15.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methyl formate.

15.1.1.2 Ethyl formate



Common Name: Ethyl formate

Synonym: ethyl methanoate, formic acid ethyl ester

Chemical Name: ethyl formate

CAS Registry No: 109-94-4

Molecular Formula: $C_3H_6O_2$, $HCOOCH_2CH_3$

Molecular Weight: 74.079

Melting Point ($^{\circ}C$):

-79.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

54.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9168 (Weast 1982-83)

0.9220, 0.9153 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

80.8 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

86.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.64; 29.94 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.205 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

88250 (Seidell 1941)

93260 (estimated, McGowan 1954)

52440 (Deno & Berkheimer 1960)

118000 (Verschueren 1983; Riddick et al. 1986)

117000 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

34530* ($25.4^{\circ}C$, isoteniscope method, measured range 25.4 – $55.4^{\circ}C$, Nelson 1928)

$\log(P/mmHg) = 7.8457 - 1621.2/(T/K)$; temp range 25.4 – $55.4^{\circ}C$ (Nelson 1928)

33050* (interpolated-regression of tabulated data, temp range -60.5 to $54.3^{\circ}C$, Stull 1947)

30844* ($23.715^{\circ}C$, temp range 3.893 – $53.56^{\circ}C$, Mertl & Polak 1964 - ref. see Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 7511.7/(T/K)] + 7.842747$; temp range -60.5 to $225^{\circ}C$ (Antoine eq., Weast 1972-73)

25590, 39990 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

30840, 32610 ($23.7^{\circ}C$, quoted exptl., interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.13263 - 1123.305/(218.177 + t/^{\circ}C)$; temp range 3.89 – $53.56^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

32540 (interpolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.0090 - 1123.94/(218.2 + t/^{\circ}C)$; temp range 4 – $54^{\circ}C$ (Antoine eq., Dean 1985, 1992)

32370 (selected, Riddick et al. 1986)

33070 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.1384 - 1151.08/[-48.94 + (T/K)]$; temp range: 213 – $336 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.4206 - 1326.4/[-26.867 + (T/K)]$; temp range: 327 – $498 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 29.9404 - 2.5263 \times 10^3/(T/K) - 7.809 \cdot \log(T/K) - 1.0111 \times 10^{-9} \cdot (T/K) + 2.7447 \times 10^{-6} \cdot (T/K)^2;$$

temp range 194–508 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

28.46	(exptl., Hine & Mookerjee 1975)
27.18, 25.96	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
17.55	(calculated-MCI χ , Nirmalakhandan & Speece 1988)
702.0	(calculated, Hoff et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

−0.38	(calculated, Iwasa et al. 1965)
0.23	(calculated, Hansch et al. 1968)
0.33	(Leo et al. 1971)
0.55	(calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)
0.26	(calculated-CLOGP, Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.19	(head-space GC, Abraham et al. 2001)
------	--------------------------------------

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (10.2 \pm 1.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a; quoted, Atkinson 1989)

$k_{\text{OH}} = 10.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{\text{OH}}(\text{calc}) = 1.17 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 15.1.1.2.1

Reported vapor pressures of ethyl formate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Nelson 1928		Stull 1947		Mertl & Polak 1964	
isotenoscope		summary of literature data		ref in Boublik et al. 1984	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
25.4	34530	−60.5	133.3	3.893	11870
28.9	40103	−42.2	666.6	5.883	13155

(Continued)

TABLE 15.1.1.2.1 (Continued)

Nelson 1928		Stull 1947		Mertl & Polak 1964	
isoteniscope		summary of literature data		ref in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
33.6	48263	-33.0	1333	8.963	15369
35.5	51982	-22.7	2666	12.395	18244
38.2	58555	-11.5	5333	16.185	21869
40.1	61608	-4.30	7999	19.290	25242
42.9	70914	5.40	13332	23.715	30844
44.2	72304	20.0	26664	28.260	37517
47.8	82193	40.0	53329	32.775	45345
50.9	91886	53.4	101325	38.220	56435
52.2	96139			43.630	69674
53.4	100392	mp/°C	-79	49.453	86066
54.2	102978			53.560	99805
55.4	109138				
eq. in Boublik et al. 1984					
bp/°C	53.8			eq. 2	P/kPa
				A	6.13263
eq. 1	P/mmHg			B	1123.305
A	7.8457			C	218.177
B	1621.6			bp/°C	54.013

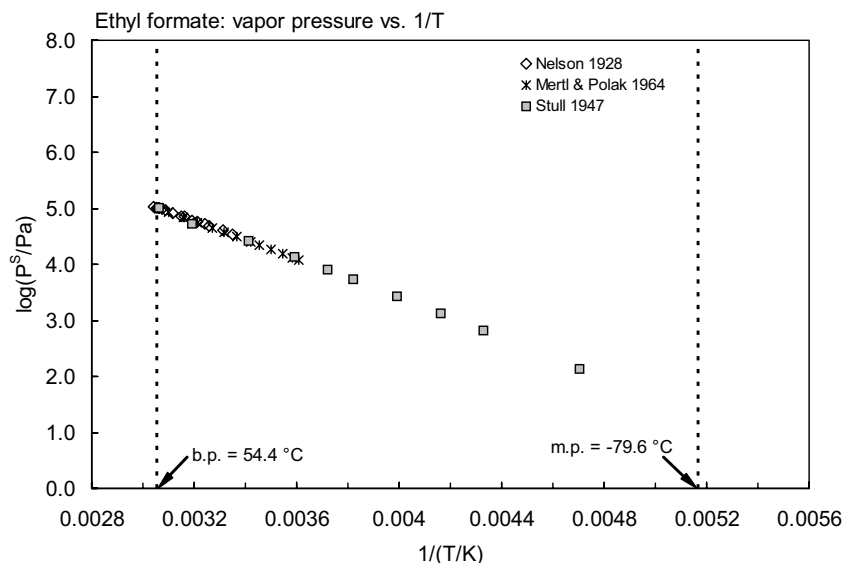
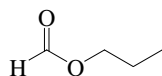


FIGURE 15.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethyl formate.

15.1.1.3 Propyl formate



Common Name: Propyl formate

Synonym: formic acid propyl ester, methanoic acid *n*-propyl ester, propyl methanoate

Chemical Name: *n*-propyl formate, propyl formate

CAS Registry No: 110-74-7

Molecular Formula: C₄H₈O₂, HCOOCH₂CH₂CH₃

Molecular Weight: 88.10 6

Melting Point (°C):

−92.9 (Stull 1947; Weast 1982–83; Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):

80.9 (Lide 2003)

Density (g/cm³ at 20°C):

0.9058 (Weast 1982–83)

0.9006 (Dean 1985)

0.9055, 0.8996 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

97.3 (20°C, calculated-density)

110.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

Enthalpy of Vaporization, ΔH_v (kJ/mol):

37.49; 33.60 (25°C; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

28445 (Seidell 1941)

27230 (Deno & Berkheimer 1960)

27300 (Hansch et al. 1968; quoted, Hine & Mookerjee 1975; Müller & Klein 1992)

20500 (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11759* (26.2°C, isotenoscope method, measured range 26.2–82.3°C, Nelson 1928)

log (P/mmHg) = 7.9925 – 1806.5/(T/K); temp range 26.2–82.3°C (Nelson 1928)

10620* (interpolated-regression of tabulated data, temp range −43 to 81.3°C Stull 1947)

log (P/mmHg) = [−0.2185 × 8208.1/(T/K)] + 7.891833; temp range −43 to 245°C (Antoine eq., Weast 1972–73)

11010 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 5.98912 – 1135.489/(204.518 + t/°C); temp range: 26.2–82.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

10710 (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 6.848 – 1127/(203 + t/°C); temp range: 26–82°C (Antoine eq., Dean 1985, 1992)

11030 (quoted lit. average, Riddick et al. 1986)

log (P/kPa) = 5.97008 – 1132.3/(204.8 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

10810 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.73268 – 1560.69/(−24.287 + T/K); temp range: 230–335 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.2378 – 1301.3/(−46.767 + T/K); temp range: 354–518 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log(P/\text{mmHg}) = 28.6983 - 2.6926 \times 10^3/(T/K) - 7.2435 \cdot \log(T/K) - 8.7226 \times 10^{-11} \cdot (T/K) + 1.9456 \times 10^{-6} \cdot (T/K)^2;$$

temp range 180–538 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 37.52 (exptl., Hine & Mookerjee 1975)
 38.39, 38.39 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 22.61 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.73 (calculated, Hansch et al. 1968)
 0.83 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1979)
 0.83 (recommended, Sangster 1989; 1993)
 0.83 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 2.66 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (2.38 \pm 2.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988; quoted, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 1.87 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 15.1.1.3.1

Reported vapor pressures of propyl formate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
<i>n</i> -propyl formate		isopropyl formate	
Nelson 1928		Stull 1947	
isoteniscope method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
26.2	11759	−43.0	133.3
30.8	14545	−22.7	666.6
35.2	17932	−12.6	1333
40.5	22718	−1.70	2666

TABLE 15.1.1.3.1 (Continued)

n-propyl formate				isopropyl formate			
Nelson 1928		Stull 1947		Nelson 1928		Stull 1947	
isoteniscope method		summary of literature data		isoteniscope method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
46.2	28864	10.8	5333	48.0	49062	0.20	5333
52.0	33717	18.8	7999	48.2	49609	7.50	7999
58.4	46516	29.5	13332	53.708	61101	17.8	13332
63.7	56235	45.3	26664	57.80	70661	33.6	26664
63.9	57422	62.6	53329	63.90	87726	50.5	53329
70.5	72034	81.3	101325	68.60	102405	68.3	101325
71.0	73967			70.30	108377		
73.5	79993	mp/°C	−92.5	77.788	113830	mp/°C	-
75.1	86513			72.100	116430		
78.9	96525						
80.5	101245			bp/°C	68.4		
82.3	106498			eq. 1	P/mmHg		
				A	7.8909		
				B	1710.5		
bp/°C	80.4						
eq. 1	P/mmHg						
A	7.99255						
B	1806.5						

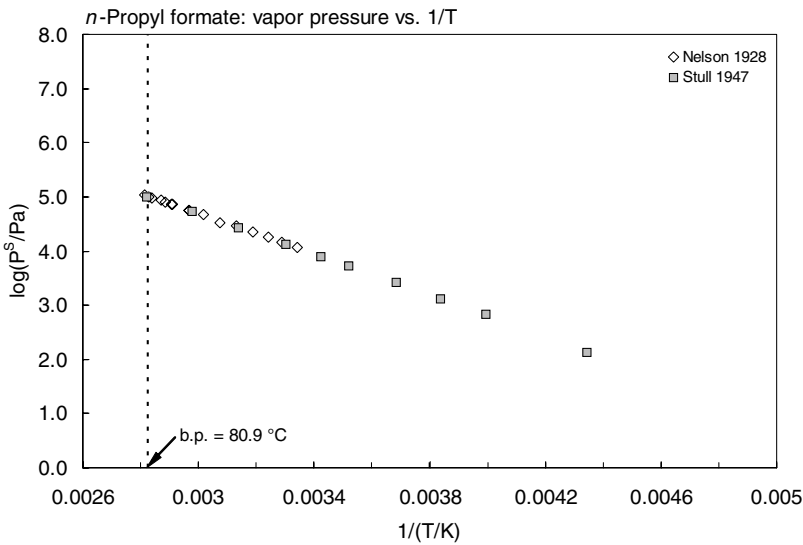


FIGURE 15.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for n-propyl formate.

15.1.1.4 Methyl acetate



Common Name: Methyl acetate

Synonym: acetic acid methyl ester, ethanoic acid methyl ester, methyl ethanoate

Chemical Name: methyl acetate

CAS Registry No: 79-20-9

Molecular Formula: $C_3H_6O_2$, CH_3COOCH_3

Molecular Weight: 74.079

Melting Point ($^{\circ}C$):

−98.25 (Lide 2003)

Boiling Point ($^{\circ}C$):

56.89 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9330 (Weast 1982–83)

0.9342 (Dean 1985)

0.9342, 0.9279 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

79.3 ($20^{\circ}C$, calculated-density)

84.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

22.50 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.30, 30.33 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

243730 ($20^{\circ}C$, shake flask-turbidity, Fühner 1924)

294920 (estimated, McGowan 1954)

243500 ($20^{\circ}C$, Stephen & Stephen 1963)

240000, 319000 ($20^{\circ}C$, Verschueren 1983)

240000 (Dean 1985)

245000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

27980* (interpolated-regression of tabulated data, -52 to $57.8^{\circ}C$, Stull 1947)

25242* ($22.060^{\circ}C$, temp range 1.758 – $55.840^{\circ}C$, Mertl & Polak 1964; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 7732.8/(T/K)] + 7.938782$; temp range -57.2 to $225^{\circ}C$ (Antoine eq., Weast 1972–73)

28830* (ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.24410 - 1183.700/(T/K) - 50.736$; temp range 259.6 – $351.3 K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

31330 (Verschueren 1983)

28830 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.25449 - 1189.608/(223.115 + t/^{\circ}C)$; temp range -13.58 to $78.12^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.19357 - 1159.358/(219.913 + t/^{\circ}C)$; temp range 1.76 – $55.84^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

28200 (calculated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.0652 - 1157.63/(219.73 + t/^{\circ}C)$; temp range: 1 – $56^{\circ}C$ (Antoine eq., Dean 1985, 1992)

28828 (lit. average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.24410 - 1183.70/(222.414 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 28830, 28840 (interpolated-Antoine eq. I and II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.190152 - 1157.622/(-53.426 + T/\text{K})$; temp range 274–331 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.18771 - 1156.219/(-53.589 + T/\text{K})$; temp range: 274–331 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 33.7235 - 2.7204 \times 10^3/(T/\text{K}) - 9.1182 \cdot \log(T/\text{K}) - 9.4316 \times 10^{-11} \cdot (T/\text{K}) + 3.3102 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 175–507 K (vapor pressure eq., Yaws 1994)
 53808 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

9.190 (volatility-partial pressure, Butler & Ramchandani 1935)
 11.65 (volatility-partial pressure-GC, Buttery et al. 1969)
 8.795 (exptl., Hine & Mookerjee 1975)
 11.59, 9.210 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
 13.06 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, $\Delta H = 39.2 \text{ kJ/mol}$, Kieckbusch & King 1979)
 9.210, 25.96 (quoted, calculated-MCI χ , Nirmalakhandan & Speece 1988)
 9.80 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 4.590 - 2048/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.18 (shake flask-CR, Collander 1951; quoted, Hansch & Leo 1979; Hansch & Leo 1985)
 0.23 (calculated, Hansch et al. 1968)
 0.70 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 0.18 (recommended, Sangster 1989, 1993)
 0.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.31 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

-0.224 (calculated-S, Lyman et al. 1982)
 -0.092 (calculated- K_{OW} , Lyman et al. 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

0.681 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1993)
 1.474 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on calculated Henry's law constant, $t_{1/2} \sim 9.1 \text{ h}$ from a model river of 1 m deep flowing at 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}} = (1.1 \pm 0.03) \times 10^{10} \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $(1.7 \pm 0.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K using relative rate technique for *n*-butane (Campbell & Parkinson 1978)

$k_{\text{OH}}(\text{exptl}) = (1.3 - 3.41) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson et al. 1979; Güesten et al. 1984; Atkinson 1987; Wallington et al. 1988a,b; quoted, Howard 1993)

$k_{\text{OH}}(\text{calc}) = 1.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = (3.41 \pm 0.29) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (absolute rate, flash photolysis-resonance fluorescence, Wallington 1988a)

$k_{\text{OH}} = 3.41 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 2.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}}(\text{calc}) = 6.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.182 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

atmospheric $t_{1/2} = 47\text{--}94 \text{ d}$, based on exptl. rate constants for the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson et al. 1979; Güsten et al. 1984; Atkinson 1987; Wallington et al. 1988; quoted, Howard 1993).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.1.4.1

Reported vapor pressures of methyl acetate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Stull 1947	Mertl & Polak 1965	Ambrose et al. 1981					
summary of literature data	ref. in Boublik et al. 1984	comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-57.2	133.3	1.758	9202	-13.581	3785	57.559	103841
-38.6	666.6	4.058	10415	-10.401	4597	61.773	119919
-29.3	1333	6.568	11870	-7.621	5426	65.575	136076
-19.1	2666	8.563	13155	-4.400	6450	70.114	157575
-7.90	5333	11.635	15369	-1.427	7733	74.442	180470
-0.50	7999	15.145	18244	1.819	9241	78.128	202007
9.40	13332	18.975	21869	4.978	10938	25.0	28828
24.0	26664	22.060	25242	8.278	12977		
40.0	53329	26.520	30844	11.635	15386	bp/K	330.018
57.8	101325	31.060	37517	14.886	18029		
		35.590	45345	19.151	22079	Antoine eq.	
mp/°C	-98.7	41.090	56435	22.787	26098	eq. 3	P/kPa
		46.500	69474	26.948	31418	A	6.24410
		52.310	86066	31.023	37456	B	1184.700
		55.840	97512	35.319	44810	C	-50.735

TABLE 15.1.1.4.1 (Continued)

Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		ref. in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				40.047	54206		
				44.148	63603	data also fitted to:	
				48.507	74964	Chebyshev equation and	
				53.215	89039	Chebyshev polynomial	
				56.821	101164	coefficients given in ref.	

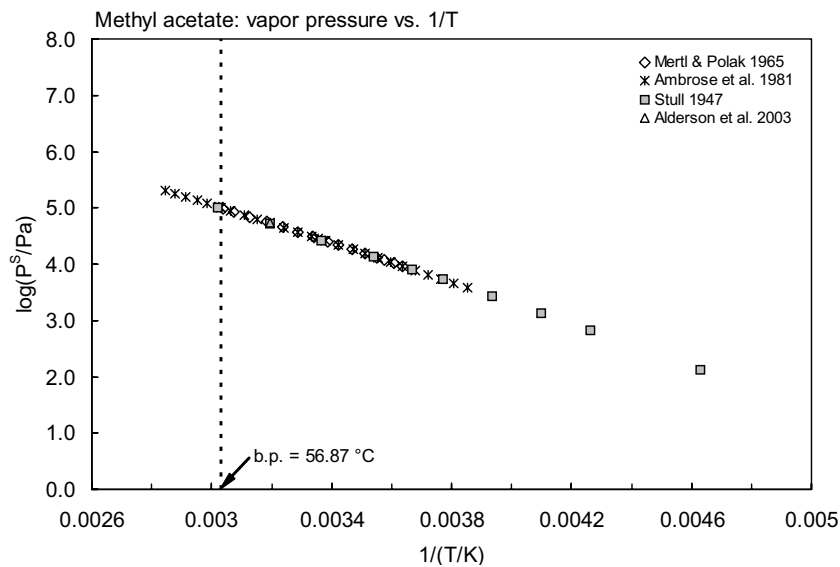
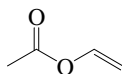


FIGURE 15.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for methyl acetate.

15.1.1.5 Vinyl acetate



Common Name: Vinyl acetate

Synonym: ethanoic acid ester, ethenyl acetate, ethenyl ethanoate

Chemical Name: ethenyl acetate, vinyl acetate

CAS Registry No: 108-05-4

Molecular Formula: $C_4H_6O_2$, $CH_3COOCH=CH_2$

Molecular Weight: 86.090

Melting Point ($^{\circ}C$):

−93.2 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

72.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9317 (Weast 1982–83)

Molar Volume (cm^3/mol):

92.2 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

101.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

37.2, 34.35 ($25^{\circ}C$, bp. Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

19722 (Deno & Berkheimer 1960)

25000 (Verschuereen 1983)

20000 (Dean 1985)

20000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

14454* (interpolated-regression of tabulated data, temp range -48 to $72.5^{\circ}C$, Stull 1947)

21.83* ($21.83^{\circ}C$, measured range 21.8 – $72.04^{\circ}C$, Capkova & Fried 1964 - ref see Boublik et al. 1984)

84406* ($67^{\circ}C$, vapor-liquid equilibrium data, measured range 67 – $82^{\circ}C$, Swamy & Van Winkle 1965)

15300 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.17023 - 1766.918/(269.951 + t/^{\circ}C)$; temp range: 67 – $82^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.3363 - 1296.847/(226.731 + t/^{\circ}C)$; temp range: 21.83 – $72.04^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

15300 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.2101 - 1296.13/(226.66 + t/^{\circ}C)$; temp range: 22 – $72^{\circ}C$ (Antoine eq., Dean 1985, 1992)

14100 (quoted lit. average, Riddick et al. 1986)

$\log(P/kPa) = 7.216 - 1798.4/(T/K)$; temp range: not specified (Antoine eq., Riddick et al. 1986)

15340, 15305 (interpolated-Antoine eq.-I, II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.3799 - 1320.2716/(-43.96 + T/K)$; temp range: 293 – 346 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.34264 - 1300.315/(-46.041 + T/K)$; temp range 294 – 346 K (Antoine eq.-II, Stephenson & Malanowski 1987)

11320 ($20^{\circ}C$, quoted, Howard 1989)

$$\log (P/\text{mmHg}) = 12.722 - 2.177 \times 10^3/(T/K) - 91.458 \cdot \log (T/K) - 4.5688 \times 10^{-3} \cdot (T/K) + 2.9673 \times 10^{-6} \cdot (T/K)^2;$$

temp range 180–524 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

48.74 (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.60 (shake flask, Fujisawa & Masuhara 1980)
0.21 (calculated-HPLC-RT, Fujisawa & Masuhara 1981)
0.73 (recommended, Sangster 1989, 1993)
0.73 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

0.32–0.37 (estimated- K_{OW} , Howard 1989)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.28–1.77 (estimated- K_{OW} , Howard 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 4.4$ h from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s, and $t_{1/2} = 2.2$ d from an environmental pond (Howard 1989).

Photolysis:

Oxidation: $t_{1/2} = 13$ and 8 d for reactions with OH radical and singlet oxygen in sunlit natural water (Howard 1989).

Hydrolysis: overall rate constant $k_h = 1.10 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 7.3$ d at 25°C and pH 7 (Mabey & Mill 1978)
degradation $t_{1/2} = 7.3$ d at 25°C and pH 7, the hydrolysis rate will increase as the pH increases (Howard 1989).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 12$ h with photochemically produced hydroxyl radical in an average atmosphere (Howard 1989).

Surface water: hydrolysis degradation $t_{1/2} = 7.3$ days at 25°C and pH 7; $t_{1/2} = 13$ and 8 d for reactions with hydroxyl radical and singlet oxygen, respectively, in natural water (Howard 1989).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.1.5.1

Reported vapor pressures of vinyl acetate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Capkova & Fried 1963		Swamy & Van Winkle 1965	
summary of literature data		in Boublik et al. 1984		V-L equil. data	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-48.0	133.3	21.83	13159	67.0	84406
-28.0	666.6	25.12	15372	69.0	90646
-18.0	1333	28.8	18252	70.0	92899
-7.0	2666	32.85	21891	72.0	100711
5.30	5333	36.13	25264	74.0	107924
13.0	7999	40.82	30864	76.0	115550
23.3	13332	45.64	37543	78.0	123643
38.4	26664	50.37	45356	80.0	132189
55.5	53329	56.12	56448	82.0	131215
72.5	101325	61.83	69487		
		67.92	86046		
mp/ $^{\circ}\text{C}$	-73	72.04	99958		
		eq. 2	P/kPa		
		A	6.33630		
		B	1296.847		
		C	226.731		
		bp/ $^{\circ}\text{C}$	71.731		

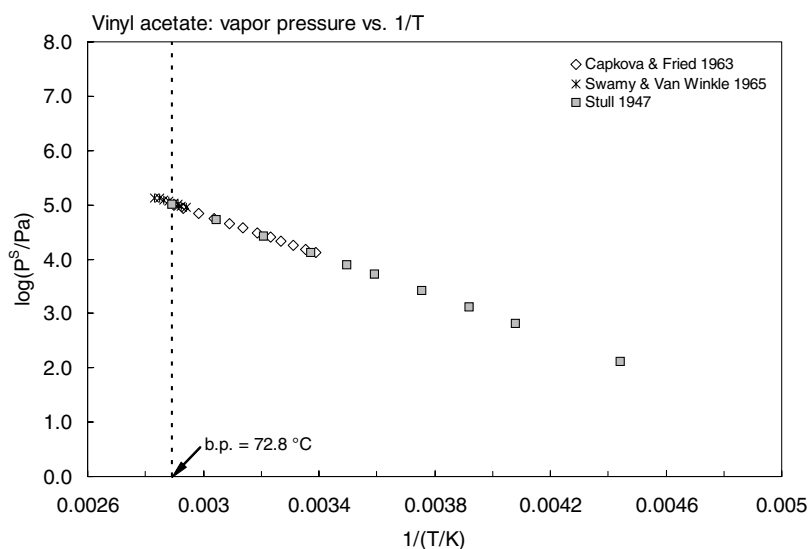
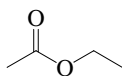


FIGURE 15.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for vinyl acetate.

15.1.1.6 Ethyl acetate



Common Name: Ethyl acetate

Synonym: acetic acid ethyl ester, acetic ether, ethanoic acid ester, ethyl ethanoate

Chemical Name: *n*-ethyl acetate, ethyl acetate

CAS Registry No: 141-78-6

Molecular Formula: $C_4H_8O_2$, $CH_3COOCH_2CH_3$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

−83.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

77.11 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9003 (Weast 1982–83)

0.9006, 0.8946 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

106.0 (exptl. at normal bp, Lee et al. 1972)

97.8 ($20^{\circ}C$, calculated-density)

108.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

22.83 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.62, 31.97 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.50 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

64408 ($20^{\circ}C$, shake flask-turbidity, Fühner 1924)

85300 ($20^{\circ}C$, synthetic method, Jones 1929)

78720 (shake flask-centrifuge, Booth & Everson 1948)

80100* (turbidimetric method, measured range 20 – $40^{\circ}C$, Altshuller & Everson 1953)

80400* (average, Altshuller & Everson 1953)

79780 (shake flask-interferometry, Donahue & Bartell 1952)

69990 (estimated, McGowan 1954)

82220 (Deno & Berkheimer 1960)

80350 (shake flask-UV, Hansch et al. 1968)

63960 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)

82500, 74000 ($20^{\circ}C$, $35^{\circ}C$, literature average, Verschuereen 1983)

80000 (shake flask-HPLC, Banerjee 1984)

97000 (Dean 1985)

95000 (shake flask-radiometric method, Lo et al. 1986)

80800 (lit. average, Riddick et al. 1986)

77900* ($20.2^{\circ}C$, shake flask-GC/TC, measured range 0 – $70^{\circ}C$, Stephenson & Stuart 1986)

73700 (solubility data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

13330*, 11860 ($27.0^{\circ}C$, interpolated-regression of tabulated data, temp range -43.4 to $78.1^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.30588 - 1357.7/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

- 13155* (25.86°C, temp range 15.58–75.830°C, Mertl & Polak 1964; quoted, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = [-0.2185 \times 8301.1/(T/K)] + 8.001170$; temp range –43.4 to 235°C (Antoine eq., Weast 1972–73)
- 12600* (ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)
 $\log(P/\text{kPa}) = 6.18799 - 1224.673/(T/K) - 57.438$; temp range: 271–372.865 K (Antoine eq., ebulliometry, Ambrose et al. 1981)
- 9704 (20°C, Verschueren 1983)
- 11220 (calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.1171 - 1245.172/(217.984 + t/^\circ\text{C})$, temp range 15.58–75.83°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.20229 - 1232.542/(216.587 + t/^\circ\text{C})$, temp range –2.08 to 99.71°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 12620 (calculated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.10179 - 1244.95/(217.88 + t/^\circ\text{C})$ temp range 15–76°C (Antoine eq., Dean 1985, 1992)
- 12600 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.18799 - 1224.673/(215.712 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
- 12620 (interpolated-Antoine eq.-I and III, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.227229 - 1245.239/(-55.239 + T/K)$; temp range: 288–351 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.38462 - 1369.41/(-37.675 + T/K)$; temp range: 350–508 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.22825 - 1245.68/(-55.193 + T/K)$; temp range: 288–351 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- 3240, 5240 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 0.6955 - 2.2498 \times 10^3/(T/K) + 5.4643 \cdot \log(T/K) - 1.9451 \times 10^{-2} \cdot (T/K) + 1.2362 \times 10^{-5} \cdot (T/K)^2$;
temp range 190–623 K (vapor pressure eq., Yaws 1994)
- 25078 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 13.42 (partial pressure, Butler & Ramchandani 1935)
- 17.78 (28°C, concn. ratio-GC, Nelson & Hoff 1968)
- 13.62 (exptl., Hine & Mookerjee 1975)
- 15.64, 13.94 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
- 17.20 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, $\Delta H = 41.4 \text{ kJ/mol}$, Kieckbusch & King 1979)
- 13.62, 24.22 (quoted, calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 41.72* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 $\ln(1/K_{\text{AW}}) = -7.28 + 3563/(T/K)$, temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)
- 13.62, 6.23 (quoted, calculated-molecular structure, Russell et al. 1992)
- 11.33 (calculated, Hoff et al. 1993)
- 13.51 (solid-phase microextraction SPME-GC, Bartelt 1997)
- 12.72 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 5.095 - 2163/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.66 (shake flask-chemical reaction CR, Collander 1951)
- 0.73 (shake flask-GC, Hansch & Anderson 1967; quoted, Leo et al. 1969, 1971; Hansch & Leo 1979)
- 0.73 (shake flask-UV, Hansch et al. 1968; Hansch & Leo 1979)
- 0.65, 0.66 (calculated- π substituent const.; calculated-fragment const., Rekker 1977)
- 0.70 (exptl., Valvani et al. 1981; quoted, Amidon & Williams 1982)
- 0.53 (calculated-activity coeff. γ , Wasik et al. 1981)
- 0.68 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
- 1.02 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
- 0.73 (recommended, Sangster 1989, 1993)
- 0.73 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.70 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

4.13 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
 0.70 (alga *Chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)
 1.48 (golden ide, Freitag et al. 1985)
 4.13 (algae, Freitag et al. 1985)
 3.52 (activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

0.361 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 10.1$ h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: rate constant $k = 6.8 \times 10^{-4} \text{ h}^{-1}$ to $2.21 \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO^- in the gas (Dilling et al. 1988).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius equation see reference:

photooxidation $t_{1/2} = 2.75\text{--}110$ yr in water, based on measured rate constant for the reaction with hydroxyl radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (1.16 \pm 0.13) \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 292 K using relative rate technique for *n*-butane (Campbell & Parkinson 1978)

$k_{OH}(\text{calc}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.82 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{calc}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (15.1 \pm 1.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 296–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a; quoted Atkinson 1989)

$k_{OH} = 1.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 1.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}(\text{calc}) = 1.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.110 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988);

overall rate constant $k_h = 1.10 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} = 2.0$ yr at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 2.02$ yr, based on measured rate constants for acid and base catalyzed and neutral hydrolysis at pH 7 and 20°C (Mabey & Mill 1978; quoted, Howard 1990; Howard et al. 1991; Kollig 1993)

$t_{1/2} = 9.5 \times 10^7$ d at pH 2, $t_{1/2} = 740$ d at pH 7 and $t_{1/2} = 97000$ d at pH 12 in natural waters at $20\text{--}25^\circ\text{C}$ (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous aerobic biodegradation screening test data (Heukelekian & Rand 1955; Price et al. 1974; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 4$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.75\text{--}110$ yr, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991);

$t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 14.6$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976)

photooxidation $t_{1/2} = 35.3\text{--}353$ h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991);

calculated lifetimes of 6.9 d and 10 yr for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 4$ d; hydrolysis $t_{1/2} = 9.5 \times 10^7$ d at pH 2, $t_{1/2} = 740$ d at pH 7 and $t_{1/2} = 97000$ d at pH 12 in natural waters at $20\text{--}25^\circ\text{C}$ (Capel & Larson 1995)

Groundwater: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 15.1.1.6.1

Reported aqueous solubilities and Henry's law constants of ethyl acetate at various temperatures

Aqueous solubility				Henry's law constant	
Altshuller & Everson 1953		Stephenson & Stuart 1986		Kolb et al. 1992	
synthetic method-turbidity		shake flask-GC/TC		equilibrium headspace-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa}\cdot\text{m}^3 \text{ mol}^{-1})$
20	83200	0	97100	40	41.72
25	80100	9.5	86200	60	94.53
30	77000	20.0	77900	70	130.9
35	73900	30.0	68100	80	167.8
40	70800	40.0	62800		
		50.0	62000	$\ln (1/K_{\text{AW}}) = A - B/(T/K)$	
eq.	$S/(\text{g}/100\text{g})$	59.9	60600	A	-7.28
$S = 9.552 - 0.0618 \cdot (t/^\circ\text{C})$		70.5	58800	B	-3563
summary of lit. average					
20	84200				
25	80400				
30	77000				
35	73900				
40	71200				

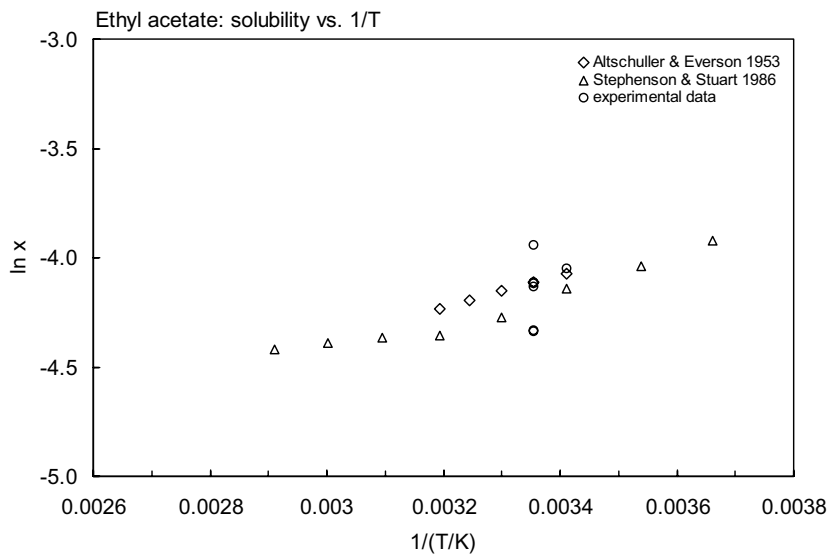


FIGURE 15.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for ethyl acetate.

TABLE 15.1.1.6.2
Reported vapor pressures of ethyl acetate at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)					
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)					
log P = A – B/(C + T/K)		(3)								
log P = A – B/(T/K) – C·log (T/K)		(4)								
Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981						
summary of literature data		in Boublik et al. 1984		comparative ebulliometry						
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa			
–43.4	133.3	15.58	7838	–2.07	2868	29.112	15339			
–23.5	666.6	18.58	9202	–0.096	3236	32.553	17990			
–13.5	1333	21.115	10415	2.398	3754	37.060	22031			
–3.0	2666	23.775	11870	5.737	4560	40.920	26056			
9.10	5333	25.86	13155	8.692	5385	45.333	31374			
16.6	7999	29.135	15369	12.098	6494	49.657	37046			
27.0	13332	32.830	18244	15.242	7683	54.214	44760			
42.0	26664	36.875	21869	18.681	9187	59.231	54168			
59.3	53329	40.175	25242	22.022	10878	63.588	63565			
77.1	101325	44.905	30844	25.532	12925	68.218	74938			
mp/°C	–82.4	49.715	37517	29.119	15336	73.224	89016			
		54.505	45345	32.599	17990	77.056	101144			
		60.320	56435	37.086	22033	77.053	103823			
		66.045	69474	40.929	26056	82.321	119902			
		72.190	86066	25.0	12600	86.359	136066			
		75.830	97272	bp/K	350.261	91.183	157571			
		eq. 2	P/kPa			95.786	180471			
				A		6.22710	Antoine eq.			

(Continued)

TABLE 15.1.1.6.2 (Continued)

Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		B	1245.172	eq. 3	P/kPa	data also fitted to:	
		C	217.904	A	6.18799	Chebyshev equation and	
		bp	77.064	B	1224.673	Chebyshev polynomial	
				C	-57.438	coefficients given in ref.	
						bp/°C	77.115
						Bublik	P/kPa
						A	6.20229
						B	1232.542
						C	216.587

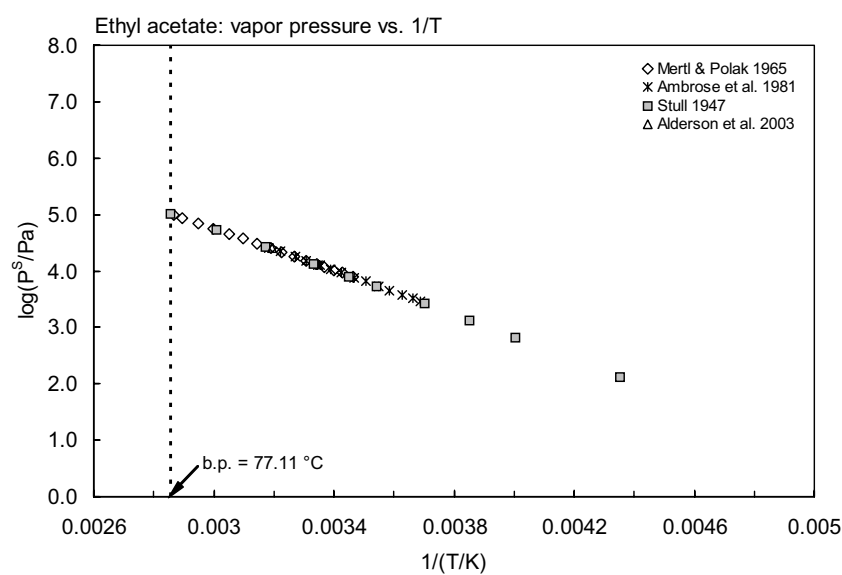
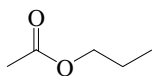


FIGURE 15.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for ethyl acetate.

15.1.1.7 Propyl acetate



Common Name: Propyl acetate

Synonym: acetic acid propyl ester, propyl ethanoate, *n*-propyl acetate

Chemical Name: propyl acetate, *n*-propyl acetate

CAS Registry No: 109-60-4

Molecular Formula: $C_5H_{10}O_2$, $CH_3COOCH_2CH_2CH_3$

Molecular Weight: 102.132

Melting Point ($^{\circ}C$):

−93 (Lide 2003)

Boiling Point ($^{\circ}C$):

101.54 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8878 (Weast 1982–83)

0.8830 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

115.0 ($20^{\circ}C$, calculated-density)

133.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

−7.18 (Perrin 1972)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.83, 33.86 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperature designated * are compiled at the end of this section):

18895 ($20^{\circ}C$, shake flask-turbidity, Fühner 1924)

18890 (Fühner 1924; quoted, Hansch et al. 1968)

20380 (estimated, McGowan 1954)

18160 (quoted, Deno & Berkheimer 1960)

18900 (Stephen & Stephen 1963; quoted, Howard 1993)

18895 (shake flask-UV, Hansch et al. 1968)

20430 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)

22450 ($20^{\circ}C$, literature average, Verschueren 1983)

23000 (Dean 1985)

23000 ($20^{\circ}C$, lit. average, Riddick et al. 1986)

22600*, 19800 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.2^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4152* (interpolated-regression of tabulated data, temp range -26.7 to $101.8^{\circ}C$ Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 8794.8/(T/K)] + 8.212268$; temp range -38.3 to $89^{\circ}C$ (Antoine eq., Weast 1972–73)

4478 (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.14362 - 1284.080/(T/K) - 64.364$; temp range 290.3 – 398.908 K (Antoine eq., ebulliometry, Ambrose et al. 1981)

4494 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.16547 - 1297.186/(210.301 + t/^{\circ}C)$; temp range 17.13 – $125.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.14152 - 1282.545/(208.628 + t/^{\circ}C)$; temp range 39.8 – $100.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- 4486 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.01615 - 1282.28/(208.6 + t/^{\circ}\text{C})$, temp range: 39–101°C (Antoine eq., Dean 1985, 1992)
 4497 (quoted lit average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.14362 - 1284.080/(208.786 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P_L/\text{kPa}) = 6.142106 - 1282.873/(-64.486 + T/\text{K})$; temp range 312–374 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.48937 - 1544.31/(-30.623 + T/\text{K})$; temp range 374–542 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.13951 - 1281.682/(-64.58 + T/\text{K})$; temp range 312–374 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 43.0548 - 3.4692 \times 10^3/(T/\text{K}) - 12.217 \cdot \log(T/\text{K}) + 2.4748 \times 10^{-10} \cdot (T/\text{K}) + 3.7508 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 178–549 K (vapor pressure eq., Yaws et al. 1994)
 9586 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 20.150 (exptl., Hine & Mookerjee 1975)
 22.092, 20.62 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
 22.09 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C, data presented in graph, $\Delta H = 43.2 \text{ kJ/mol}$, Kieckbusch & King 1979)
 30.50 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 82.91, 203.7, 290.5, 387.3 (40, 60, 70 80°C, equilibrium headspace-GC, Kolb et al. 1992)
 $\ln(1/K_{\text{AW}}) = -9.27 + 3971/(T/\text{K})$, temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)
 10.10 (calculated-molecular structure, Russell et al. 1992)
 16.13 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 5.519 - 2257/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.23 (calculated, Hansch et al. 1968; quoted, Leo et al. 1969)
 1.11 (calculated-activity coeff. γ , Wasik et al. 1981)
 1.24 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
 1.23 (Hansch & Leo 1985)
 1.24 (recommended, Sangster 1989, 1993)
 1.24 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 3.17 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.380, 0.708 (calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.288, 2.045 (soil, calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on Henry's law constant, $t_{1/2} \sim 6.5 \text{ h}$ from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

exptl. photooxidation rate constant of 2.4 to $4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with the photochemically produced hydroxyl radicals in the atmosphere (Conkle et al. 1975; Atkinson et al. 1979; Ambrose et al. 1981; Atkinson 1985, 1987; Drossman et al. 1988; quoted, Howard 1993)

photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}} = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ using relative rate technique for 2-methylpropene (Winer et al. 1977; quoted, Atkinson 1985)

$k_{\text{OH}} = (1.7 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Zetzsch 1982; quoted, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 2.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = (34.5 \pm 3.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{\text{OH}} = 3.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.087 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976);

$t_{1/2} = 3.39\text{--}6.69 \text{ d}$, based on exptl. rate constant for the vapor-phase reaction with the photochemically produced hydroxyl radical in the atmosphere (Conkle et al. 1975; Atkinson et al. 1979; Ambrose et al. 1981; Atkinson 1985, 1987; Drossman et al. 1988; quoted, Howard 1993).

TABLE 15.1.1.7.1
Reported aqueous solubilities of propyl acetate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
0	32100
9.5	27800
20.0	22600
30.0	19800
40.0	18700
50.0	17200
60.1	16400
70.5	17200
80.0	16600
90.2	13500

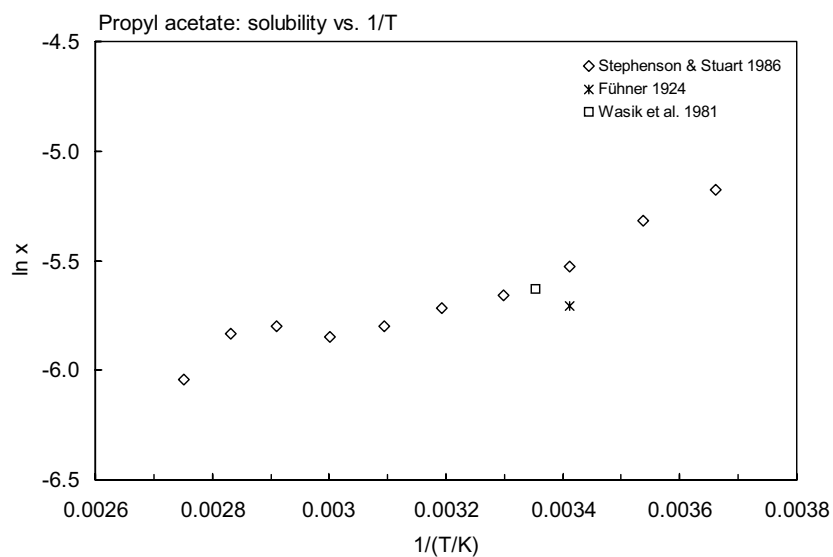


FIGURE 15.1.1.7.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for propyl acetate.

TABLE 15.1.1.7.2

Reported vapor pressures of propyl acetate at various temperatures

Stull 1947

summary of literature data

t/°C	P/Pa
-26.7	133.3
-5.40	666.6
5.0	1333
16.0	2666
28.8	5333
37.0	7999
47.8	13332
64.0	26664
82.0	53329
101.8	101325
mp/°C	-92.5

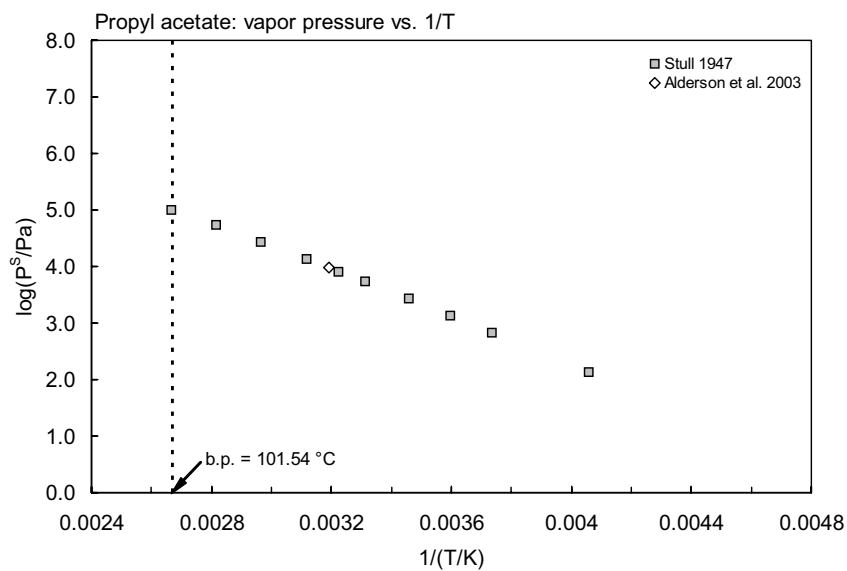
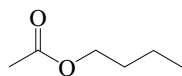


FIGURE 15.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for propyl acetate.

15.1.1.8 Butyl acetate



Common Name: Butyl acetate

Synonym: acetic acid butyl ester, butyl ethanoate, *n*-butyl acetate, ethanoic acid butyl ester

Chemical Name: butyl acetate, *n*-butyl acetate

CAS Registry No: 123-86-4

Molecular Formula: $C_6H_{12}O_2$, $CH_3COOCH_2CH_2CH_2CH_3$

Molecular Weight: 116.158

Melting Point ($^{\circ}C$):

-78 (Lide 2003)

Boiling Point ($^{\circ}C$):

126.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8825 (Weast 1982-83)

0.8764 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

132.5 ($20^{\circ}C$, calculated-density)

155.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

23.28 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

43.64, 35.81 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

23550 (Seidell 1941)

23180 (estimated, McGowan 1954)

4955 (Deno & Berkheimer 1960)

23580 (shake flask-spectrophotometry, Hansch et al. 1968)

7040 ($20^{\circ}C$, quoted, Amidon et al. 1975)

6702 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)

3936 (Hine & Mookerjee 1975)

5000, 14000 (Verschuereen 1983)

4300 (Dean 1985)

8400 (shake flask-radiometric method, Lo et al. 1986)

6800 ($20^{\circ}C$, quoted lit. average, Riddick et al. 1986)

6400*, 5200 ($19.7^{\circ}C$, $30.3^{\circ}C$, shake flask-GC/TC, measured range $0-90.5^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

$\log(P/mmHg) = 8.099 - 1964/(253 + t/^{\circ}C)$ (Davis 1941)

1560* ($24.5^{\circ}C$, measured range $24.5-94.1^{\circ}C$, Usanovich & Dembicij 1959)

9210* ($59.74^{\circ}C$, temp range $59.74-126.09^{\circ}C$, Kliment et al. 1964; quoted, Boublik et al. 1984)

3386* ($67.9^{\circ}C$, ebulliometry, measured range $67.9-124.0^{\circ}C$, Sheehan & Langer 1969)

1505 (Hoy 1970)

$\log(P/mmHg) = 6.9688 - 1326.7/(199.2 + t/^{\circ}C)$; temp range $67.0-130^{\circ}C$ (ebulliometry, Sheehan & Langer 1969)

$\log(P/mmHg) = [-0.2185 \times 9300.8/(T/K)] + 8.095046$; temp range -21.2 to $118^{\circ}C$ (Antoine eq., Weast 1972-73)

1440 (quoted, Hine & Mookerjee 1975)

- 1333 (20.0°C, Verschueren 1983)
 1530, 1138 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.25496 - 1432.217/(210.936 + t/^\circ\text{C})$; temp range 59.74–126°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 4.7514 - 669.809/(117.657 + t/^\circ\text{C})$; temp range 24.5–94.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 1529 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.12712 - 1430.418/(210.746 + t/^\circ\text{C})$; temp range 60–126°C (Antoine eq., Dean 1985, 1992)
 1664 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.151445 - 1368.051/(203.9298 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P_L/\text{kPa}) = 6.176 - 1385.8/(-67.05 + T/\text{K})$; temp range 332–399 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.13505 - 1355.816/(-70.705 + T/\text{K})$; temp range: 341–399 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 2000, 635 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 4.383 - 2.7134 \times 10^3/(T/\text{K}) + 3.9835 \cdot \log(T/\text{K}) - 1.6575 \times 10^{-2} \cdot (T/\text{K}) + 9.7246 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 200–579 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 33.44 (exptl., Hine & Mookerjee 1975)
 30.50, 31.21 (calculated-group contribution, calculated-group contribution, Hine & Mookerjee 1975)
 28.51 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, $\Delta H = 47.6 \text{ kJ/mol}$, Kieckbusch & King 1979)
 38.39 (predicted-MCI χ , Nirmalakhandan & Speece 1988)
 82.91* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 20.2 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 6.400 - 2486/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.73 (calculated, Hansch et al. 1968; quoted, Leo et al. 1969)
 1.69 (calculated-activity coeff. γ , Wasik et al. 1981)
 1.82 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
 1.78 (24°C, shake flask-GC, Catz & Friend 1989)
 1.82 (recommended, Sangster 1989, 1993)
 1.78 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C:

- 3.65 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.602, 1.146 (calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.531, 2.367 (soil, calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 6.1 \text{ h}$ was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s and an estimated $t_{1/2} \sim 7.4 \text{ d}$ for a 10 m deep similar model river (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}}(\text{calc}) = 4.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 4.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp.
(SAR structure-activity relationship, Atkinson 1987)

photooxidation $t_{1/2} = 6.0 \text{ d}$ in air was estimated for the vapor-phase reaction with an average atmospheric OH of $8 \times 10^5/\text{cm}^3$ (GEMS 1986; quoted, Howard 1990)

$k_{\text{OH}} = (41.5 \pm 3.0) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988)

$k_{\text{OH}} = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.087 \text{ M}^{-1}\cdot\text{s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988);

$t_{1/2} = 3.1 \text{ yr}$, 114 d, 11.4 d at pH 7.0, 8.0, 9.0 were estimated, respectively, based on observed acid and base-catalyzed rate constants at 20°C (Mabey & Mill 1978; quoted, Howard 1990).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 6.0 \text{ d}$ was estimated for the vapor-phase reaction with an average atmospheric hydroxyl radical of $8 \times 10^5 \text{ per cm}^3$ (GEMS 1986; quoted, Howard 1990).

TABLE 15.1.1.8.1
Reported aqueous solubilities and Henry's law constants of
butyl acetate at various temperatures

Aqueous solubility		Henry's law constant	
Stephenson & Stuart 1986		Kolb et al. 1992	
shake flask-GC/TC		equilibrium headspace-GC	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ mol ⁻¹)
0	9600	40	82.91
9.1	7600	60	203.7
19.7	6400	70	290.5
30.3	520	80	387.3
39.6	500		
50.0	500	$\ln (1/K_{\text{AW}}) = A - B/(T/K)$	
60.2	500	A	-9.27
70.2	470	B	-3971
80.1	480		
90.5	480		

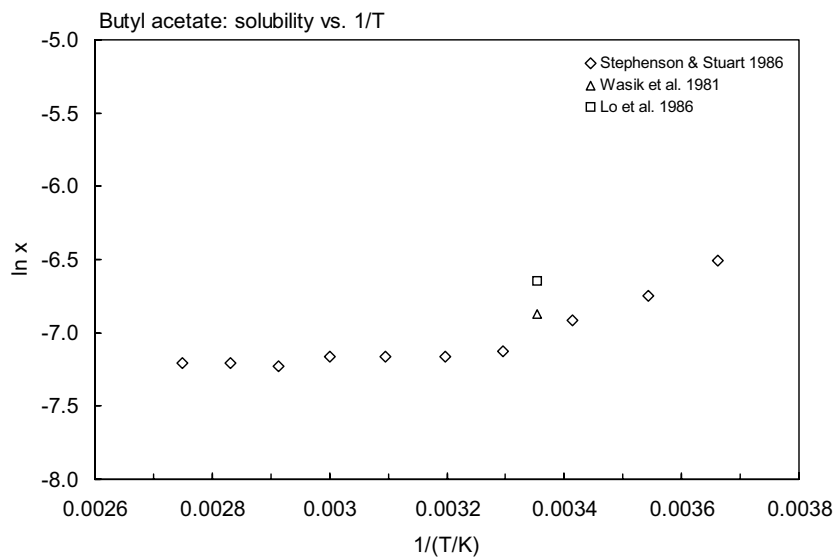
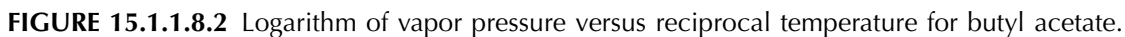


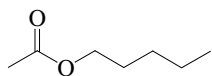
FIGURE 15.1.1.8.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for butyl acetate.

TABLE 15.1.1.8.2
Reported vapor pressures of butyl acetate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Usanovich & Dembicij 1959		Kliment et al. 1964		Sheehan & Langer 1969	
in Boublik et al. 1984		in Boublik et al. 1984		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.5	1560	59.74	9210	67.9	13386
33.0	2533	62.35	10426	96.3	40183
43.0	4133	65.52	11876	100	45663
51.2	6199	67.96	13159	124.0	97325
57.7	8533	71.70	15372	Antoine eq. eq. 2 A B C	
65.2	11999	75.88	18252		
71.1	15332	80.49	21891		
77.5	20132	84.21	25264		
83.7	25598	89.58	30864		
88.8	31064	95.06	37543	P/mmHg	
94.1	42130	100.53	45356		
		107.07	56448		
eq in Boublik et al. 1984		113.62	69487		
eq. 2	P/kPa	120.62	86053		
A	4.75140	126.09	101325		
B	669.609	eq in Boublik et al. 1984			
C	117.657				
bp/°C	60.892				
at 10 mmHg		eq. 2	P/kPa		
		A	6.25496		
		B	1432.217		
		C	218.936		
		bp/°C	126.116		



15.1.1.9 Pentyl acetate



Common Name: Pentyl acetate

Synonym: acetic acid pentyl ester, amyl acetate, amylacetic ester, pentyl ethanoate, *n*-pentyl acetate, ethanoic acid pentyl ester

Chemical Name: *n*-amyl acetate, *n*-pentyl acetate

CAS Registry No: 628-63-7

Molecular Formula: $C_7H_{14}O_2$, $CH_3COOCH_2CH_2CH_2CH_2CH_3$

Molecular Weight: 130.185

Melting Point ($^{\circ}C$):

-70.8 (Weast 1982–83; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

149.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8756 (Weast 1982–83)

0.8766, 0.8719 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

148.5 ($20^{\circ}C$, calculated-density)

177.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

24.25 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.0 (at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1730 (shake flask-turbidimeter, McBain & Richards 1946)

1800 ($20^{\circ}C$, Verschueren 1983)

1700 (Dean 1985)

1700 ($20^{\circ}C$, Riddick et al. 1986)

2200*, 1600 ($19.7^{\circ}C$, $30.3^{\circ}C$, shake flask-GC/TC, measured range 0 – $80^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 8.078 - 2077/(253 + t/^{\circ}C)$ (Davis 1946)

547 (quoted, Hine & Mookerjee 1975)

546 (quoted, Abraham 1984)

1290 (selected lit., Riddick et al. 1986)

$\log(P/kPa) = 5.4315 - 1197/(200 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 7.356 - 2258.3/(T/K)$; temp range 329–423 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 7.8848 - 3.0696 \times 10^3/(T/K) + 2.7085 \cdot \log(T/K) - 1.5165 \times 10^{-2} \cdot (T/K) + 8.7135 \times 10^{-6} \cdot (T/K)^2$;
temp range 202–598 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

39.29 (exptl., Hine & Mookerjee 1975)

42.10, 42.16 (calculated-group contribution, calculated-group contribution, Hine & Mookerjee 1975)

35.94 (vapor-liquid equilibrium, headspace-GC, measured range 25 – $40^{\circ}C$ data presented in graph,
 $\Delta H = 51.4\ kJ/mol$, Kieckbusch & King 1979)

48.33 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

- 38.39 (calculated-molecular structure, Russell et al. 1992)
 24.86 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 7.167 - 2685/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.70 (calculated, Iwasa et al. 1965)
 2.23 (Leo et al. 1969)
 2.42 (calculated- V_1 and solvatochromic parameters, Leahy 1986)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 4.12 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

photooxidation $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976).

Hydrolysis:

Biodegradation: biodegradation rates $k = 0.054\text{ d}^{-1}$ with $t_{1/2} = 13$ d in Lester river, $k = 0.069\text{ d}^{-1}$ with $t_{1/2} = 10$ d in Superior harbor waters and $k = 0.014\text{ d}^{-1}$ with $t_{1/2} = 50$ d in groundwater (Vaishnav & Babeu 1987).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water: biodegradation $t_{1/2} = 13$ d in Lester river and $t_{1/2} = 10$ d in Superior harbor waters (Vaishnav & Babeu 1987).

Groundwater: biodegradation $t_{1/2} = 50$ d (Vaishnav & Babeu 1987).

Sediment:

Soil:

Biota:

TABLE 15.1.1.9.1
Reported aqueous solubilities of pentyl acetate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	2900
19.7	2200
30.6	1600
39.5	1600
50.0	1000
60.3	1000
70.2	1700
80.1	1700

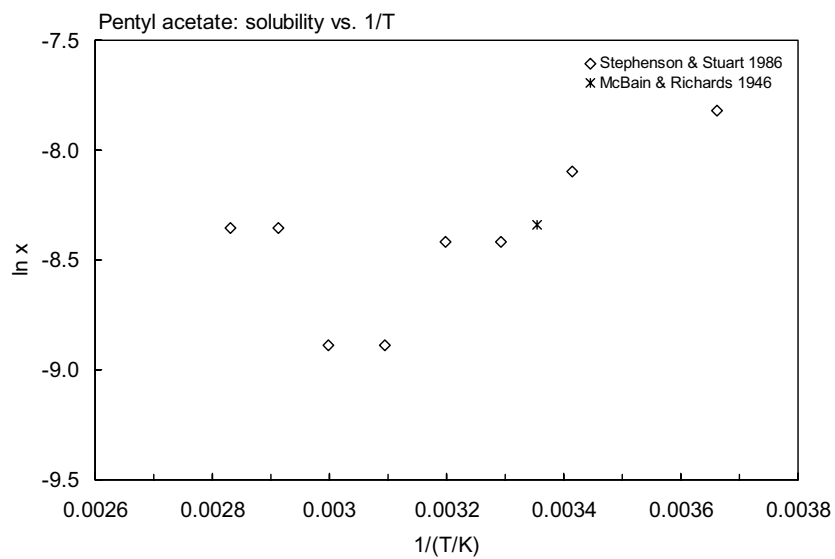
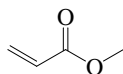


FIGURE 15.1.1.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for pentyl acetate.

15.1.1.10 Methyl acrylate



Common Name: Methyl acrylate

Synonym: acrylic acid methyl ester, methyl 2-propenoate

Chemical Name: methyl acrylate

CAS Registry No: 96-33-3

Molecular Formula: $C_4H_6O_2$, $CH_2=CHCOOCH_3$

Molecular Weight: 86.090

Melting Point ($^{\circ}C$):

-76.5 (Dean 1985)

Boiling Point ($^{\circ}C$):

80.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9535 (Weast 1982-83; Riddick et al. 1986)

0.9561 (Dean 1985)

Molar Volume (cm^3/mol):

90.3 ($20^{\circ}C$, calculated-density)

99.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

29.20, 33.1 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

60000 (Dean 1985)

49400 (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

11250 (interpolated-regression of tabulated data, temp range -43.7 to $80.2^{\circ}C$, Stull 1947)

13330 ($28.0^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 8598.0/(T/K)] + 8.226778$; temp range -43.7 to $80.2^{\circ}C$ (Antoine eq., Weast 1972-73)

9330, 14660 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

11000 (Riddick et al. 1986)

3120, 5400, 9090, 11000, 14500, 30000, 70700 (0, 10, 20, 25, 30, 50, $70^{\circ}C$, Riddick et al. 1986)

$\log(P_1/kPa) = 6.5561 - 1467.93/(-30.849 + T/K)$; temp range: 316-354 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 47.0416 - 3.1218 \times 10^3/(T/K) - 14.86 \cdot \log(T/K) + 7.1646 \times 10^{-3} \cdot (T/K) + 3.4547 \times 10^{-6} \cdot (T/K)^2$; temp range 196-536 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

19.17 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.21 (Tute 1971; Laurence et al. 1972)

0.36 (HPLC-RT correlation, Fujisawa & Masuhara 1981)

0.80 (shake flask-GC, Tani & Hashimoto 1982)

0.80 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.7\text{--}27$ h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991)

Hydrolysis: first order hydrolysis $t_{1/2} = 2.8$ yr at pH 7 and 25°C, based on measured base rate constant; acid rate constant $k = 1.2 \times 10^{-7} \text{ M}^{-1}\cdot\text{h}^{-1}$ using measured rate constant for ethyl acrylate, resulting a $t_{1/2} = 280$ yr; base rate constant $k = 0.0779 \text{ M}^{-1}\cdot\text{h}^{-1}$ at pH 9 and 25°C with $t_{1/2} = 10$ d (Roy 1972; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on biological screening test data (Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.7\text{--}27$ h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 to $1\text{--}5$ d (Kelly et al. 1994).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

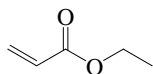
Groundwater: $t_{1/2} = 48\text{--}336$ h, based on measured hydrolysis data and estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

15.1.1.11 Ethyl acrylate



Common Name: Ethyl acrylate

Synonym: acrylic acid ethyl ester, ethyl 2-propenoate, propenoic acid ethyl ester

Chemical Name: ethyl acrylate, *n*-ethyl acrylate

CAS Registry No: 140-88-5

Molecular Formula: $C_5H_8O_2$, $CH_2=CHCOOCH_2CH_3$

Molecular Weight: 100.117

Melting Point ($^{\circ}C$):

-71.2 (Stull 1947; Weast 1982–83; Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

99.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9234 (Weast 1982–83; Riddick et al. 1986)

0.9405 (Dean 1985)

Molar Volume (cm^3/mol):

109.2 (Stephenson & Malanowski 1987)

123.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

34.7 (at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

20000 (Verschuereen 1983)

15000 (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4860* (interpolated-regression of tabulated data, temp range -29.5 to $99.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 9259.4/(T/K)] + 8.347017$; temp range -29.5 to $99.5^{\circ}C$ (Antoine eq., Weast 1972–73)

3866, 6532 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

5100 (lit average, Riddick et al. 1986)

$\log(P/kPa) = 7.2103 - 1939.49/(T/K)$, temp range: not specified, (Antoine eq., Riddick et al. 1986)

5140 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.25041 - 1354.65/(-53.603 + T/K)$; temp range: 244–373 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 55.0109 - 3.5904 \times 10^3/(T/K) - 17.694 \cdot \log(T/K) + 8.051 \times 10^{-3} \cdot (T/K) - 4.8864 \times 10^{-13} \cdot (T/K)^2$; temp range 202–553 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ $25^{\circ}C$):

34.041 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.73 (Tute 1971; Laurence et al. 1972)

0.88 (calculated-fragment const. per Rekker 1977, Hermens & Leeuwangh 1982)

0.66 (HPLC-RT correlation, Fujisawa & Masuhara 1981)

1.33 (shake flask-GC, Tanii & Hashimoto 1982)

1.32 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.37\text{--}22.7$ h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: overall rate constant $k_h = 6.3 \times 10^{-9} \text{ s}^{-1}$ with $t_{1/2} = 3.5$ yr at 25°C and pH 7; acid rate constant $k_A = 1.2 \times 10^{-13} \text{ s}^{-1}$ and base rate constant $k_B = 7.8 \times 10^{-9} \text{ s}^{-1}$ at 25° and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 2.8$ yr at pH 7 and 25°C , based on acid and base catalyzed hydrolysis rate constants; acid rate constant $k_A = 1.2 \times 10^{-6} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 244$ yr at pH 5; measured base rate constant $k_B = 0.078 \text{ M}^{-1} \cdot \text{h}^{-1}$ with $t_{1/2} = 10.4$ d at pH 9 and 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991);

calculated rate constant for base-catalyzed hydrolysis $k_B = 5.0 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ and estimated $t_{1/2} \sim 25$ d in aqueous solutions at pH 8.8 (Freidig et al. 1999).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on aqueous aerobic screening test data (Price et al. 1974; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.37\text{--}22.7$ h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: hydrolysis $t_{1/2} = 3.5$ yr at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 15.1.1.11.1
Reported vapor pressures of ethyl acrylate at various temperatures

Stull 1947	
summary of literature data	
$t/^\circ\text{C}$	P/Pa
−29.5	133.3
−8.70	666.6
2.0	1333
13.0	2666
26.0	5333
33.5	7999
44.5	13332
61.5	26664
80.0	53329
99.5	101325
mp/ $^\circ\text{C}$	−71.2

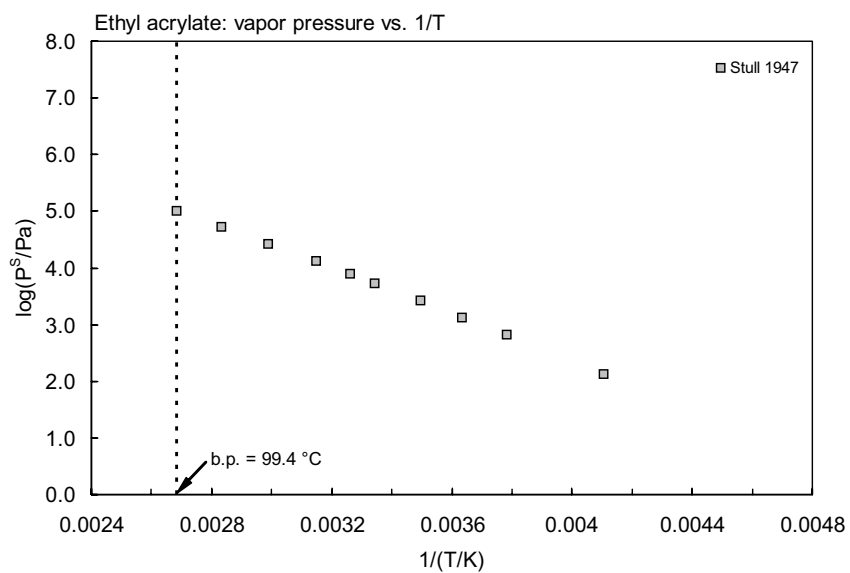
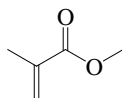


FIGURE 15.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for ethyl acrylate.

15.1.1.12 Methyl methacrylate



Common Name: Methyl methacrylate

Synonym: methyl 2-methyl-2-propenoate, methyl ester methacrylic acid, methacrylic acid methyl ester, MMA

Chemical Name: 2-methyl-2-propenoic acid methyl ester

CAS Registry No: 80-62-6

Molecular Formula: $C_5H_8O_2$, $H_2C=C(CH_3)COOCH_3$

Molecular Weight: 100.117

Melting Point ($^{\circ}C$):

−47.55 (Lide 2003)

Boiling Point ($^{\circ}C$):

100.5 (Lide 2003)

Flash Point ($^{\circ}C$): 10

Density (g/cm^3 at $20^{\circ}C$):

0.9440 (Weast 1982–83)

Molar Volume (cm^3/mol):

106.6 ($25^{\circ}C$, Stephenson & Malanowski 1987)

121.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.7, 36.0 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

16000 (Dean 1985)

15000 (USEPA 1985; ENVIROFATE; ISHOW)

15900 (Yalkowsky et al. 1987)

15600 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5332*, 4888 ($25.5^{\circ}C$, interpolated-regression of tabulated data, temp range -30.5 to $101^{\circ}C$, Stull 1947)

1315* ($3.44^{\circ}C$, temp range -45.26 to $3.44^{\circ}C$, Bywater 1952; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 8794.9/(T/K)] + 8.140942$; temp range -30.5 to $101^{\circ}C$ (Antoine eq., Weast 1972–73)

3732, 5333 ($20^{\circ}C$, $26^{\circ}C$, Verschuere 1977, 1983)

7003* ($32.489^{\circ}C$, temp range 32.489 – $99.855^{\circ}C$, Boublik & Aim 1979; quoted, Boublik et al. 1984)

5333 ($25.5^{\circ}C$, Weast 1982–83)

4440 (extrapolated average-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 3.20496 - 4017.882/(126.685 + t/^{\circ}C)$; temp range -45.26 to $3.44^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.19400 - 1315.670/(213.490 + t/^{\circ}C)$; temp range: 32.41 – $99.855^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

4846 (extrapolated-Antoine equation, Dean 1985)

$\log(P/mmHg) = 8.4092 - 2050.5/(274.4 + t/^{\circ}C)$; temp range: 39 – $89^{\circ}C$ (Antoine eq., Dean 1985, 1992)

5100 (lit. average, Riddick et al. 1986)

$\log(P/kPa) = 7.83859 - 2126.21/(T/K)$, temp range 0 – $30^{\circ}C$ (Antoine eq., Riddick et al. 1986)

5081, 5020 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.63751 - 1597.9/(-28.76 + T/K)$; temp range: 293 – 374 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.43088 - 1461.197/(-43.15 + T/\text{K})$; temp range: 293–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 106.896 - 5.2741 \times 10^3/(T/\text{K}) - 37.654 \cdot \log(T/\text{K}) + 1.862 \times 10^{-2} \cdot (T/\text{K}) - 3.6507 \times 10^{-13} \cdot (T/\text{K})^2$;
temp range 225–564 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

24.31 (calculated-P/C, USEPA 1985)
32.823 (calculated-P/C, Howard 1989)
32.09 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.73 (Tute 1971; Laurence et al. 1972)
0.70 (shake flask, Fujisawa & Masuhara 1981)
0.67 (HPLC-RT correlation, Fujisawa & Masuhara 1981)
1.36 (CLOGP, Hansch & Leo 1982)
1.38 (shake flask-GC, Tanii & Hashimoto 1982)
0.79 (calculated-f const. as per Lyman et al. 1982, USEPA 1985)
1.38 (recommended, Sangster 1989)
1.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

−0.03 (correlated as per Veith et al. 1979 for aquatic organisms, USEPA 1985)
0.55 (calculated- K_{OW} , Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

1.80 (calculated- K_{OW} as per Lyman et al. 1982, USEPA 1985)
1.94 (calculated- K_{OW} , Howard 1989)
0.74 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 6.3$ h from model river water (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: photodegradation $t_{1/2} = 2.7$ h in air of urban areas and $t_{1/2} > 3$ h in rural areas (Joshi et al. 1982; quoted, Howard 1989) (CHEMFATE; Hazardous Substance Databank).

Oxidation: photooxidation $t_{1/2} = 1.1$ – 9.7 h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: alkaline hydrolysis rate constant at 25°C, $k = 171 \text{ M}^{-1} \text{ h}^{-1}$ (Sharma & Sharma 1970; quoted, Ellington et al. 1987; Ellington 1989);

alkaline catalyzed rate constant $k(\text{exptl}) = 200 \text{ M}^{-1} \cdot \text{h}^{-1}$ at 25°C with estimated $t_{1/2} \sim 3.9$ yr at pH 7 and $t_{1/2} = 14$ d at pH 9 (Ellington et al. 1987; quoted, Ellington 1989; Howard 1989; Howard et al. 1991; Kollig 1993);

hydrolysis $t_{1/2} = 4$ yr at pH 7 and 25°C; base rate constant $k = 200 \text{ M}^{-1} \text{ h}^{-1}$ with $t_{1/2} = 14.4$ d at pH 9 based on measured rate constant at 25°C and pH 11 (Howard et al. 1991)

$k(\text{calc}) = 9.0 \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$, $2.6 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ for neutral and base-catalyzed hydrolysis and estimated $t_{1/2} \sim 8$ d in aqueous solutions at pH 8.8 (Freidig et al. 1999)

Biodegradation: completely degraded by activated sludge in approximately 20 h (Slave et al. 1974; quoted, EPA 1985; Howard 1989; Hazardous Substance Databank);

expert systems survey found that both aerobic ultimate degradation in receiving waters and anaerobic ultimate degradation were within a month and aerobic primary degradation in receiving waters was within few days (Boethling et al. 1989);

aqueous aerobic $t_{1/2} = 168$ – 672 h, based on unacclimated screening test data (Pahren & Bloodgood 1961; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ – 2688 h, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 1.1\text{--}9.7$ h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 to $1\text{--}5$ d (Kelly et al. 1994).

Surface water: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 336\text{--}1344$ h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 15.1.1.12.1

Reported vapor pressures of methyl methacrylate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Bywater 1952		Boublik & Aim 1979	
summary of literature data		in Boublik et al. 1984		in Boublik et al. 1984	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
-30.5	133.3	-45.26	17	32.489	7003
-10.0	666.6	-43.46	25	37.962	9160
1.0	1333	-40.16	43	38.307	9306
11.0	2666	-35.16	64	43.731	12004
25.5	5333	-32.06	95	43.834	12049
34.5	7999	-27.96	140	47.951	14515
47.0	13332	-22.96	223	48.225	14680
63.0	26664	-20.46	260	53.954	18815
82.0	53329	-16.76	347	53.289	18290
101.0	101325	-10.56	547	55.846	20379
		-3.46	893	61.670	25849
mp/ $^{\circ}\text{C}$	-	-0.16	1053	65.350	29910
		3.44	1315	69.772	35421
				74.142	41676
		in Boublik et al. 1984		79.113	49831
		eq. 2	P/kPa	84.938	61430
		A	3.20496	91.998	77126
		B	401.882	99.855	98890
		C	126.685		
		bp/ $^{\circ}\text{C}$	-1.292	in Boublik et al. 1984	
		at 1 mmHg		eq. 2	P/kPa
				A	6.19400
				B	1315.670
				C	215.490
				bp/ $^{\circ}\text{C}$	100.641

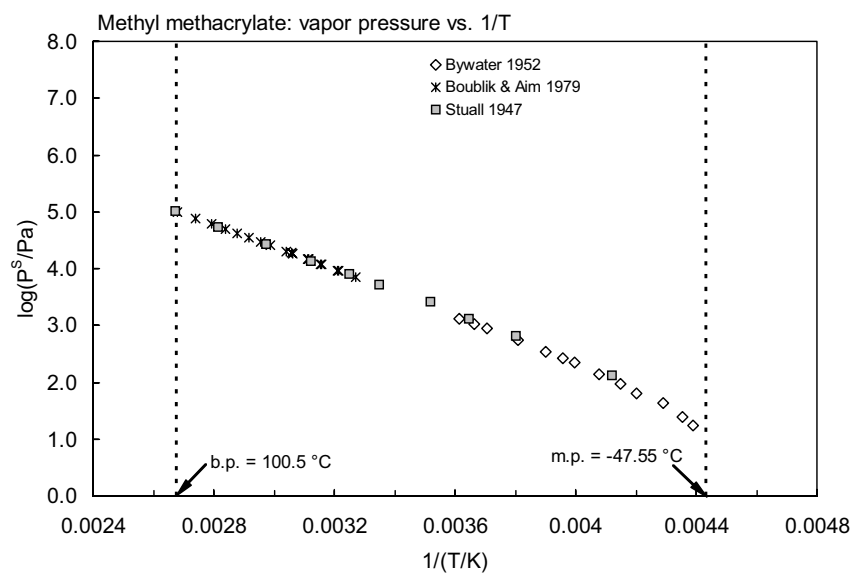
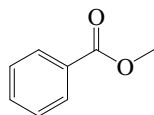


FIGURE 15.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for methyl methacrylate.

15.1.2 AROMATIC ESTERS

15.1.2.1 Methyl benzoate



Common Name: Methyl benzoate

Synonym: benzoic acid methyl ester

Chemical Name: methyl benzoate

CAS Registry No: 93-58-3

Molecular Formula: $C_8H_8O_2$, $C_6H_5COOCH_3$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

-12.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

199 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.08854, 1.08377 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

Molar Volume (cm^3/mol):

125.0 (Stephenson & Malanowski 1987)

151.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.18, 55.84 (normal bp, $25^{\circ}C$, Dreisbach 1955)

43.18, 55.568 (normal bp, $25^{\circ}C$, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.736 (Dreisbach 1955; Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1524 (titration, Booth & Everson 1948)

4018 (Hine & Mookerjee 1975)

2100 ($20^{\circ}C$, quoted, Riddick et al. 1986)

1600 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

2130*, 2820 ($20.1^{\circ}C$, $29.6^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.5^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/mmHg) = 7.48253 - 1974.6/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

52.58 (calculated by formula, Dreisbach 1955)

$\log (P/mmHg) = 7.07832 - 1656.25/(195.23 + t/^{\circ}C)$; temp range: 100 – $260^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log (P/mmHg) = [-0.2185 \times 12077.2/(T/K)] + 8.509910$; temp range: 39 – $199.5^{\circ}C$ (Antoine eq., Weast 1972–73)

77.6 (extrapolated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 6.60743 - 1974.6/(230.0 + t/^{\circ}C)$; temp range 111 – $199^{\circ}C$ (Antoine eq., Dean 1985, 1992)

52.58 (quoted lit. average, Riddick et al. 1986)

$\log (P/kPa) = 6.60743 - 1974.6/(230 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

54.5 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 8.183 - 2816.6/(T/K)$; temp range 283 – $323 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.20322 - 1656.25/(-77.92 + T/\text{K})$; temp range: 383–533 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -13.6342 - 2.9133 \times 10^3/(T/\text{K}) + 11.773 \cdot \log (T/\text{K}) - 2.3979 \times 10^{-2} \cdot (T/\text{K}) + 1.1324 \times 10^{-5} \cdot (T/\text{K})^2$;
temp range 261–693 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 1.80 (calculated- C_w/C_A , Hine & Mookerjee 1975)
- 2.48 (calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.15 (HPLC-RT correlation, D'Amboise & Hanai 1982)
- 2.22 (HPLC- k' correlation, Haky & Young 1984)
- 2.14 (shake flask-HPLC, Nielson & Bundgaard 1988)
- 2.10 (recommended, Klein et al. 1988)
- 2.15 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
- 2.20 (recommended, Sangster 1989)
- 2.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.30, 2.01, 1.98 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 1.89 (calculated-MCI χ , Meylan et al. 1992)
- 2.10 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 2.14; 2.57, 2.14, 1.94, 2.16, 1.89 (soil: calculated- K_{ow} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: overall rate constant $k_h = 1.90 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 118 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)
alkaline hydrolysis rate constant $k = 0.0794 \text{ M}^{-1} \text{ s}^{-1}$ (Drossman et al. 1988, quoted, Collette 1990)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants::

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} = 118 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.2.1.1
Reported aqueous solubilities of methyl benzoate at various temperatures
 Stephenson & Stuart 1986

shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	2210
9.7	2210
20.1	2130
29.6	2820
40.2	2470
49.8	2580
60.1	2860
70.2	3250
80.3	3580
90.5	4080

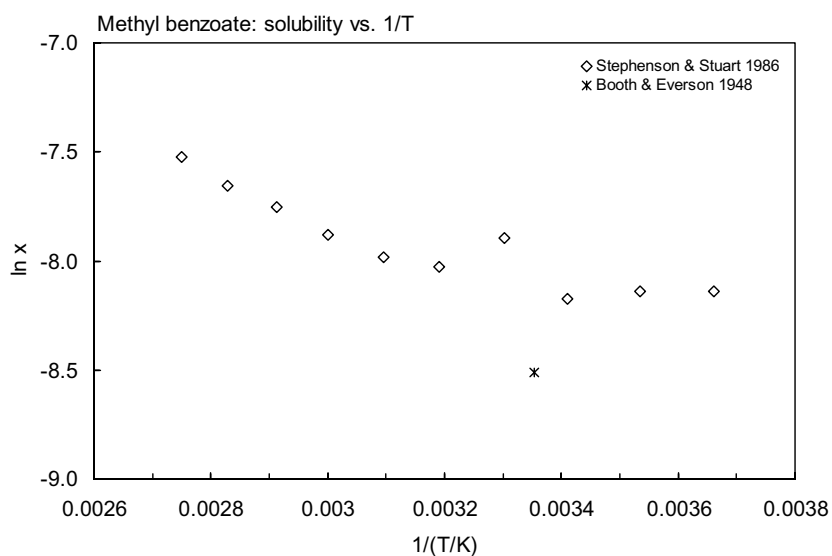
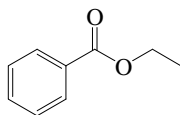


FIGURE 15.1.2.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for methyl benzoate.

15.1.2.2 Ethyl benzoate



Common Name: Ethyl benzoate

Synonym: benzoic acid ethyl ester, ethyl benzenecarboxylate

Chemical Name: benzoic acid ethyl ester, ethyl benzenecarboxylate, ethyl benzoate

CAS Registry No: 93-89-0

Molecular Formula: $C_9H_{10}O_2$, $C_6H_5COOC_2H_5$

Molecular Weight: 150.174

Melting Point ($^{\circ}C$):

-34 (Lide 2003)

Boiling Point ($^{\circ}C$):

212 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0468 (Weast 1982-83)

1.0511, 1.0372 ($15^{\circ}C$, $30^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

175.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.5 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

720 (Seidell 1941; quoted, Andrews & Keefer 1950)

598 (Deno & Berkheimer 1960)

702 (calculated- K_{ow} , Hansch et al. 1968)

510 (calculated- K_{ow} , Yalkowsky & Morozowich 1980)

2026 (calculated- K_{ow} and mp, Amidon & Williams 1982),

807 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)

1090 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Kamlet et al. 1987)

464 (calculated-intrinsic molar volume V_1 and mp, Kamlet et al. 1987)

500 ($20^{\circ}C$, Riddick et al. 1986)

926 (calculated-fragment const., Wakita et al. 1986)

398 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

850*, 810 ($19.6^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range $0-90.3^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

42.1 (extrapolated-regression of tabulated data, temp range $44-213.4^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11981.5/(T/K)] + 8.279591$; temp range $44-213.4^{\circ}C$ (Antoine eq., Weast 1972-73)

24.0 ($20^{\circ}C$, quoted lit., Riddick et al. 1986)

$\log(P/kPa) = 7.7579 - 2750.0/(T/K)$; temp range $90-140^{\circ}C$ (Antoine eq., Riddick et al. 1986)

$\log(P/kPa) = 7.1599 - 2500.0/(T/K)$; temp range $140-220^{\circ}C$ (Antoine eq., Riddick et al. 1986)

27.5 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.81152 - 2174.3/(-34.071 + T/K)$; temp range $358-487 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.23958 - 2922.167/(T/K)$; temp range $288-333 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 40.8047 - 3.9985 \times 10^3/(T/K) - 11.793 \cdot \log (T/K) + 4.0697 \times 10^{-3} \cdot (T/K) - 1.2372 \times 10^{-13} \cdot (T/K)^2;$$

temp range 238–698 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

10.298 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log K_{ow}:

2.62 (calculated, Hansch et al. 1968)
 2.20 (shake flask-spectrophotometry, Yaguzhinskii et al. 1973)
 2.64 (Valvani et al. 1981, Amidon & Williams 1982)
 2.64 (shake flask-HPLC, Nielsen & Bundgaard 1988)
 2.60 (recommended, Klein et al. 1988)
 2.64 (recommended, Sangster 1989)
 2.66, 2.89, 2.90 (centrifugal partition chromatography CPC-RV, Gluck & Martin 1990)
 2.70 ± 0.15, 2.63 ± 0.57 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k' correlation, Cichna et al. 1995)
 2.64 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

2.25, 2.17, 2.43 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
 2.16 (calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 2.30 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: overall rate constant k_h = 3.0 × 10⁻⁹ s⁻¹ with t_{1/2} = 7.3 yr at 25°C and pH 7 (Mabey & Mill 1978)
 alkaline hydrolysis rate constant k = 0.0316 M⁻¹ s⁻¹ (Drossman et al. 1988, quoted, Collette 1990)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis t_{1/2} = 7.3 yr at 25°C and pH 7 (Mabey & Mill 1978)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.2.2.1

Reported aqueous solubilities of ethyl benzoate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

t/°C	S/g·m ⁻³
0	1080
19.6	850
30.5	810
40.0	1060
50.0	1080
60.1	1170
70.5	1210
80.2	1210
90.3	1430

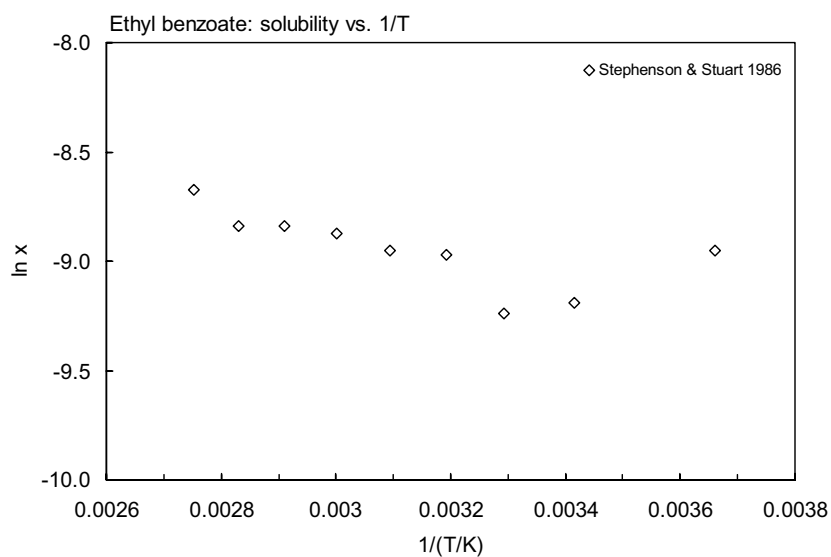
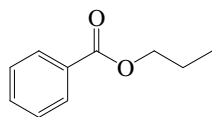


FIGURE 15.1.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for ethyl benzoate.

15.1.2.3 *n*-Propyl benzoate

Common Name: *n*-Propyl benzoate

Synonym: benzoic acid *n*-propyl ester, propyl benzenecarboxylate

Chemical Name: benzoic acid *n*-propyl ester, propyl benzenecarboxylate, propyl benzoate

CAS Registry No: 2315-68-6

Molecular Formula: $C_{10}H_{12}O_2$, $C_6H_5COOCH_2CH_2CH_3$

Molecular Weight: 164.201

Melting Point ($^{\circ}C$):

−51.6 (Weast 1982–83; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

211 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0232 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

160.5 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

199.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

51.92; 49.75 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

350 (quoted exptl., Kamlet et al. 1987)

292 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Kamlet et al. 1987)

140 (calculated-intrinsic molar volume V_1 and mp, Kamlet et al. 1987)

966 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

133.3 ($54.6^{\circ}C$, summary of literature data, temp range 54.6 – $231^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 12318.7/(T/K)] + 8.237827$; temp range 54.6 – $231^{\circ}C$ (Antoine eq., Weast 1972–73)

100 ($54.6^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 7.42756 - 2172.71/(T/K)$; temp range 80 – $160^{\circ}C$ (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.68614 - 2165.28/(-41.593 + T/K)$; temp range 327 – 504 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.80 (shake flask-HPLC, Nielsen & Bundgaard 1988)

3.18 (recommended, Sangster 1989)

3.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

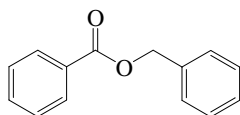
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

15.1.2.4 Benzyl benzoate



Common Name: Benzyl benzoate

Synonym: benzoic acid benzyl ester, phenylmethyl benzoate, benzyl benzenecarboxylate, benzyl phenylformate, benzenoate

Chemical Name: benzyl benzoate, phenylmethyl benzoate, benzyl benzenecarboxylate

CAS Registry No: 120-51-4

Molecular Formula: $C_{14}H_{12}O_2$, $C_6H_5COOCH_2C_6H_5$

Molecular Weight: 212.244

Melting Point ($^{\circ}C$):

19.4 (Riddick et al. 1986)

Boiling Point ($^{\circ}C$):

323.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1121 ($25^{\circ}C$, Weast 1982–83)

1.120, 1.1121 ($19.5^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

190.9 ($25^{\circ}C$, calculated-density)

243.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

53.56 (at normal bp, Hon et al. 1976)

77.8; 53.6 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

15.73 (Seidell 1941; quoted, Deno & Berkheimer 1960)

61.21 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/mmHg) = 6.42726 - 1594.49/(126.36 + t/^{\circ}C)$; temp range 224.7 – $329.09^{\circ}C$ (Antoine eq., from twin ebulliometry measurement, Hon et al. 1976)

0.0137 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.59354 - 1628.726/(130.735 + t/^{\circ}C)$; temp range 224.7 – $329^{\circ}C$ (Antoine eq. from reported exptl. data of Hon et al. 1976, Boublik et al. 1984)

461 ($150^{\circ}C$, quoted lit., Riddick et al. 1986)

0.0104 (calculated-Antoine eq., Riddick et al. 1986)

$\log (P/kPa) = 5.55216 - 1594.49/(126.36 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

0.043 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 9.240 - 4057/(T/K)$; temp range 297 – 353 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.63847 - 1666.706/(-137.564 + T/K)$; temp range 497 – 602 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/mmHg) = -1.654 - 4.6284 \times 10^3/(T/K) + 7.363 \cdot \log (T/K) - 1.8259 \times 10^{-2} \cdot (T/K) + 7.4580 \times 10^{-6} \cdot (T/K)^2$; temp range 293 – 820 K (vapor pressure eq., Yaws et al. 1994)

0.0178, 0.0107, 0.0135, 0.295, 0.0603 (GC-RT correlation, Sugden's parachor method, McGowan's parachor method, calculated-MCI, calculated-MW, Tsuzuki 2001)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.57 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.86 (quoted, calculated- V_I and solvatochromic parameters, Taft et al. 1985)

4.00 (quoted, calculated- V_I and solvatochromic parameters, Leahy 1986)

3.97 (recommended value, Sangster 1989)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Hydrolysis: overall rate constant $k_h = 8.0 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 27 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

alkaline hydrolysis rate constant $k = 0.00794 \text{ M}^{-1} \text{ s}^{-1}$ (Mabey et al. 1978; quoted, Collette 1990)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} = 27 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

Groundwater:

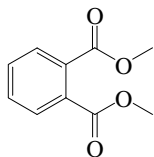
Sediment:

Soil:

Biota:

15.1.3 PHTHALATE ESTERS

15.1.3.1 Dimethyl phthalate (DMP)



Common Name: Dimethyl phthalate

Synonym: DMP, 1,2-benzenedicarboxylic acid dimethyl ester, dimethyl-1,2-benzenedicarboxylate, methyl Common phthalate, *o*-dimethylphthalate, phthalic acid dimethyl ester

Chemical Name: dimethyl phthalate, dimethyl-*o*-phthalate, methyl phthalate

CAS Registry No: 131-11-3

Molecular Formula: $C_{10}H_{10}O_4$, $o\text{-}C_6H_4(COOCH_3)_2$

Molecular Weight: 194.184

Melting Point ($^{\circ}C$):

5.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

283.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.189 ($25^{\circ}C$, Fishbein & Albro 1972)

1.1905 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

162.8 (calculated-density, Stephenson & Malanowski 1987)

206.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.66 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K) F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3965 (Deno & Berkheimer 1960)

5000 ($20^{\circ}C$, Fishbein & Albro 1972)

4000 ($32^{\circ}C$, from Monsanto Chemical Co. data sheets, Peakall 1975)

4320 ± 37 (shake flask-GC, Wolfe et al. 1980b; Wolfe et al. 1980a)

4248 (shake flask-LSC, Veith et al. 1980)

4290 ($20^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)

5000, 1744 ($20^{\circ}C$, Verschueren 1983)

4000 ± 60 (shake flask-HPLC/UV, Howard et al. 1985)

2810 ($21^{\circ}C$, shake flask-HPLC/UV, Nielsen & Bundgaard 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

40* ($82^{\circ}C$, ebulliometry, measured range $82\text{--}151^{\circ}C$, Gardner & Brewer 1937)

$\log(P/\text{mmHg}) = 9.117 - 1496.375/(T/K)$; temp range $82\text{--}151^{\circ}C$ (Antoine eq. derived by Kim 1985 from exptl data of Gardner & Brewer 1937)

0.863* (extrapolated-regression of tabulated data, temp range $100.3\text{--}288.7^{\circ}C$ Stull 1947)

0.245 (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log(P/\text{mmHg}) = 11.06 - 4113/(T/K)$; temp range $32\text{--}55^{\circ}C$ or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, data presented in graph and Antoine eq., Small et al. 1948)

0.559 ($20^{\circ}C$, calculated-Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 14922.2/(T/K)] + 8.747053$; temp range $100.3\text{--}287^{\circ}C$ (Antoine eq., Weast 1972–73)

0.445 (gas saturation, extrapolated, measured range $60\text{--}100^{\circ}C$, Potin-Gautier et al. 1982)

$\log (P/\text{mmHg}) = 8.899 - 3332.764/(T/K)$; temp range 60–100°C (Antoine eq., Potin-Gautier et al. 1982)
 $\log (P/\text{kPa}) = 3.64598 - 699.876/(51.372 + t/^{\circ}\text{C})$; temp range 82–151°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 4.52232 - 700.31/(51.42 + t/^{\circ}\text{C})$; temp range 82–151°C (Antoine eq., Dean 1985, 1992)
 0.220 (gas saturation-HPLC/UV, Howard et al. 1985; quoted, Howard et al. 1986; Howard 1989; Banerjee et al. 1990)
 0.245, 0.863 (extrapolated-Antoine eq.-I, II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 10.185 - 4113/(T/K)$; temp range 304–371 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.095 - 3327/(T/K)$; temp range 371–547 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 1.190 (GC-RT correlation, Hinckley et al. 1990)
 $\log (P/\text{mmHg}) = 12.6974 - 4.1989 \times 10^3/(T/K) + 0.3463 \cdot \log(T/K) - 7.6524 \times 10^{-3} \cdot (T/K) + 3.349 \times 10^{-6} \cdot (T/K)^2$;
 temp range 272–766 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.111 (calculated-P/C, Fishbein & Albro 1972)
 0.111 (calculated-P/C, Wolfe et al. 1980a)
 0.011 (calculated as per Lyman et al. 1982; quoted, Howard 1989)
 0.218 (20°C, calculated-P/C, Mabey et al. 1982)
 0.012 (selected, Staples et al. 1997)
 0.00978 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.61 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1983)
 1.56 (HPLC-RT correlation, Veith et al. 1980)
 1.62, 1.82 (HPLC- k' correlations, McDuffie 1981)
 1.53 (20°C, shake flask-UV, Leyder & Boulanger 1983)
 1.47, 1.90 (shake flask-HPLC/UV, HPLC-RT correlation, Howard et al. 1985)
 1.56 (shake flask, unpublished data, Hansch & Leo 1985; 1987)
 1.66 (shake flask, average from interlaboratory study, Renberg et al. 1985)
 1.74, 1.61 (HPLC, RP-TLC, average from interlaboratory study, Renberg et al. 1985)
 1.62 (HPLC-RT correlation, Eadsforth 1986)
 1.46 (shake flask-HPLC/UV, Nielsen & Bundgaard 1989)
 1.56 (recommended, Sangster 1993)
 1.56 (recommended, Hansch et al. 1995)
 1.61 (recommended, Staples et al. 1997)
 1.54 (micro-emulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.01 (calculated-QSPR, Cousin & Mackay 2000)

Bioconcentration Factor, $\log \text{BCF}$:

0.67 (calculated- K_{OW} , Veith et al. 1979, 1980)
 1.76 (bluegill sunfish, Barrows et al. 1980)
 1.76 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1983)
 1.42 (bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
 0.49–0.8, 0.67–0.78 (shrimp, fish, Wofford et al. 1981)
 1.20 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 0.77 (sheepshead minnow, quoted from Wofford et al. 1981, Zaroogian et al. 1985)
 1.76, 2.22 (quoted, calculated-MCI χ , Sabljic 1987)
 0.67, 0.73 (brown shrimp, sheepshead minnow, quoted, Howard 1989)
 1.76 (fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

1.64 (soil, estimated, Kenaga 1980)
 2.20 (soil, estimated- K_{OW} , Wolfe et al. 1980a)

- 1.74 (soil/sediment, Osipoff et al. 1981)
 1.24 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 1.52 (sediment, calculated- K_{OW} , Pavlou & Weston 1983, 1984)
 2.69 (activated carbon, calculated- MCI χ , Blum et al. 1994)
 1.20 (calculated- K_{OW} , Kollig 1993)
 1.60 (quoted or calculated-QSAR MCI χ , Sabljic et al. 1995)
 4.70 (suspended solids, calculated- K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)
 1.64, 2.14; 2.16, 1.87, 2.53, 1.83, 1.67 (soil: quoted lit., calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constant, k , and Half-Lives $t_{1/2}$:

- Volatilization: estimated $t_{1/2} = 46$ d from a river of 1 m deep with 1.0 m/s current and a 3.0 m/s wind using calculated Henry's law constant and considering the volatilization rate being controlled by the diffusion through the air layer (Lyman et al. 1982; quoted, Howard 1989).
- Photolysis: direct $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a);
 abiotic degradation $t_{1/2} = 3500$ h for direct sunlight in surface waters and $t_{1/2} = 12.7$ h in pure water but reduced to 2.8 h in the presence of NO_2 when irradiated with a UV lamp through a Pyrex filter (Howard 1989)
 Indirect photolysis rate $k = 0.048 \text{ d}^{-1}$ with $t_{1/2} = 14.4$ d in air (Peterson & Staples 2003)
- Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k(\text{aq.}) = 18 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with free radical in aqueous environment (Wolfe et al. 1980a)
 $k(\text{aq.}) \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $0.05 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)
 photooxidation $t_{1/2} = 23.8$ h (estimated, Howard 1989)
 atmospheric $t_{1/2} = 112\text{--}1118$ h, based on estimated rate data for the reaction with OH radical in air (Howard et al. 1991)
 $k(\text{aq.}) = (0.20 \pm 0.10) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $21 \pm 1^\circ\text{C}$, with a $t_{1/2} = 1.9$ d at pH 7 (Yao & Haag 1991).
 $k(\text{aq.}) = 4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (Haag & Yao 1992)
 photooxidation $t_{1/2}(\text{predicted}) = 9.3\text{--}93$ d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)
 $k_{OH} = 5.74 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 14.4$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)
- Hydrolysis: $k(\text{acid-catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1}$, $k(\text{alkaline}) = 2.5 \times 10^2 \text{ M}^{-1} \text{ h}^{-1}$; phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2} = 4$ month to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)
 $k(\text{second-order alkaline}) = 6.9 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at pH 8 and 30°C , and $t_{1/2} = 4$ months for hydrolytic degradation in the eutrophic lake system (Wolfe et al. 1980b; quoted, Kollig 1993)
 $k(\text{second-order alkaline}) = 6.9 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at pH 10–12 and 30°C in water with $t_{1/2}(\text{calc}) = 3.2$ yr at pH 7 (Callahan et al. 1979)
 hydrolysis half-lives: $t_{1/2} = 3.2$ yr under natural conditions at 30°C , $t_{1/2} = 11.6$ d at 30°C and $t_{1/2} = 25$ d at 18°C and at pH 9 (Howard 1989; selected, Staples et al. 1997);
 first-order hydrolysis $t_{1/2} = 1163$ d based on a second-order rate constant at pH 7 and 30°C ; and a base rate constant $k = 111.6 \text{ M}^{-1} \text{ h}^{-1}$ corresponding to $t_{1/2} = 1.2$ d at pH 9 and 18°C (Howard et al. 1991)
 $t_{1/2} = 1200$ d at pH 7, $t_{1/2} = 0.026$ d at pH 12 in natural waters (Capel & Larson 1995)
- Biodegradation: calculated rate constant $k = (9.49 \pm 0.41) \times 10^2 \text{ min}^{-1}$ from retention times in reverse phase chromatography (Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985);
 significant degradation with rapid adaption within 7 d in an aerobic environment with a rate $k > 0.5 \text{ d}^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);
 biodegradation rate constant $k = 1.2 \times 10^{-4} \text{ mL-cell}^{-1} \cdot \text{d}^{-1}$ in river die-away test (Scow 1982);
 58–88% mineralization in 7 d in municipal digested sludge (Horowitz et al. 1982);
 rate constant $k = 0.364 \text{ d}^{-1}$ which corresponds to $t_{1/2} = 1.90$ d in shake flask biodegradation experiments (Sugatt et al. 1984);
 greater than 90% of DMP was degraded within 40 d in digested sludge (Shelton et al. 1984);
 biodegraded in excess of 90% in activated sludge systems in less than 24 h (O'Grady et al. 1985);
 soil-water biodegradation studies showed that 85% loss in Broome County soil after 120 hours and 75% loss in leachate sprayed soil after 48 h (Russell et al. 1985);

anaerobic digestion of sludge with a first-order $k = 8.9 \times 10^{-3} \text{ h}^{-1}$ and $t_{1/2} = 78 \text{ h}$ (Ziogou et al. 1989); aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aerobic river die-away test data and acclimated aerobic soil grab sample data; aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 3 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

$k = 0.0290 \text{ h}^{-1}$ with $t_{1/2} = 23.9 \text{ h}$ for microbial degradation by anaerobic sludge (Wang et al. 2000)

Aerobic biodegradation in aquatic environments, first order $k = 0.5 \text{ d}^{-1}$ with $t_{1/2} = 1.39 \text{ d}$ in river water, $k = 0.5 \text{ d}^{-1}$ with $t_{1/2} = 1.39 \text{ d}$ in MITI inoculum (Peterson & Staples 2003)

Aerobic biodegradation in soil, pseudo-first-order rate $k = 0.36 \text{ d}^{-1}$ with $t_{1/2} = 1.93 \text{ d}$ in agitated aqueous suspension, and $k = 0.40 \text{ d}^{-1}$ with $t_{1/2} = 1.70 \text{ d}$ at 30°C in garden soil. For anaerobic degradation, first order rate $k = 0.25\text{--}0.696 \text{ d}^{-1}$ with $t_{1/2} = 2.8\text{--}1.0 \text{ d}$ in digester sludge, batch incubation; $k = 0.033 \text{ d}^{-1}$ with $t_{1/2} = 21 \text{ d}$ in flood soil (Peterson & Staples 2003)

Biotransformation: estimated rate constant $k \sim 5.2 \times 10^{-6} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a; quoted, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

depuration $t_{1/2} = 24\text{--}48 \text{ h}$ from bluegill sunfish (Barrows et al. 1980).

$k_2 = 27.7 \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 2.37 \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} = 23.8 \text{ h}$ for reaction with hydroxyl radicals (Howard 1989);

$t_{1/2} = 112\text{--}1118 \text{ h}$, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

$t_{1/2} = 14.41 \text{ d}$ based on photooxidation reaction rate with OH radical, indirect photolysis $t_{1/2} = 14.4 \text{ d}$ (Peterson & Staples 2003)

Surface water: estimated $t_{1/2} < 0.3 \text{ d}$ in river waters (Zoeteman et al. 1980);

mineralization $t_{1/2} \sim 7 \text{ d}$ in municipal digested sludge (Horowitz et al. 1982);

biodegradation $t_{1/2} = 1.90 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984);

$t_{1/2} < 192\text{--}264 \text{ h}$ by biodegradation in fresh river water, $t_{1/2} = 12 \text{ h}$ in Rhine River, an estimated $t_{1/2} \sim 13\text{--}27 \text{ h}$ in a modelling study of simulated ecosystem; abiotic degradation $t_{1/2} = 12.7 \text{ h}$ in pure water and $t_{1/2} = 2.8 \text{ h}$ in the presence of nitrogen dioxide when irradiated with a UV lamp (Howard 1989);

overall degradation $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated river die-away test data (Howard et al. 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 4 \text{ d}$ in natural waters (Capel & Larson 1995)

$k(\text{exptl}) = (0.20 \pm 0.10) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $21\text{--}1^\circ\text{C}$, with $t_{1/2} = 1.9 \text{ d}$ at pH 7 (Yao & Haag 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 4 \text{ d}$ and $t_{1/2} = 1200$ at pH 7, $t_{1/2} = 0.026 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

$t_{1/2} = 0.5\text{--}1.39 \text{ d}$ for biodegradation in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 48\text{--}336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: biodegradation $t_{1/2} < 5 \text{ d}$ (aerobic) and $t_{1/2} \sim 20 \text{ d}$ (anaerobic) in a garden soil (Shanker et al. 1985);

$t_{1/2} = 10\text{--}50 \text{ d}$, via volatilization subject to plant uptake from soil (Ryan et al. 1988);

$t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aerobic river die-away test data and acclimated aerobic soil grab sample data (Howard et al. 1991)

Biodegradation in aerobic soil: $t_{1/2} = 1.93 \text{ d}$ in agitated aqueous suspension and $t_{1/2} = 1.70 \text{ d}$ in garden soil (Peterson & Staples 2003)

Biota: $24 < t_{1/2} < 48 \text{ h}$ depuration half-life in tissues of bluegill sunfish in 21 d-exposure experiment (Barrows et al. 1980; quoted, Howard 1989);

$t_{1/2} = 23.9 \text{ h}$ for microbial degradation by anaerobic sludge (Wang et al. 2000).

TABLE 15.1.3.1.1

Reported vapor pressures of dimethyl phthalate at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & \end{aligned}$$

Gardner & Brewer 1937		Stull 1947	
ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
82.0	40.0	100.3	133.3
85.0	53.3	131.8	666.6
90.0	66.7	147.6	1333
99.0	80.0	164.0	2666
103.0	120	182.8	5333
105.3	160	194.0	7999
107.4	213	210.0	13332
110.6	227	232.7	26664
115.0	267	257.8	53329
118.0	333	283.7	101325
123.8	440		
129.5	587	mp/°C	
136.9	813		
146.5	1293		
146.9	1293		
150.6	1533		
151.0	1547		
bp/°C	140.586		
	at 1 mmHg		

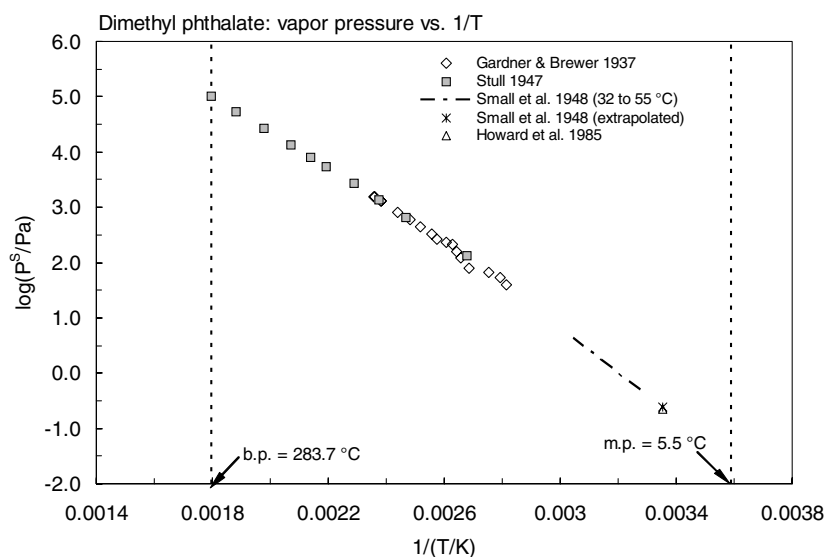
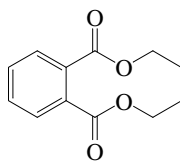


FIGURE 15.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl phthalate.

15.1.3.2 Diethyl phthalate (DEP)



Common Name: Diethyl phthalate

Synonym: DEP, ethyl phthalate

Chemical Name: phthalic acid diethyl ester, ethyl phthalate, 1,2-benzenedicarboxylic acid ethyl ester

CAS Registry No: 84-66-2

Molecular Formula: $C_{12}H_{14}O_4$, $C_6H_4(COOC_2H_5)_2$

Molecular Weight: 222.237

Melting Point ($^{\circ}C$):

−40.5 (Patty 1963; Fishbein & Albro 1972; Lide 2003)

Boiling Point ($^{\circ}C$):

295 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.123 ($25^{\circ}C$, Fishbein & Albro 1972)

1.1175 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

198.9 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

254.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

82.42 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$) F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

598 (Deno & Berkheimer 1960)

1000 ($20^{\circ}C$, Fishbein & Albro 1972)

1000 ($32^{\circ}C$, from Monsanto Chemical Co. data sheets, Peakall 1975)

896 (shake flask-GC, Wolfe et al. 1980b)

1200* ($20^{\circ}C$, elution chromatography, UV, Schwarz & Miller 1980)

7028 (shake flask-LSC, Veith et al. 1980)

928 ($20^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)

1080 (shake flask-HPLC/UV, Howard et al. 1985)

680 (measured, Russell & McDuffie 1986)

938* (shake flask-surface tension measurement, measured range 10 – $35^{\circ}C$ Thomsen et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.467* (extrapolated-regression of tabulated data, temp range 108.8 – $294^{\circ}C$, Stull 1947)

0.086 (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log(P/mmHg) = 11.26 - 4308/(T/K)$; temp range 32 – $60^{\circ}C$ or pressure range 5×10^{-2} to 10^{-4} mmHg (effusion method, data presented in graph and Antoine eq., Small et al. 1948)

0.052 ($20^{\circ}C$, torsion-effusion method, Balson 1958)

0.0195 ($20^{\circ}C$, aerosol saturation, measured range 25 – $70^{\circ}C$, Frostling 1970)

$\log(P/mmHg) = 11.13 - 4275/(T/K)$; temp range 25 – $70^{\circ}C$ (aerosol saturation, Frostling 1970)

0.467 (calculated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 15383.0/(T/K)] + 8.18275$; temp range 108.8 – $294^{\circ}C$ (Antoine eq., Weast 1972–73)

- 0.046* (20°C, extrapolated, gas-saturation method, measured range 34.2–60.5°C, Grayson & Fosbraey 1982)
 $\ln(P/\text{Pa}) = 32.50 - 10436/(T/\text{K})$; temp range 34.2–60.5°C (Antoine eq., gas saturation-GC, Grayson & Fosbraey 1982)
- 1.867 (gas saturation, measured range 60–120°C. Potin-Gautier et al. 1982)
 $\log(P/\text{mmHg}) = 8.806 - 1443.039/(T/\text{K})$; temp range 60–120°C (Potin-Gautier et al. 1982)
- 0.220 (gas saturation-HPLC/UV, Howard et al. 1985)
- 0.0064 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.04308 - 1866.05/(-115.9 + T/\text{K})$; temp range 345–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 10.6902 - 6768.3/(-209.45 + T/\text{K})$; temp range 421–570 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- 0.280 (GC-RT correlation, Hinckley et al. 1990)
 $\log(P/\text{mmHg}) = 72.1438 - 7.0747 \times 10^3/(T/\text{K}) - 21.029 \cdot \log(T/\text{K}) - 3.2404 \times 10^{-10} \cdot (T/\text{K}) + 3.4691 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 269–757 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.0020 (calculated-P/C, Wolfe et al. 1980a)
- 0.0486 (Lyman et al. 1982; quoted, Howard 1989)
- 0.1220 (calculated-P/C, Mabey et al. 1982)
- 4.7100 (quoted from WERL Treatability Data, Ryan et al. 1988)
- 0.0269 (selected, Staples et al. 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.22 (calculated as per Leo et al. 1971)
- 3.15 (RP-HPLC-RT correlation, Veith et al. 1979)
- 1.40 (shake flask-LSC, Veith et al. 1980)
- 2.67 (RP-HPLC-RT correlation, Veith et al. 1980)
- 2.21 (HPLC-RT correlation, McDuffie 1981)
- 2.70 (quoted from Veith et al. 1980, Veith & Kosian 1983; Davies & Dobbs 1984; Saito et al. 1992)
- 2.35 (20°C, shake flask-UV, Leyder & Boulanger 1983)
- 2.24, 2.29 (shake flask-HPLC/UV, HPLC-RT correlation, Howard et al. 1985)
- 2.47 (shake flask, unpublished data, Hansch & Leo 1985; 1987)
- 3.00 (RP-HPLC-RT correlation, De Koch & Lord 1987)
- 2.47 (recommended, Sangster 1993)
- 2.47 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 7.55 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.49–1.56 (calculated- K_{OW} , Veith et al. 1979, 1980)
- 2.07 (bluegill sunfish, Veith et al. 1980; Barrows et al. 1980; Veith & Kosian 1983)
- 1.86 (bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
- 1.08, 1.64 (calculated-S, calculated- K_{OW} , Lyman et al. 1982)
- 2.04 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.19 (mullet, Shimada et al. 1983)
- 2.10 (Davies & Dobbs 1984)
- 2.07 (fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.65 (calculated- K_{OW} , Wolfe et al. 1980a)
- 2.72 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1989)
- 1.97 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)
- 2.15 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.34	(sediment, calculated- K_{ow} , Pavlou & Weston 1983, 1984)
1.84	(Broome County of New York soil, shake flask-GC, Russell & McDuffie 1986)
3.00, 2.85, 3.24	(sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
2.03	(activated carbon, calculated-MCI χ , Blum et al. 1994)
1.99	(calculated- K_{ow} , Kollig 1993)
1.84	(quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
1.84	(sediment/soil, selected, Staples et al. 1997)
4.90	(suspended solids, calculated- K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k(aq.) = 18 \text{ M s}^{-1}$ in aquatic environment (Wolfe et al. 1980a)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1.4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{OH} = 1.08 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ corresponding to $t_{1/2} = 22.2 \text{ h}$ and the alkyl peroxy reaction $t_{1/2}(\text{calc}) = 6.5 \text{ yr}$ (Howard 1989)

photooxidation $t_{1/2} = 21\text{--}212 \text{ h}$ in air, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

photooxidation $t_{1/2} = 2.4\text{--}12.2 \text{ yr}$ in water, based on estimated rate data for the reaction with alkyloxyl radical in aqueous solution (Howard et al. 1991)

$k(aq.) = (0.14 \pm 0.05) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} = 2.8 \text{ d}$ at pH 7 (Yao & Haag 1991).

$k_{OH}(aq.) = 4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

predicted atmospheric photooxidation $t_{1/2} = 1.8\text{--}18 \text{ d}$ from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)

$k_{OH} = 3.466 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 2.39 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis: $k(\text{acid-catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1}$, $k(\text{alkaline}) = 79 \text{ M}^{-1} \text{ h}^{-1}$; phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2} = 4$ months to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)

$k(\text{second-order alkaline}) = 2.5 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C (Wolfe et al. 1980b; quoted, Kollig 1993)

$k(\text{alkaline}) = 2.5 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C and $k(\text{second-order alkaline rate}) = 1.2 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at pH 10–12 at 30°C, with a calculated $t_{1/2} = 18.3 \text{ yr}$ at pH 7 (Callahan et al. 1979)

First order hydrolysis $t_{1/2} = 8.8 \text{ yr}$ based on base rate constant at 30°C and pH 7; base rate constant $k = 90 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 32 \text{ d}$ based on measured rate constant at 30°C and pH from 10 to 12 (Howard et al. 1991)

$t_{1/2} = 3200 \text{ d}$, $t_{1/2} = 0.032 \text{ d}$ in natural waters (Capel & Larson 1995)

first-order hydrolysis $t_{1/2} = 8.8 \text{ yr}$ at pH 7 and $t_{1/2} = 32 \text{ d}$ at pH 10–12 based on base rate constant at 30°C (Howard et al. 1991; selected, Staples et al. 1997)

Biodegradation: microbial degradation $t_{1/2} = 10.5 \text{ d}$ by microorganisms isolated from soil and waste water at 30°C (Kurane et al. 1977, quoted, Russell et al. 1985);

estimated rate constant $k \sim (6.59 \pm 0.43) \times 10^2 \text{ min}^{-1}$ from retention times of reverse phase chromatography (Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985);

microbial degradation $k = 2 \times 10^{-4} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a);

0 to 32% mineralization in > 8 wk in municipal digested sludge (Horowitz et al. 1982);

complete degradation in 7.0 d for 5 and 10 ppm DEP in domestic waste water under aerobic conditions at 25°C (Tabak et al. 1981; quoted, Howard 1989);

$k = 0.315 \text{ d}^{-1}$ corresponding to $t_{1/2} = 2.21 \text{ d}$ with a mixed microbial population and underwent > 99% degradation in 28-d in shake flask biodegradation experiment (Sugatt et al. 1984);

greater than 90% of DEP was degraded within 40 d in digested sludge (Shelton et al. 1984); 85% biodegraded after 14 d incubation in aerobic freshwater sediments at 22°C (Johnson et al. 1984);

biodegraded in excess of 90% in less than 24 h in activated sludge systems (O'Grady et al. 1985);

soil-water biodegradation studies showed the 86% loss after 120 h in Broome County soils and 67% loss in leachate sprayed soil after 48 h (Russell et al. 1985);

anaerobic digestion of sludge with first-order $k = 6.0 \times 10^{-3} \text{ h}^{-1}$ and $t_{1/2} = 115 \text{ h}$ (Ziogou et al. 1989)

aqueous aerobic $t_{1/2} = 72\text{--}1344 \text{ h}$, based on aerobic aqueous grab sample data for fresh and marine water (Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672\text{--}5376 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life and anaerobic screening test data (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 3 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

Aerobic biodegradation in aquatic environments, first order $k = 1.8 \text{ d}^{-1}$ with $t_{1/2} = 0.39 \text{ d}$ in river water, $k = 0.16 \text{ d}^{-1}$ with $t_{1/2} = 4.33 \text{ d}$ in MITI inoculum, and $k = 0.98 \text{ d}^{-1}$ with $t_{1/2} = 0.71 \text{ d}$ (Peterson & Staples 2003)

biodegradation in aerobic soil, pseudo-first-order $k = 0.38 \text{ d}^{-1}$ with $t_{1/2} = 1.83 \text{ d}$ in agitated aqueous suspension.

For anaerobic degradation, first order rate $k = 0.069$ to $> 0.3 \text{ d}^{-1}$ with $t_{1/2} = 10.0$ to $< 2.3 \text{ d}$ in digester sludge, batch incubation; $k = 0.036 \text{ d}^{-1}$ with $t_{1/2} = 19.3 \text{ d}$ in flood soil; $k = 0.27 \text{ d}^{-1}$ with $t_{1/2} = 2.6 \text{ d}$ in pond sediment, $k = 0.13 \text{ d}^{-1}$ with $t_{1/2} = 5.3 \text{ d}$ in 10% freshwater sediment and $k = 0.31 \text{ d}^{-1}$ with $t_{1/2} = 2.2 \text{ d}$ in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: experimentally determined microbial $k = 3.2 \times 10^{-9} \text{ mL organism}^{-1} \text{ h}^{-1}$ (Wolfe et al. 1980a,c); estimated $k \sim 1 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982);

mean microbial $k = (7.2 \pm 15.4) \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ for 54 batch aufwuchs cultures (Lewis & Holm 1981; Lewis et al. 1984).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

depuration half-life $24 \text{ h} < t_{1/2} < 48 \text{ h}$ in tissues of bluegill sunfish (Barrows et al. 1980).

$k_2 = 6.83 \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.584 \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: an estimated $t_{1/2} = 22.2 \text{ h}$ for the vapor reaction with photochemically generated $8 \times 10^5 \text{ molecules}\cdot\text{cm}^{-3}$ OH radical in air at 25°C with an estimated $k \sim 1.08 \times 10^{-11} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ (Howard 1989);

$t_{1/2} = 21\text{--}212 \text{ h}$, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

photodegradation $t_{1/2} = 2.39 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 2.21 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984); $t_{1/2} \sim 2 \text{ d}$ to $> 2 \text{ wk}$ for aerobic biodegradation in water; $t_{1/2} = 3 \text{ d}$ when incubated in dirty river water (Howard 1989);

overall degradation $t_{1/2} = 72\text{--}1344 \text{ h}$, based on aerobic aqueous grab sample data for fresh and marine water (Howard et al. 1991);

$k(\text{exptl}) = (0.14 \pm 0.5) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C , with $t_{1/2} = 2.8 \text{ d}$ at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 144\text{--}2688 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} < 14 \text{ d}$ in freshwater sediment (Johnson et al. 1984).

Soil: degradation $t_{1/2} = 10.5 \text{ d}$ by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977);

$t_{1/2} = 10\text{--}50 \text{ d}$ via volatilization subject to plant uptake from soil (Ryan et al. 1988);

$t_{1/2} = 72\text{--}1344 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $24 \text{ h} < t_{1/2} < 48 \text{ h}$ in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 15.1.3.2.1
Reported vapor pressures and aqueous solubilities of diethyl phthalate at various pressures and solubilities

Aqueous solubility				Vapor pressure			
Schwarz & Miller 1980		Thomsen et al. 2001		Stull 1947		Grayson & Fosbraey 1982	
elution chromatography-UV		shake flask-surface tension		summary of literature data		gas saturation-GC	
t/°C	g m ⁻³	t/°C	g m ⁻³	t/°C	P/Pa	t/°C	P/Pa
20	1200	10	1113	108.8	133.3	34.2	0.222
20	1240	25	838	140.7	666.6	40.0	0.470
20	1160	35	741	156.0	1333	44.8	0.784
30	1370			173.6	2666	50.7	1.368
30	1400			192.1	5333	60.5	3.320
30	1340			204.1	7999	20	0.046
				219.5	13332		
				243.0	26664	ln P = A – B/(T/K)	
				267.5	53329		P/Pa
				294.0	101325	A	32.5
						B	10436

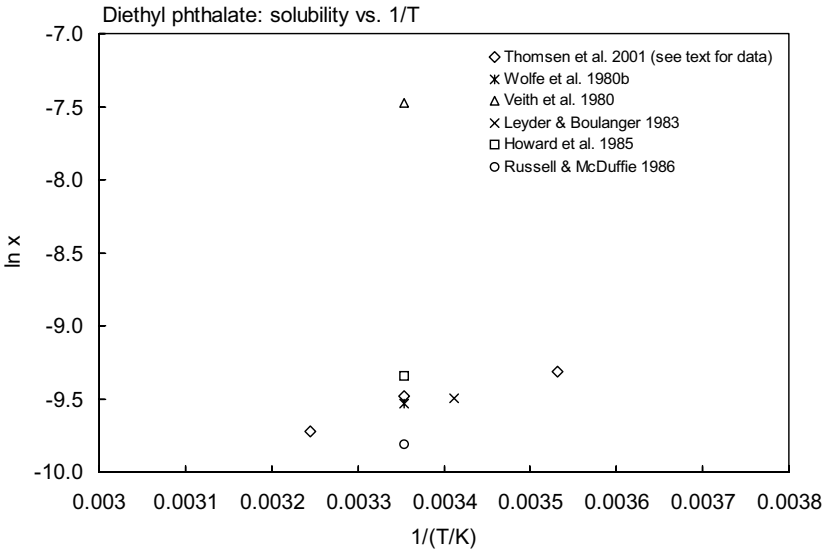


FIGURE 15.1.3.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for diethyl phthalate.

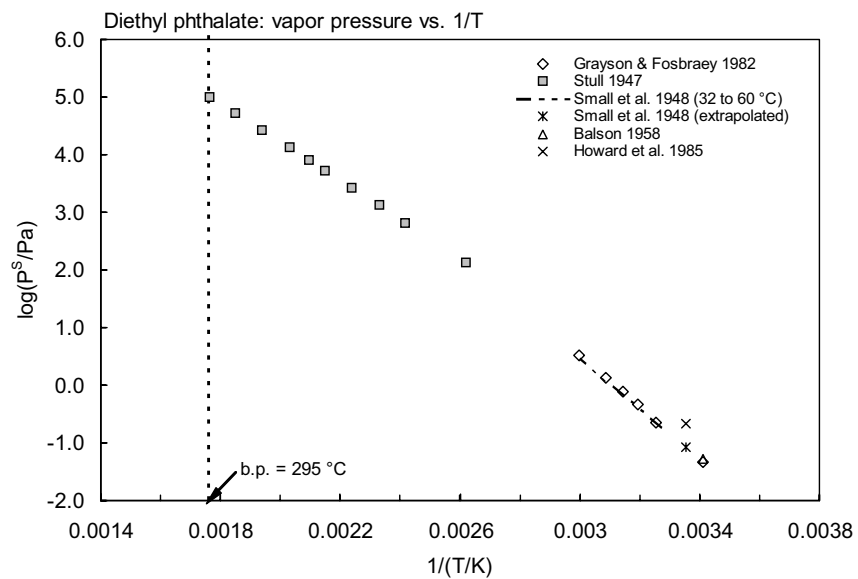
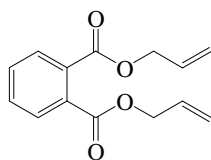


FIGURE 15.1.3.2.2 Logarithm of vapor pressure versus reciprocal temperature for diethyl phthalate.

15.1.3.3 Diallyl phthalate (DAP)



Common Name: Diallyl phthalate

Synonym: DAP

Chemical Name: di(2-propenyl) phthalate, bis(2-propenyl)ester, 1,2-benzenedicarboxylic acid

CAS Registry No: 131-17-9

Molecular Formula: $C_{14}H_{14}O_4$, $C_6H_4-1,2-(CO_2CH_2CH=CH_2)_2$

Molecular Weight: 246.259

Melting Point ($^{\circ}C$):

-77 (Fishbein & Albro 1972)

Boiling Point ($^{\circ}C$):

290 (Fishbein & Albro 1972)

Density (g/cm^3 at $20^{\circ}C$):

1.121 (Fishbein & Albro 1972)

Molar Volume (cm^3/mol):

219.7 ($20^{\circ}C$, calculated-density)

288.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

< 100 (Fishbein & Albro 1972)

182 ($20^{\circ}C$, shake flask-GC, Leyder & Boulanger 1983)

182; 43, 100 (recommended; calculated-QSAR, Staples 1997)

94 (calculated-UNIFAC, Thomsen et al. 1999)

156 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0213; 0.00493, 0.155 (recommended; calculated-QSAR, Staples et al. 1997)

0.0271 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0289 (selected, Staples et al. 1997)

0.0428 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.23 (shake flask, Leyder & Boulanger 1983)

3.23 (recommended value, Sangster 1993)

3.23 (recommended, Hansch et al. 1995)

3.23; 3.37, 3.63 (recommended; calculated-QSAR, Staples 1997)

3.61 (calculated-UNIFAC, Thomsen et al. 1999)

3.11 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.87 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} = 0.04\text{--}0.4$ d (Staples et al. 1997).

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 2.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} = 0.04\text{--}0.4$ d (Staples et al. 1997).

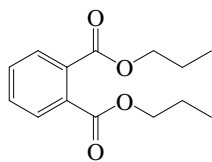
Surface water:

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 2.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

15.1.3.4 Di-*n*-propyl phthalate (DnPP)

Common Name: Di-*n*-propyl phthalate

Synonym: DPP, DNPP, dipropyl phthalate

Chemical Name: phthalic acid dipropyl ester; 1,2-benzenedicarboxylic acid dipropyl ester

CAS Registry No: 131-16-8

Molecular Formula: C₁₄H₁₈O₄, C₆H₄[COOCH₂CH₂CH₃]₂

Molecular Weight: 250.291

Melting Point (°C):

−31.0 (Lide 2003)

Boiling Point (°C):

304.5 (Lide 2003)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

232.2 (20°C, calculated-density, Stephenson & Malanowski 1987)

302.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.70 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

108 (shake flask-UV, Leyder & Boulanger 1983)

108; 38, 47 (recommended; calculated-structure activity program, QSAR, Staples et al. 1997)

77 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.0175 (effusion method, extrapolated-Antoine eq., Small et al. 1948)

log (P/mmHg) = 11.66 − 4634/(T/K); temp range 32–75°C or pressure range 5 × 10^{−2} to 10^{−4} mmHg (Antoine eq., effusion method, Small et al. 1948). Additional data at other temperatures designated * are compiled at the end of this section

log (P/kPa) = 8.625 − 3824/(T/K); temp range 403–578 K (Antoine eq., Stephenson & Malanowski 1987)

0.0119, 0.138 (calculated-QSAR, Staples et al. 1997)

0.0175 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.0309 (recommended, Staples et al. 1997)

0.0569 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{ow}:

3.27 (shake flask, Leyder & Boulanger 1983)

4.05 (HPLC-RT correlation, Hayward et al. 1990)

4.20 (HPLC-RT correlation, Jenke et al. 1990)

3.27, 4.05 (lit. values, Hansch et al. 1995)

3.27; 3.57, 3.63 (recommended; calculated-structure activity program, QSAR, Staples et al. 1997)

3.636 (Thomsen & Carlsen 1998)

3.40 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.04 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} = 0.9\text{--}9.0$ d (calculated, Staples et al. 1997).

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 6.5$ d by microorganisms (*Pseudomonas acidovorans* 256-1) from soil or waste water at 30°C (Kurane et al. 1977);

rate constant $k = (10.71 \pm 0.73) \times 10^{-2} \text{ min}^{-1}$ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979).

Aerobic biodegradation in aquatic environments, first order $k = 1.3 \text{ d}^{-1}$ with $t_{1/2} = 0.53$ d in river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} = 0.9\text{--}9.0$ d (calculated, Staples et al. 1997).

Surface water: $t_{1/2} = 0.53$ d in river water (Peterson & Staples 2003)

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 6.5$ d by microorganisms (*Pseudomonas acidovorans* 256-1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

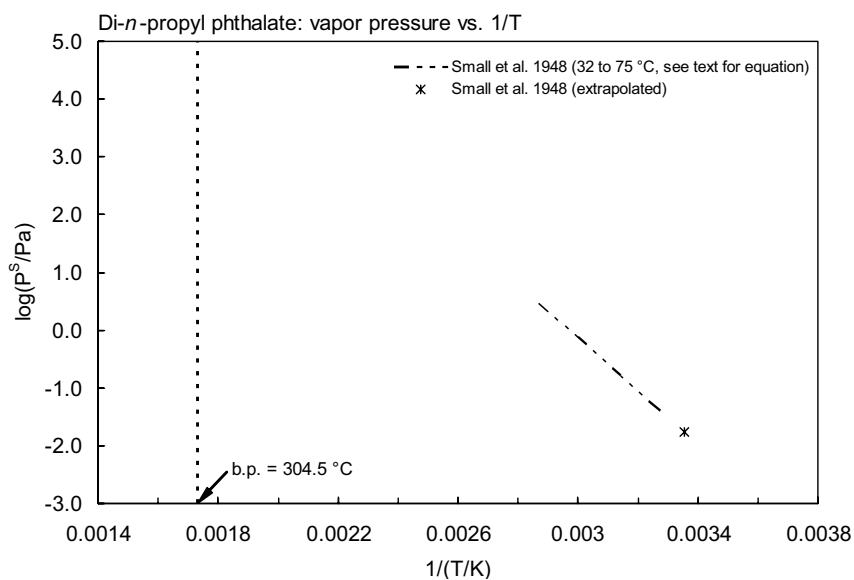
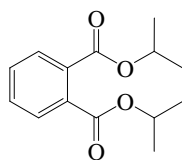


FIGURE 15.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-propyl phthalate.

15.1.3.5 Di-isopropyl phthalate (DIPP)



Common Name: Di-isopropyl phthalate

Synonym: DIPP

Chemical Name: phthalic acid dipropyl ester, bis(1-methylethyl)ester, 1,2-benzenedicarboxylic acid diisopropyl ester

CAS Registry No: 605-45-8

Molecular Formula: $C_{14}H_{18}O_4$, 1,2- $C_6H_4(CO_2C_3H_7)_2$

Molecular Weight: 250.291

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

304–305 (Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

302.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

322 (shake flask-UV, Leyder & Boulanger 1983)

136 (calculated-UNIFAC, Thomsen et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.83 (shake flask-UV, Leyder & Boulanger 1983)

2.83 (recommended, Sangster 1993)

2.83 (recommended, Hansch et al. 1995)

3.59 (calculated-UNIFAC, Thomsen et al. 1999)

Bioconcentration Factor, $\log BCF$:

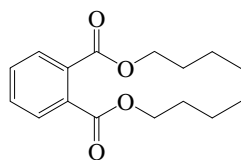
Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Biodegradation: degradation $t_{1/2} = 1.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at $30^{\circ}C$ (Kurane et al. 1977).

Half-Lives in the Environment:

Soil: degradation $t_{1/2} = 1.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at $30^{\circ}C$ (Kurane et al. 1977).

15.1.3.6 Di-*n*-butyl phthalate (DBP)

Common Name: Dibutyl phthalate

Synonym: *n*-butyl phthalate, di-*n*-butyl phthalate, DBP, dibutyl *o*-phthalate, *o*-benzenedicarboxylic acid dibutyl ester, benzene-*o*-dicarboxylic acid dibutyl ester

Chemical Name: phthalic acid dibutyl ester, di-*n*-butyl phthalate

CAS Registry No: 84-74-2

Molecular Formula: $C_{16}H_{22}O_4$, $o-C_6H_4(COOC_4H_9)_2$

Molecular Weight: 278.344

Melting Point ($^{\circ}C$):

-35.0 (Fishbein & Albro 1972; Verschueren 1977, 1983; Dean 1985; Howard 1989; Lide 2003)

Boiling Point ($^{\circ}C$):

340.0 (Stull 1947; Fishbein & Albro 1972; Weast 1982-83; Verschueren 1983; Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0465 (21 $^{\circ}C$, Fishbein & Albro 1972)

1.047 (Weast 1982-83)

Molar Volume (cm^3/mol):

267.1 (calculated-density, Stephenson & Malanowski 1987)

347.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

93.3 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K) F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

11.08 (Deno & Berkheimer 1960)

4500 (Patty 1967)

4500 (Fishbein & Albro 1972)

10.0 (30 $^{\circ}C$, from Monsanto Chemical Co. data sheets, Peakall 1975)

13.0 (Wolfe et al. 1979; Wolfe et al. 1980a)

10.8, 11.1, 10.5 (20 $^{\circ}C$: quoted average, elution chromatography, UV, Schwarz & Miller 1980)

11.4, 11.5, 11.2 (30 $^{\circ}C$: quoted average, elution chromatography, UV, Schwarz & Miller 1980)

13 ± 1.6 , 4.45 (shake flask-GC, quoted, Wolfe et al. 1980b; quoted, Staples et al. 1997)

3.25 (solubility in 35 liter instant ocean, Giam et al. 1980)

10.1 (20 $^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)

400, 4500 (Verschueren 1983)

28.0 (26 $^{\circ}C$, Verschueren 1983)

11.2 ± 0.3 (shake flask-HPLC/UV, Howard et al. 1985)

100 (Dean 1985)

11.2 (Howard et al. 1985)

9.40 (best estimate by turbidity inflection, DeFoe et al. 1990)

8.70, 9.40 (centrifugation-HPLC/UV, turbidity inflection-HPLC/UV, DeFoe et al. 1990)

11.2 (recommended, Staples et al. 1997)

9.90 (calculated-QSPR, Cousin & Mackay 2000)

13.3, 14.6, 5.50 (10, 25, 35 $^{\circ}C$, shake flask-surface tension measurement, Thomsen et al. 2001). Additional data at other temperatures designated * are compiled at the end of this section

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

- 13.33* (89°C, ebulliometry, measured range 89–176°C, Gardner & Brewer 1937)
 0.00233 (20°C, extrapolated, tensimeter, measured range 52–97°C, Hickman et al. 1937)
 $\log(P/\mu\text{mHg}) = 14.215 - 4680/(T/K)$; temp range 52–97°C (Hickman et al. 1937)
 0.0171* (20°C, extrapolated, effusion, measured range 40–95°C, Verhoek & Marshall 1939)
 $\log(P/\mu\text{mHg}) = 15.589 - 5122/(T/K)$; temp range 40–95°C (Verhoek & Marshall 1939)
 0.00253* (ebulliometry, extrapolated from graph, measured range 50–172°C, Burrows 1946)
 0.0217* (extrapolated-regression of tabulated data, temp range 148.2–340°C, Stull 1947)
 0.00345, 0.0043 (effusion method, extrapolated-Antoine eq., Small et al. 1948)
 $\log(P/\text{mmHg}) = 11.75 - 4871/(T/K)$; temp range ~ 32–75°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, Small et al. 1948)
 $\log(P/\text{mmHg}) = 11.86 - 4875/(T/K)$; temp range ~ 40–95°C or pressure range 5×10^{-2} to 10^{-4} mmHg (redistilled technical grade, Antoine eq., effusion method, Small et al. 1948)
 0.00276 (extrapolated-combined vapor pressure eq., Small et al. 1948)
 $\log(P/\text{mmHg}) = 7.065 - 1666/(T/K) - 547700/(T/K)^2$; temp range ~ 35–352°C (combined vapor pressure eq. derived from effusion measurement results and other published data, Small et al. 1948)
 0.0033 (20°C, extrapolated, tensimeter, measured range 55–102°C, Perry & Weber 1949)
 $\log(P/\mu\text{mHg}) = 13.58 - 4450/(T/K)$; temp range 55–102°C (pendulum-tensimeter method, Perry & Weber 1949)
 0.00364* (effusion method, measured range 19.9–44°C, Birks & Bradley 1949)
 7.6×10^{-5} (dew-point method and tensimeter method, temp range of 72–185°C, extrapolated-Antoine eq., Werner 1952)
 $\log(P/\mu\text{mHg}) = 11.008 - 2872/(176.5 + t/^{\circ}\text{C})$; temp range 72–185°C (Antoine eq., dew-point method and tensimeter method, Werner 1952)
 32* (125.7°C, vapor-liquid equilibrium data, measured range 125.7–202.5°C, Hammer & Lydersen 1957)
 $\log(P/\text{kPa}) = 6.439 - 1011/(T/K) - 720000/(T/K)^2$; temp range 125.7–202.5°C, Hammer & Lydersen 1957)
 1.53* (86.5°C, transpiration method, measured range 86.5–144°C, Franck 1969)
 $\log(P/\text{mmHg}) = [-0.2185 \times 17747.0/(T/K)] + 9.217428$; temp range: 148.2–340°C, (Antoine eq., Weast 1972–73)
 3.87×10^{-4} (6.55°C, submicron droplet evaporation, measured range 6.55–12.55°C, Ray et al. 1979)
 $\log(P/\text{mmHg}) = 12.217 - 4993/(T/K)$; temp range 6.55–12.55°C (submicron droplet evaporation, Ray et al. 1979)
 0.00206* (20°C, transpiration-GC “collection” measurement, Hales et al. 1981)
 $\ln(P/\text{Pa}) = 27.5178 - 8739.43/(T/K) - 330691/(T/K)^2$; temp range 293–373 K (empirical vapor pressure eq., from transpiration-GC measurement, Hales et al. 1981)
 0.0023* (20°C, vapor pressure balance, temp range 10–50°C, OECD 1981)
 0.00277 (20°C, evaporation rate-gravimetric method, Gückel et al. 1982)
 0.00133 (gas saturation, Jaber et al. 1982)
 0.40, 0.0653, 1.0 (structure-based estimation methods, Tucker et al. 1983)
 1.55×10^{-4} (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 576561 - 1744.128/(188.880 + t/^{\circ}\text{C})$, temp range 125.8–202.5°C (Antoine eq. derived from exptl. data of Hammer & Lydersen 1957, Boublik et al. 1984)
 0.00230 (OECD 1981 Guidelines, Dobbs et al. 1984)
 0.0011 (saturated column-HPLC/UV, Howard et al. 1985)
 0.00355 (extrapolated, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.8788 - 2538.4/(-92.25 + T/K)$; temp range 314–469 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.97157 - 3385.9/(-37.18 + T/K)$; temp range 468–605 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 0.0244 (calculated-solvatochromic parameters, Banerjee et al. 1990)
 0.0056 (GC-RT correlation, Hinckley et al. 1990)
 $\log(P/\text{mmHg}) = 6.63980 - 1744.20/(113.69 + t/^{\circ}\text{C})$, temp range 126–202°C (Antoine eq., 1992)
 $\log(P/\text{mmHg}) = 152.675 - 1.0754 \times 10^4/(T/K) - 51.17 \cdot \log(T/K) + 1.6933 \times 10^{-2} \cdot (T/K) + 2.4948 \times 10^{-14} \cdot (T/K)^2$; temp range 238–781 K (vapor pressure eq., Yaws et al. 1994)
 0.0027 (liquid P_L , GC-RT correlation, Donovan 1996)

- 0.0036 (recommended, Staples et al. 1997)
 0.0473 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 0.1320 (calculated-P/C, Wolfe et al. 1980a)
 0.0466 (Lyman et al. 1982; quoted, Howard 1989)
 0.0284 (calculated-P/C, Mabey et al. 1982)
 0.1835 (Atlas et al. 1983)
 0.456, 0.446 (calculated-P/C, calculated-group contribution, Tucker et al. 1983)
 0.0297 (quoted from WERL Treatability Data, Ryan et al. 1988)
 0.0895 (selected, Staples et al. 1997)
 0.133 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 5.20 (calculated as per Leo et al. 1971, Callahan et al. 1979)
 5.15 (RP-HPLC-RT correlation, Veith et al. 1979)
 4.13 (HPLC-RT correlation; McDuffie 1981)
 4.11, range 3.23–4.45 (shake flask-concn ratio, OECD 1981)
 4.08 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
 4.39, 4.56 (HPLC-extrapolated, Harnish et al. 1983)
 4.57 (20°C , shake flask-UV, Leyder & Boulanger 1983)
 4.79, 3.74 (shake flask-HPLC/UV, HPLC-RT, Howard et al. 1985)
 4.11 (OECD value, Howard et al. 1985)
 4.72 (shake flask, Hansch & Leo 1985; 1987)
 4.57 (HPLC- k' correlation, Eadsforth 1986)
 4.30 (HPLC-RT correlation, Haky & Leja 1986)
 4.72 (measured value, DeFoe et al. 1990)
 4.72 (recommended, Sangster 1993)
 4.72 (recommended, Hansch et al. 1993)
 4.01 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 8.54 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log \text{BCF}$:

- 3.15 (fish, Mayer & Sanders 1973)
 3.82, 3.70, 3.83, 3.28, 3.70, 3.43 (midge larvae, waterflea, scud, mayfly, grass shrimp, damselfly, Sanders et al. 1973)
 3.83 (fish, Sanders et al. 1973)
 1.32 (calculated, Kenaga 1980)
 3.90 (bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
 1.32–1.62, 0.46–1.49, 1.07 (oyster, shrimp, fish, Wofford et al. 1981)
 1.50, 1.22, 1.07 (American oyster, brown shrimp, sheephead minnow, Wofford et al. 1981)
 4.67 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 4.36 (*Selenastrum capricornutum*, Casserly et al. 1983)
 1.32 (oyster, quoted from Wofford et al. 1981, Zaroogian et al. 1985)
 3.68, 3.68 (oyster, estimated values, Zaroogian et al. 1985)
 1.08 (fish, highest BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.20 (soil, estimated-S, Kenaga 1980)
 3.81 (soil, estimated-S, Wolfe et al. 1980a)
 2.17 (marine sediment/seawater with 1% organic carbon, Bouwer et al. 1981)
 1.60, 1.30, 0.602 (between montmorillonite, kaolinite, calcium montmorillonite and seawater at concn. of 3–4 ppm, Sullivan et al. 1981)

- 0.301, 0.602, 1.556 (between montmorillonite, kaolinite, calcium montmorillonite and seawater at concn. of 20 ppb, Sullivan et al. 1981)
- 5.23 (sediment-water, calculated- K_{OW} , Mabey et al. 1982).
- 4.17 (sediment/soil, Sullivan et al. 1982; selected, Staples et al. 1997)
- 4.54 (sediment, calculated- K_{OW} , Pavlou & Weston 1983,84)
- 3.14 (Broome County soil in New York, shake flask-GC, Russell & McDuffie 1986)
- 4.37 (calculated- K_{OW} , Kollig 1993)
- 3.14 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 3.09, 5.20 (suspended solids, calculated- K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)
- 3.14; 3.76, 2.46, 2.86, 3.09, 3.12, 3.11 (quoted lit.; values obtained from HPLC- k' correlation on different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2} = 28$ d from a stirred seawater solution 1.0 m deep (Atlas et al. 1982; quoted, Howard 1989)
 evaporation rate $k = 3.42 \times 10^{-10}$ mol cm^{-2} h^{-1} at 20°C (Gückel et al. 1982);
 $t_{1/2} \sim 47$ d in a river of 1.0 m deep with 1 m/s current and a 3 m/s wind using Henry's law constant while the rate of volatilization being controlled by the diffusion through air (Lyman et al. 1982; quoted, Howard 1989).
- Photolysis: direct photolysis (near surface) rate constant $k \sim 2 \times 10^{-4}$ h^{-1} in natural water (Wolfe et al. 1980a)
 aqueous photolysis rate $k = 0.23$ h^{-1} and $t_{1/2} = 3$ h (Jin et al. 1999, quoted, Peterson & Staples 2003)
 Indirect photolysis $k = 0.29$ d^{-1} with $t_{1/2} = 2.4$ d in air (Peterson & Staples 2003).
- Oxidation:
 $k = 18$ M s^{-1} , the free radical oxidation rate constant (EXAMS model, Wolfe et al. 1980a)
 photooxidation $t_{1/2} = 2.4\text{--}12.2$ yr in water, based on estimated rate data for the reaction with alkyloxyl radical in aqueous solution (Wolfe et al. 1980a; quoted, Howard et al. 1991)
 $k \ll 360$ M $^{-1}$ h^{-1} for singlet oxygen and $k = 1.4$ M $^{-1}$ h^{-1} for peroxy radical (Mabey et al. 1982)
 photooxidation $t_{1/2} = 18.4$ h with reaction with OH radical (Howard 1989)
 photooxidation $t_{1/2} = 7.4\text{--}74$ h in air, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)
 Atmospheric photooxidation $t_{1/2} = 0.6\text{--}6.0$ d from Atkinson 1988 atmospheric-oxidation program (estimated, Staples et al. 1997).
 $k_{OH} = 9.277 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} and $t_{1/2} = 0.89$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis:

- $k(\text{second-order alkaline}) = 2.2 \times 10^{-2}$ M $^{-1}$ s^{-1} for pH 10–12 at 30°C, with calculated half-life of 10 yr at pH 7 (calculated as per Radding et al. 1977, Callahan et al. 1979)
- $k(\text{acid catalyzed}) = 0.04$ M $^{-1}$ h^{-1} , $k(\text{second order alkaline}) = 38$ M $^{-1}$ h^{-1} in an aquatic environment (Wolfe et al. 1980a)
- $k(\text{second-order alkaline}) = (1.0 \pm 0.05) \times 10^{-2}$ M $^{-1}$ s^{-1} at pH 7 and 30°C, with first-order hydrolysis $t_{1/2} = 10$ yr (Wolfe et al. 1980b; quoted, Kollig 1993);
- $t_{1/2} = 76$ d at pH 9 and $t_{1/2} = 10$ yr at neutral pH (estimated, Howard 1989)
- $t_{1/2} = 10$ yr, based on the overall hydrolysis rate constant (Howard et al. 1991)
- aqueous abiotic $t_{1/2} = 22$ yr (selected, Staples et al. 1997)
- $t_{1/2} = 3700$ d at pH 7, $t_{1/2} = 76$ d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation:

- $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)
- DBP was rapidly degraded, 3% left after 5 d, but under anaerobic conditions required 30 d for the degradation freshwater hydrosol, under aerobic conditions (Johnson et al. 1979, quoted, Russell et al. 1985)
- a 90% loss in 3 d from river water (Brinkman et al. 1979, quoted, Russell et al. 1985)
- $k = (13.26 \pm 0.73) \times 10^2$ min $^{-1}$ (reversed phase-GC-RT correlation, Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985)
- $k = 2.9 \times 10^{-8}$ mL organism $^{-1}$ h^{-1} (Wolfe et al. 1980a);
- $k > 0.5$ d $^{-1}$, significant degradation with rapid adaptation within 7 d in an aerobic environment (Tabak et al. 1981; quoted, Mills et al. 1982);
- $k = 7.4 \times 10^{-7}$ mL cell $^{-1}$ d $^{-1}$ (river die-away test, Scow 1982);

32–85% degraded after 2–3 wk in municipal digested sludge (Horowitz et al. 1982)

decomposed within 80 d under both aerobic and anaerobic conditions when approximately 90% added to soils (Inman et al. 1984)

$k = (0.1\text{--}7.6) \times 10^{-4} \text{ h}^{-1}$ to $(4.9\text{--}36.5) \times 10^{-4} \text{ h}^{-1}$ for water and water/sediment systems (under sterile conditions); and $k = (29.3\text{--}409) \times 10^{-4} \text{ h}^{-1}$ to $(38.2\text{--}456) \times 10^{-4} \text{ h}^{-1}$ for water and water/sediment systems (under active conditions) samples from six estuarine and freshwater sites, actual $t_{1/2} = 1.0\text{--}4.8 \text{ d}$ for active sediment treatment, $t_{1/2} = 1.7\text{--}13.0 \text{ d}$ for active water treatment and $t_{1/2} = 8\text{--}23 \text{ d}$ for sterile sediment (Walker et al. 1984)

$k = 0.050 \text{ d}^{-1}$ and $a_{t_{1/2}} = 15.4 \text{ d}$ in a shake flask biodegradation experiment (Sugatt et al. 1984)

> 90% of DBP was degraded within 40 d in digested sludge (Shelton et al. 1984)

> 90% biodegraded in less than 24 h in activated sludge systems (O'Grady et al. 1985)

81% loss in Broome County soils after 24 h and 70% loss in leachate sprayed soil after 24 h in soil-water biodegradation studies (Russell et al. 1985);

$k = 10.6 \times 10^{-3} \text{ h}^{-1}$ and $t_{1/2} = 65 \text{ h}$, anaerobic digestion of sludge (Ziogou et al. 1989);

$t_{1/2} < 5 \text{ d}$, aerobic conditions, $t_{1/2} = 20 \text{ d}$ under anaerobic conditions in a garden soil (Shanker et al. 1985)

$t_{1/2} = 24\text{--}552 \text{ h}$, aqueous aerobic based on unacclimated aerobic river die-away test and soil grab sample data (Howard et al. 1991);

$t_{1/2} = 48\text{--}552 \text{ h}$, aqueous anaerobic, based on unacclimated anaerobic grab sample data for soil and sediment (Johnson & Lulves 1975; Verschueren 1983; Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2 \text{ d}$ in natural waters (Capel & Larson 1995)

$k = 0.0216 \text{ h}^{-1}$ with $t_{1/2} = 32.1 \text{ h}$ for microbial degradation by anaerobic sludge (Wang et al. 2000)

aerobic biodegradation in aquatic environments, first order $k = 0.8 \text{ d}^{-1}$ with $t_{1/2} = 0.87 \text{ d}$ in river water, $k = 0.51$

d^{-1} with $t_{1/2} = 1.56 \text{ d}$ in estuarine and river water, $k = 0.29 \text{ d}^{-1}$ with $t_{1/2} = 2.40 \text{ d}$ in sediment microcosm,

$k = 0.22 \text{ d}^{-1}$ with $t_{1/2} = 3.15 \text{ d}$ in MITI inoculum, $k = 0.14 \text{ d}^{-1}$ with $t_{1/2} = 4.95 \text{ d}$ in river water, low sediment,

and $k = 0.98 \text{ d}^{-1}$ with $t_{1/2} = 0.71 \text{ d}$ river water only (Peterson & Staples 2003)

biodegradation in aerobic soil, pseudo-first-order $k = 1.61 \text{ d}^{-1}$ with $t_{1/2} = 0.43 \text{ d}$ in agitated aqueous suspension,

$k = 0.39 \text{ d}^{-1}$ with $t_{1/2} = 1.8 \text{ d}$ at 30°C garden soil; $k = 0.103 \text{ d}^{-1}$ with $t_{1/2} = 6.7 \text{ d}$ in soil with 2% OC;

$k = 0.044 \text{ d}^{-1}$ with $t_{1/2} = 11.2 \text{ d}$ in soil with 3.3% OC and $k = 0.62 \text{ d}^{-1}$ with $t_{1/2} = 15.8 \text{ d}$ in soil with 1.6%

OC. For anaerobic degradation, first order rate $k = 0.26\text{--}0.581 \text{ d}^{-1}$ with $t_{1/2} = 1.19\text{--}2.7 \text{ d}$ in undiluted

digester sludge, $k = 0.025\text{--}0.073 \text{ d}^{-1}$ with $t_{1/2} = 27.7\text{--}9.5 \text{ d}$ in 10% diluted sludge, batch incubation;

$k = 0.076 \text{ d}^{-1}$ with $t_{1/2} = 9 \text{ d}$ in 10% freshwater sediment and $k = 0.051 \text{ d}^{-1}$ with $t_{1/2} = 13 \text{ d}$ in 10% salt

marsh sediment (Peterson & Staples 2003)

Biotransformation: $k = (1.9\text{--}4.4) \times 10^{-8} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Steen et al. 1979; quoted, Mabey et al. 1982; Steen 1991);

$k = 2.9 \times 10^{-8} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or half-Lives:

$t_{1/2} = 3 \text{ d}$ in *Daphnia magna* (Mayer & Sanders 1973).

$k_2 = 0.237 \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.0114 \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} \sim 18 \text{ h}$ for the vapor phase reaction with hydroxyl radicals in air (Howard 1989);

$t_{1/2} = 7.4\text{--}74 \text{ h}$, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

Photodegradation $t_{1/2} = 0.89 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air and indirect photolysis $t_{1/2} = 2.4 \text{ d}$ (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 15.4 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984)

$t_{1/2} = 2\text{--}12 \text{ d}$ in water alone (Howard 1989);

$t_{1/2} = 24\text{--}336 \text{ h}$, based on unacclimated aerobic river die-away test and fresh water/sediment grab sample data (Howard et al. 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2 \text{ d}$; hydrolysis $t_{1/2} = 3700 \text{ d}$ at pH 7 and $t_{1/2} = 76 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

biodegradation $t_{1/2} = 0.87\text{--}5.78 \text{ d}$ in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 48\text{--}552$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: 97% degradation in 5 d in an aerobic pond water-sediment mixture; $t_{1/2} = 7\text{--}30$ d under anaerobic conditions, $t_{1/2} = 1\text{--}5$ d in sediment-water systems of estuarine and freshwater sites (Howard 1989).

Soil: degradation $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977) degradation $t_{1/2} = 11$ to 53 d as affected by soil type, pH, temperature, aeration status and sterilization (Inman et al. 1984);

biodegradation $t_{1/2}(\text{aerobic}) < 5$ d and $t_{1/2}(\text{anaerobic}) \sim 20$ d in a garden soil (Shanker et al. 1985);

$t_{1/2} = 10\text{--}50$ d via volatilization subject to plant uptake from soil (Ryan et al. 1988);

overall $t_{1/2} = 48\text{--}552$ h, based on unacclimated aerobic soil grab sample data (Howard et al. 1991)

Aerobic biodegradation in soil, $t_{1/2}$ ranging from 0.43 to 19.8 d in aqueous suspension, garden soil and soils with different organic carbon contents (Peterson & Staples 2003)

Biota: elimination $t_{1/2} = 3$ d for waterfleas *Daphnia magna* (Mayer & Sanders 1973).

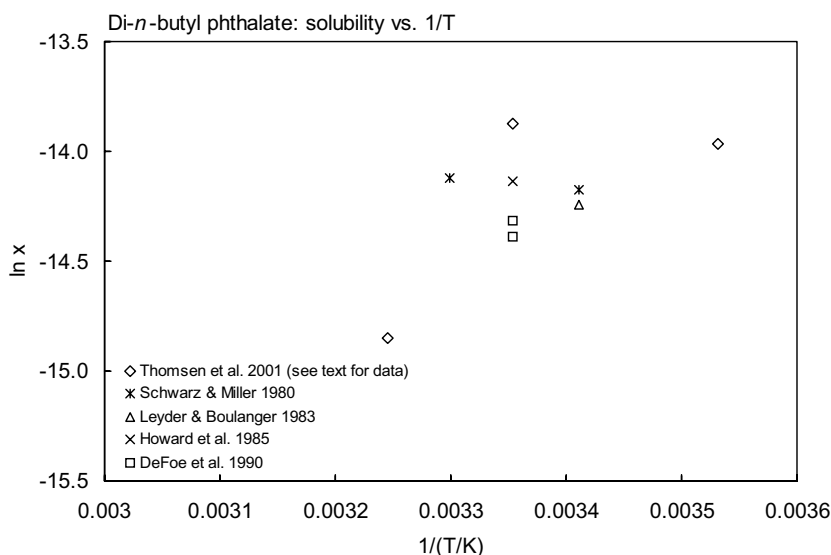


FIGURE 15.1.3.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for di-*n*-butyl phthalate.

TABLE 15.1.3.6.1

Reported vapor pressures of di-*n*-butyl phthalate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log(T/K)$	(4)		
$\log P = A - B/(T/K) - C/(T/K)^2$	(5)	$\ln P = A - B/(T/K) - C/(T/K)^2$	(5a)

1.

Gardner & Brewer 1937		Verhoek & Marshall 1939		Burrows 1946		Stull 1947	
ebulliometry		static and dynamic methods		ebulliometry		summary of literature data	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
89.0	13.33	40	0.0223	50	0.0667	148.2	133.3
98.8	53.33	55	0.137	82	1.333	182.1	666.6
106.1	79.99	55	0.109	120	26.66	198.2	1333

TABLE 15.1.3.6.1 (Continued)

Gardner & Brewer 1937		Verhoek & Marshall 1939		Burrows 1946		Stull 1947	
ebulliometry		static and dynamic methods		ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
111.3	106.7	59.7	0.237	147	133.3	216.2	2666
122.5	120.0	64.7	0.393	172	533.3	235.8	5333
132.0	133.3	65.0	0.409	25	0.00253*	247.8	7999
134.5	120.0	69.7	0.612		*extrapolated	263.7	13332
137.2	133.32	70.0	0.601			287.0	26664
138.0	133.32	74.6	0.981			313.5	53329
141.0	146.7	75.0	1.076			340.0	101325
141.2	146.7	75.0	0.904				
144.8	160.0	85.0	2.880			mp/°C	—
145.4	146.7	85.0	2.520				
147.5	173.3	85.0	2.520				
148.0	160.0	95.0	6.040				
149.5	173.3						
150.0	186.7						
151.0	173.3	eq. 1	P/microns				
153.5	200.0	A	15.589				
162.9	280.0	B	5122				
164.4	293.3						
167.2	373.3	$\Delta H_v = 98.07$ kJ/mol					
168.0	373.3						
168.6	386.6						
171.8	426.6						
176.3	546.6						
bp/°C	340.7						

2.

Small et al. 1948		Birks & Bradley 1949		Hammer & Lydersen 1957		Franck 1969	
effusion		effusion		vapor-liquid equilibrium		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
exptl data presented in graph		19.9	0.001907	125.7	32.0	86.5	1.53
		23.0	0.002733	131.55	49.06	86.5	1.63
eq. 2	P/mmHg	25.0	0.003640	139.21	73.86	86.5	1.76
A	11.75	30.0	0.006666	147.02	120	105.5	9.42
B	4871	35	0.01180	156.70	205	105.6	9.88
measured pressure range:		40	0.02106	158.89	228	105.5	10.5
0.05 to 0.001 mmHg		43	0.02933	162.12	277	125.5	37.8
$\Delta H_v = 93.30$ kJ/mol		43.5	0.02959	172.76	480	125.5	36.9
		44	0.03346	180.18	671	125.5	34.9
for redistilled tech. grade				180.36	667	144.5	136.0
eq. 2	P/mmHg	eq. 2	P/mmHg	186.87	921	144.5	109.0
A	11.86	A		195.88	1353	144.5	103.0
B	4875	B		202.05	1739		
$\Delta H_v = 93.30$ kJ/mol		C					

(Continued)

TABLE 15.1.3.6.1 (Continued)

Small et al. 1947		Birks & Bradley 1949		Hammer & Lydersen 1957		Franck 1969	
effusion		effusion		vapor-liquid equilibrium		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
<div>Werner 1952</div> <div>dew-point/tensimeter method</div> <div>t/°C</div> <div>P/Pa</div>				eq. 5	P/kPa	OECD 1981	
				A	6.439	vapor pressure balance	
				B	1011	t/°C	P/Pa
				C	720000	10	6.5×10^{-4}
						20	2.3×10^{-3}
exptl data presented in graph				In Boublik et al. 1984		30	7.8×10^{-3}
				A	5.76561	40	2.4×10^{-2}
				B	1744.128	50	7.0×10^{-2}
				C	113.731		
				bp/°C	188.880		
eq. 2	P/mmHg						
A	11.008						
B	2872						
C	176.5						
temp range: 70–170°C							

3.

Hales et al. 1981

transpiration-GC analysis							
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
collection		continued		continued		overall best fit equation:	
39.89	0.02398	80.02	1.162	19.90	2.064×10^{-3}	eq. 5a	P/Pa
39.92	0.02333	79.95	1.089	20.0	2.065×10^{-3}	A	21.5178
39.92	0.02273	99.93	5.335	30.1	7.252×10^{-3}	B	8739.43
39.92	0.02321	100.2	5.648	30.15	7.428×10^{-3}	C	330691
60.18	0.1917	99.94	5.833	40.7	0.02461		
60.03	0.1734	for small saturator		60.01	0.1826		
60.06	0.1858	19.85	0.002224	79.96	1.130		
60.06	0.1779	19.90	0.002160	79.92	1.112		
60.16	0.1842	30.11	0.007276	100.09	5.798		
79.98	1.104	30.13	0.007481				
79.96	1.099	60.27	0.1996				

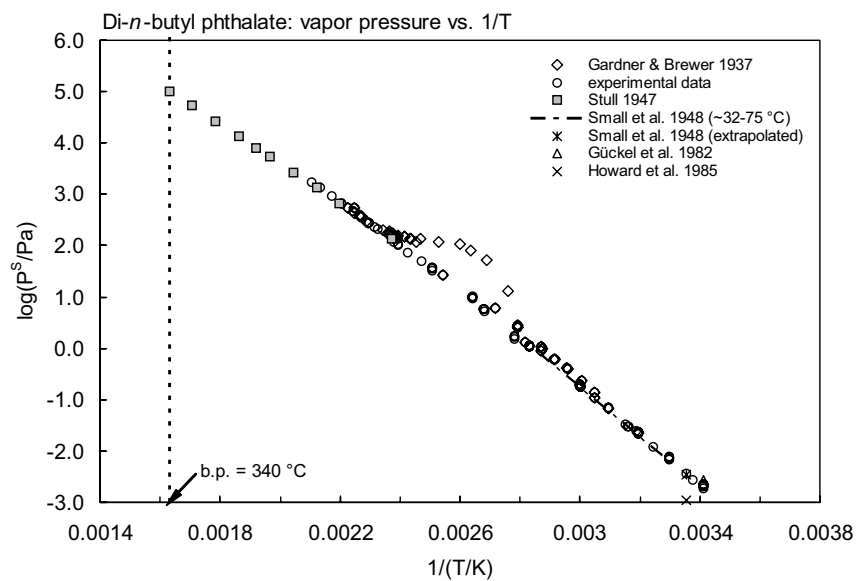
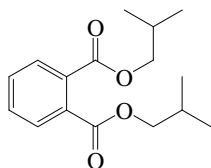


FIGURE 15.1.3.6.2 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-butyl phthalate.

15.1.3.7 Di-isobutyl phthalate (DIBP)



Common Name: Di-isobutyl phthalate

Synonym: DIBP

Chemical Name: phthalic acid diisobutyl ester, bis(2-methylpropyl)ester, 1,2-benzenedicarboxylic acid

CAS Registry No: 84-69-5

Molecular Formula: $C_{16}H_{22}O_4$

Molecular Weight: 278.344

Melting Point ($^{\circ}C$):

-58 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

296.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.040 (Fishbein & Albro 1972)

1.049 ($15^{\circ}C$, Weast 1982-83)

Molar Volume (cm^3/mol):

347.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

100 (Fishbein & Albro 1972)

6.20 (shake flask-nephelometry, Hollifield 1979)

20.3 (Leyder & Boulanger 1983)

20.0; 5.1, 9.6 (recommended; calculated-QSAR, Staples et al. 1997)

21.6 (calculated-UNIFAC, Thomsen et al. 1999)

9.90 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

2.4×10^{-4} , 0.0773 (calculated-QSAR, Staples et al. 1997)

0.00473 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.0185 (recommended, Staples et al. 1997)

0.133 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.11 (shake flask, Leyder & Boulanger 1983)

4.43 (calculated-QSAR, Matthiessen et al. 1992)

4.11 (quoted and recommended, Sangster 1993)

4.11 (recommended, Hansch et al. 1995)

4.11; 4.31, 4.46 (recommended; calculated-QSAR, Staples et al. 1997)

4.46 (calculated-UNIFAC, Thomsen et al. 1999)

4.27 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

3.10 (calculated-QSAR, fish, Matthiessen et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.14 (calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
3.01 (suspended solids, Staples et al. 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} = 0.6\text{--}6.0$ d (calculated, Staples et al. 1997)

$k_{OH} = 9.280 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.89$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003).

Hydrolysis:

$k(\text{second-order alkaline}) = (1.4 - 0.2) \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C in water (Wolfe et al. 1980b)

Biodegradation: degradation $t_{1/2} = 3.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Aerobic biodegradation in aquatic environments, first order $k = 0.8 \text{ d}^{-1}$ with $t_{1/2} = 0.87$ d in river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.134 \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.0114 \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: atmospheric photooxidation half-life of $0.6\text{--}6.0$ d (calculated, Staples et al. 1997).

photodegradation $t_{1/2} = 0.89$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 0.87$ d in river water (Peterson & Staples 2003)

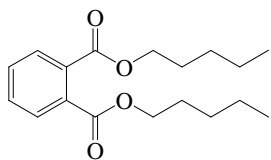
Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 3.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

15.1.3.8 Dipentyl phthalate (DPP)



Common Name: Dipentyl phthalate

Synonym: DPpP, di-*n*-amyl phthalate

Chemical Name: dipentyl phthalate, phthalic acid diphenyl ester, 1,2-benzenedicarboxylic acid diphenyl ester

CAS Registry No: 131-18-0

Molecular Formula: C₁₈H₂₆O₄

Molecular Weight: 306.397

Melting Point (°C):

< -54.5 (Stephenson & Malanowski 1987)

Boiling Point (°C):

342 (Stephenson & Malanowski 1987)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

299.8 (16°C, Stephenson & Malanowski 1987)

391.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

99.16 (Small et al. 1948)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

0.082 (shake flask-nephelometry, Hollifield 1979)

0.1–0.8 (shake flask-GC, Leyder & Boulanger 1983)

0.522, 1.69 (quoted, calculated-UNIFAC, Thomsen et al. 1999)

1.30 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

5.68×10^{-4} (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log (P/\text{mmHg}) = 12.04 - 5191/(T/K)$; temp range 55–102°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion, data presented in graph, Small et al. 1948) (See figure at the end of this section.)

0.0014 (20°C, extrapolated, tensimeter, measured range 63–111°C, Perry & Weber 1949)

$\log (P/\mu\text{mHg}) = 13.57 - 4560/(T/K)$; temp range 63–111°C (pendulum-tensimeter method, Perry & Weber 1949)

5.68×10^{-4} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 11.165 - 5191/(T/K)$; temp range 303–500 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

0.00128 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.302 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{ow}:

4.85 (shake flask, Leyder & Boulanger 1983; quoted, Sangster 1993, Hansch et al. 1995)

5.33 (calculated-UNIFAC, Thomsen et al. 1999)

5.12, 5.62 (calculated-QSPR, quoted lit., Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.03 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 9.0$ d by microorganisms (*Pseudomonas acidovorans* 256-1) from soil or waste water at 30°C (Kurane et al. 1977);

rate constant $k = (9.12 \pm 1.51) \times 10^{-2} \text{ min}^{-1}$ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979).

aerobic biodegradation in aquatic environments, first order $k = 1.3 \text{ d}^{-1}$ with $t_{1/2} = 5.3$ d in river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: biodegradation $t_{1/2} = 5.3$ d in aerobic aquatic environments (Peterson & Staples 2003)

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 9.0$ d by microorganisms (*Pseudomonas acidovorans* 256-1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

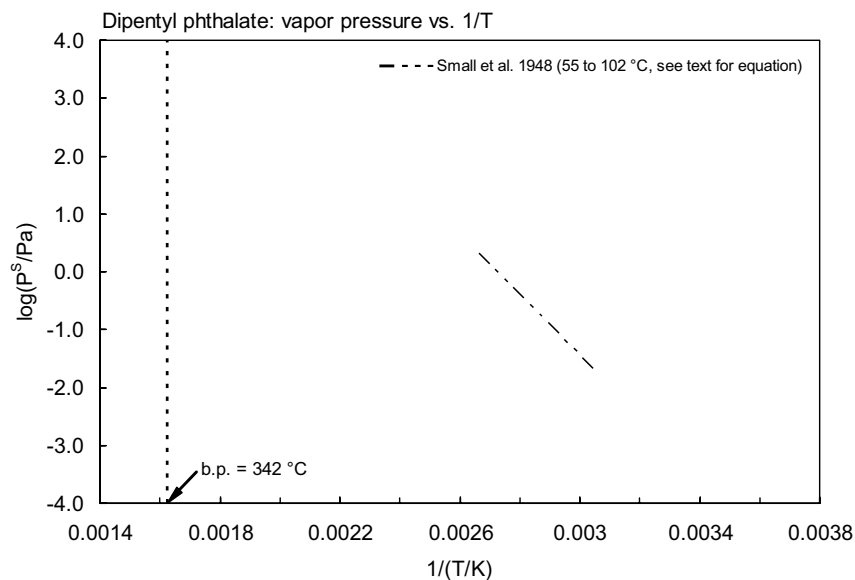
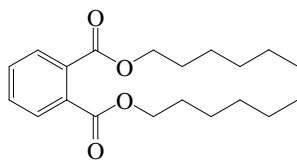


FIGURE 15.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for dipentyl phthalate.

15.1.3.9 Di-*n*-hexyl phthalate (DHP)

Common Name: Di-*n*-hexyl phthalate

Synonym: DHP, DnH(6)P

Chemical Name: Di-*n*-hexyl phthalate, dihexyl ester, 1,2-benzenedicarboxylic acid

CAS Registry No: 84-75-3, 68515-50-4

Molecular Formula: $C_{20}H_{30}O_4$, $C_6H_4[COOCH_2(CH_2)_4CH_3]_2$

Molecular Weight: 334.450

Melting Point ($^{\circ}C$):

-27.4 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

0.990 (Fishbein & Abro 1972)

Molar Volume (cm^3/mol):

227.8 ($20^{\circ}C$, calculated-density)

436.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

102.9 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

insoluble (Fishbein & Abro 1972)

0.24 (shake flask-HPLC/UV, Howard et al. 1985)

0.05; 0.19, 0.049 (recommended; calculated-QSAR, Staples et al. 1997)

0.046 (shake flask-GC, Ellington 1999)

0.47 (calculated-UNIFAC method, Thomsen et al. 1999)

0.159 (calculated-QSPR, Cousins & Mackay 2000)

0.94, 0.52, 0.38 (10, 25, $35^{\circ}C$, shake flask-surface tension measurement, Thomsen et al. 2001) (See figure at the end of this section.)

0.070 ($20^{\circ}C$, shake flask-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 11.98 - 5381/(T/K)$; temp range 72 – $112^{\circ}C$ or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, data presented in graph, Small et al. 1948) (See figure at the end of this section.)

667 (at $210^{\circ}C$, Fishbein & Abro 1972)

1.03×10^{-3} (Antoine eq., interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = -1.01167 - 1483.636/(T/K)$; temp range 288 – 303 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 11.105 - 5382/(T/K)$; temp range 343 – 387 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = -9.785 - 4805/(T/K)$; temp range 453 – 533 K (Antoine eq.-III for liquid, Stephenson & Malanowski 1987)

1.90×10^{-3} (gas saturation-GC, Howard et al. 1985)

0.267 (quoted, Giam et al. 1994)

0.67; 2.53×10^{-6} , 1.6×10^{-3} (recommended; calculated-QSAR, Staples et al. 1997)

0.000345 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

4.46	(recommended, Staples et al. 1997)
0.726	(calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

5.65–5.91	(HPLC-RT correlation, Howard et al. 1985)
5.80	(quoted value of Howard et al. 1985, Sangster 1993)
5.80	(Hansch et al. 1995)
6.30; 6.57, 6.67	(recommended; calculated-QSAR, Staples et al. 1997)
6.20	(calculated-UNFAC, Thomsen et al. 1999)
6.00	(calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

9.53	(calculated-QSPR, Cousins & Mackay 2000)
------	--

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

4.72	(soil/sediment, Staples et al. 1997)
------	--------------------------------------

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} = 0.4\text{--}4.0$ d (calculated, Staples et al. 1997).

$k_{\text{OH}} = 14.929 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.55$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: rate constant $k = (6.86 \pm 0.23) \times 10^{-2} \text{ min}^{-1}$ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979);
primary biodegradation rate constant $k = 0.241 \text{ d}^{-1}$ and $t_{1/2} = 2.93$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} = 0.4\text{--}4.0$ d (calculated, Staples et al. 1997).

Photodegradation $t_{1/2} = 0.55$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: primary biodegradation rate constant $k = 0.241 \text{ d}^{-1}$ and $t_{1/2} = 2.93$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

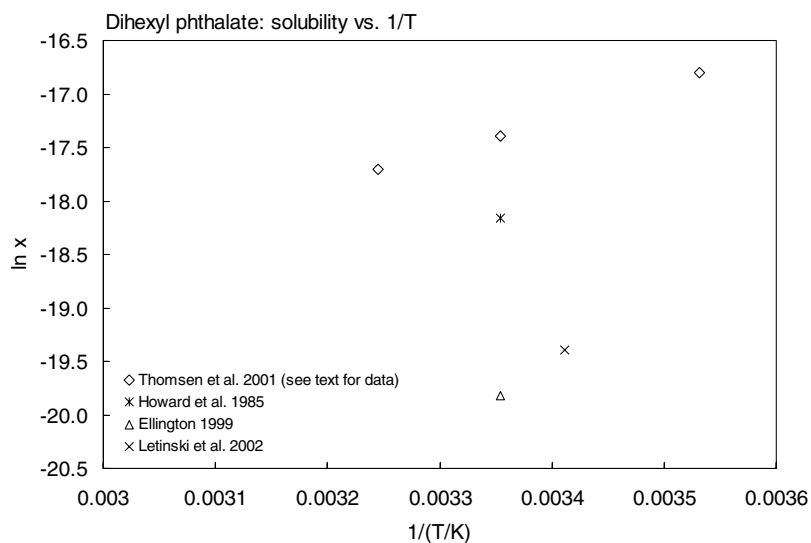


FIGURE 15.1.3.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for dihexyl phthalate.

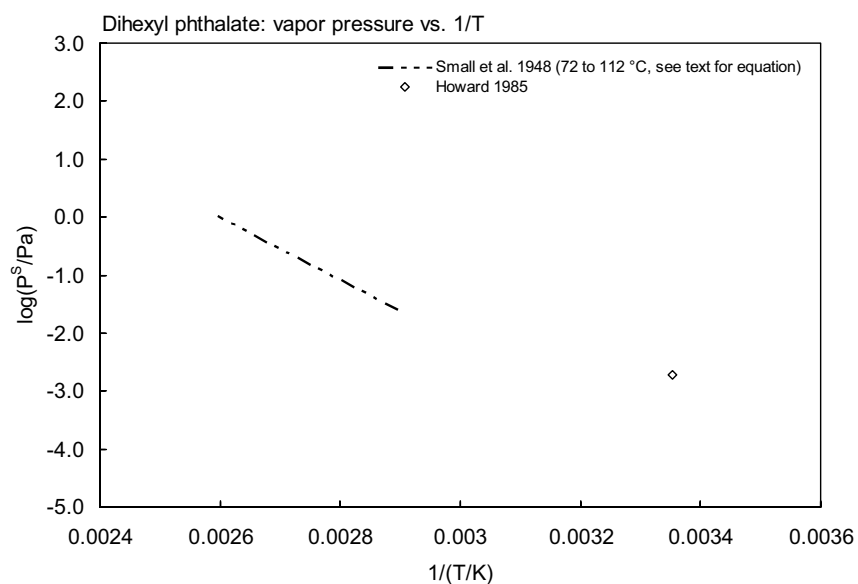
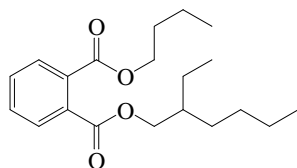


FIGURE 15.1.3.9.2 Logarithm of vapor pressure versus reciprocal temperature for dihexyl phthalate.

15.1.3.10 Butyl-2-ethylhexyl phthalate (BOP)

Common Name: Butyl-2-ethylhexyl phthalate

Synonym: BEHP, BOP

Chemical Name: Butyl-2-ethylhexyl phthalate

CAS Registry No: 85-69-8

Molecular Formula: $C_{20}H_{30}O_4$, $(C_4H_9OOC)C_6H_4(COOCH_2CH(C_2H_5)(CH_2)_3CH_3)$

Molecular Weight: 333.450

Melting Point ($^{\circ}C$):

-37 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

446.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

< 1.0 (shake flask-HPLC/UV spec., Howard et al. 1985)

0.11; 0.02 (recommended; calculated-QSAR, Staples et al. 1997)

0.075 (calculated-UNIFAC, Thomsen et al. 1999)

0.385 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

1.47×10^{-5} ; 3.2×10^{-3} , 0.016 (recommended; calculated-QSAR, Staples et al. 1997)

5.37×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0405 (recommended, Staples et al. 1997)

0.466 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.93 (av. from OECD, Howard et al. 1985)

3.70–7.88 (calculated-HPLC-RT, Howard et al. 1985)

6.28; 6.5 (recommended, calculated-QSAR, Staples et al. 1997)

6.20 (calculated-UNIFAC, Thomsen & Carlsen 1998)

5.64 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.37 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

6.30 (suspended solids, Staples et al. 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photolysis rate $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a)Oxidation: atmospheric photooxidation $t_{1/2} = 0.4\text{--}4.0 \text{ d}$ (calculated, Staples et al. 1997).

Hydrolysis:

 $k(\text{second-order alkaline}) = (1.1 \pm 0.1) \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ for pH 10–12 at 30°C, with $t_{1/2}(\text{calc}) = 2000 \text{ yr}$ at pH 7 (calculated as per Radding et al. 1977, Callahan et al. 1979) $k(\text{acid catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1}$, $k(\text{second order alkaline}) = 0.4 \text{ M}^{-1} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a) $k(\text{second-order alkaline}) = (1.1 \pm 0.1) \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C in water with $t_{1/2} = 100\text{--}2000 \text{ yr}$ (Wolfe et al. 1980b)Biodegradation: primary biodegradation rate constant $k = 0.153 \text{ d}^{-1}$ and $t_{1/2} = 4.55 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

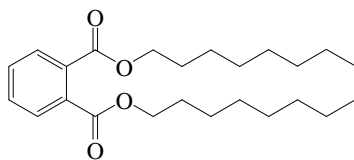
Air: atmospheric photooxidation $t_{1/2} = 0.4\text{--}4.0 \text{ d}$ (calculated, Staples et al. 1997).Surface water: hydrolysis $t_{1/2} = 100\text{--}2000 \text{ yr}$ (Wolfe et al. 1980b; Callahan et al. 1979);primary biodegradation rate constant $k = 0.153 \text{ d}^{-1}$ and $t_{1/2} = 4.55 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.11 Di-*n*-octyl phthalate (DOP)

Common Name: Di-*n*-octyl phthalate

Synonym: di-*n*-octyl phthalate, DOP, *o*-benzenedicarboxylic acid dioctyl ester, *n*-dioctyl phthalate, octyl phthalate, dioctyl-*o*-benzenedicarboxylate

Chemical Name: di-*n*-octyl phthalate

CAS Registry No: 117-84-0

Common Molecular Formula: $C_{24}H_{38}O_4$, $C_6H_4(COOC_8H_{17})_2$

Molecular Weight: 390.557

Melting Point ($^{\circ}C$):

-25.0 (Patty 1963; Fishbein & Albro 1972; Callahan et al. 1979; Mabey et al. 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

220.0 (Patty 1963; Fishbein & Albro 1972; Callahan et al. 1979; Mabey et al. 1982)

Density (g/cm^3 at $20^{\circ}C$):

0.978 (Fishbein & Albro 1972; Ellington 1999)

Molar Volume (cm^3/mol):

399.3 ($20^{\circ}C$, calculated-density)

524.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

50.0	($20^{\circ}C$, Fishbein & Albro 1972)
3.0	(shake flask-GC, Wolfe et al. 1979)
3.0	(shake flask-GC, Wolfe et al. 1980a,b)
0.285	($24^{\circ}C$, tech. grade, Verschueren 1983)
0.022	(generator column-HPLC/UV, DeFoe et al. 1990)
0.020, 0.040	(synthesized phthalates by turbidity inflection-HPLC/UV, DeFoe et al. 1990)
1.96	(calculated-molar volume, Wang et al. 1992)
0.0005	(recommended, Staples et al. 1997)
0.00051; 0.00049	(shake flask: slow stirring; no-stirring, GC/FID, Ellington 1999)
0.0092	(calculated-UNIFAC method, Thomsen et al. 1999)
0.0249	(calculated-QSPR, Cousins & Mackay 2000)
0.00040	($20^{\circ}C$, shake flask-GC/MS, Letinski et al. 2002)
0.00040, 0.00042	(QSAR estimates-SPARC model, WSKOWWIN model, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.21×10^{-6}	($20^{\circ}C$, tensimeter, extrapolated, measured range 113 – $162^{\circ}C$, Perry & Weber 1949)
$\log(P/\mu mHg) = 14.68 - 5620/(T/K)$; temp range 113 – $162^{\circ}C$ (tensimeter, Perry & Weber 1949)
0.0187	(estimated by analogy to Henry's law constant, Mabey et al. 1982)
2.92×10^{-5}	(extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log(P_L/kPa) = 9.897 - 5197.4/(T/K)$; temp range: 423 – 523 K, (Antoine eq., Stephenson & Malanowski 1987)
1.33×10^{-5}	(recommended, Staples et al. 1997)
2.52×10^{-5}	(calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

0.557	(calculated-P/C, Wolfe et al. 1980a)
1.722	(calculated-P/C, Mabey et al. 1982)
0.0297	(quoted from WERL Treatability Data, Ryan et al. 1988)

- 10.435 (selected, Staples et al. 1997)
 0.0249 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 9.2 (calculated as per Leo et al. 1971, Callahan et al. 1979)
 9.2 (calculated, Wolfe et al. 1979)
 8.06 (HPLC-RT correlation; McDuffie 1981)
 8.92 (calculated-CLOGP for synthesized phthalate, DeFoe et al. 1990)
 5.22 (shake flask, $\log P$ database, Hansch & Leo 1987)
 8.06 (recommended, Staples et al. 1997)
 6.99 (calculated-UNIFAC method, Thomsen et al. 1999)
 7.73 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 10.53 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

- 2.82, 3.97, 0.064, 3.72, 2.64 (in lab. model ecosystem after 3 d: alga, daphnia, mosquito fish, mosquito larvae, snails, Sanborn et al. 1975)
 4.45, 3.41, 3.97, 3.97, 4.13 (in lab. model ecosystem after 33 d: alga, daphnia, mosquito fish, mosquito larvae, snails, Sanborn et al. 1975)
 3.46 (bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
 8.59 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.28 (calculated, Wolfe et al. 1980a)
 9.56 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 7.91 (sediment, calculated- K_{OW} , Pavlou & Weston 1983, 1984)
 7.60 (calculated- K_{OW} , Kollig 1993)
 6.30 (suspended solids, calculated- K_d assuming a 0.1 org. carbon fraction, Staples et al. 1997)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photolysis rate $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a)

Oxidation: $k = 18 \text{ M s}^{-1}$, free radical oxidation rate constant in an aquatic environment (Wolfe et al. 1980a)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1.4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

photooxidation $t_{1/2} = 4.5\text{--}44.8 \text{ h}$ in air, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

photooxidation $t_{1/2} = 0.3\text{--}3.0 \text{ d}$ from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)

$k_{OH} = 20.581 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.40 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2} = 4 \text{ months to } 100 \text{ yr}$ at pH 8 and 30°C (Wolfe et al. 1980a)

$k(\text{acid catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1}$, $k(\text{second order alkaline}) = 59 \text{ M}^{-1} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a)

$k(\text{base}) = 7.4 \text{ M}^{-1} \text{ h}^{-1}$ at pH 7 and 25°C (Ellington et al. 1987)

$t_{1/2} = 107 \text{ yr}$ at pH 7, $t_{1/2} = 1 \text{ yr}$ at pH 9 and 25°C (Howard et al. 1991; selected, Staples et al. 1997).

Biodegradation: the pseudo first-order degradation rate constant $k = 0.14 \text{ d}^{-1}$ corresponding to $t_{1/2} = 5 \text{ d}$ in a model ecosystem (Sanborn et al. 1975);

degradation $t_{1/2} = 8 \text{ d}$ by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

rate constant $k \sim (1.57 \pm 0.17) \times 10^2 \text{ min}^{-1}$ from retention times of reverse phase chromatography (estimated, Urushigawa & Yonezawa 1979);

microbial degradation rate constant $k = 2 \times 10^{-4} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a)

significant degradation with gradual adaptation from 7 to 21 d in an aerobic environment with a rate $k < 0.5 \text{ d}^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);

biodegradation rate constant $k = 7.4 \times 10^{-9} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{d}^{-1}$ at 30°C in water (Scow 1982);

aqueous aerobic $t_{1/2} = 168\text{--}672 \text{ h}$, based on unacclimated and acclimated aqueous screening test data; aqueous anaerobic $t_{1/2} = 4320\text{--}8760 \text{ h}$, based on acclimated anaerobic screening test data (Howard et al. 1991);

rate constant $k = 0.0014 \text{ h}^{-1}$ with $t_{1/2} = 513.4 \text{ h}$ for microbial degradation by anaerobic sludge (Wang et al. 2000)

aerobic biodegradation in aquatic environments, first order $k = 0.7 \text{ d}^{-1}$ with $t_{1/2} = 1.0 \text{ d}$ in river water (Peterson & Staples 2003)

anaerobic biodegradation, first order rate $k = 0.006\text{--}0.0336 \text{ d}^{-1}$ with $t_{1/2} = 115\text{--}20.6 \text{ d}$ in undiluted digester sludge of different DOP concn, batch incubation (Peterson & Staples 2003)

Biotransformation: $k = 3.1 \times 10^{-10} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a);

microbial transformation $k = (3.7 \pm 0.6) \times 10^{-13} \text{ L} \cdot \text{organism}^{-1} \cdot \text{h}^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_2 = 3.69 \times 10^{-5} \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 3.16 \times 10^{-6} \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} = 4.5\text{--}44.8 \text{ h}$, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

photodegradation $t_{1/2} = 0.40 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: degradation $t_{1/2} = 5 \text{ d}$ in an aquatic model ecosystem (Sanborn et al. 1975);

overall degradation $t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

biodegradation $t_{1/2} = 1.0 \text{ d}$ in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 336\text{--}8760 \text{ h}$, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

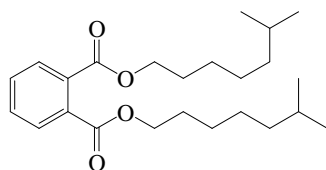
Soil: degradation $t_{1/2} = 8 \text{ d}$ by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

$t_{1/2} = 10\text{--}50 \text{ d}$ via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

degradation $t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

15.1.3.12 Di-isooctyl phthalate (DIOP)



Common Name: Di-isooctyl phthalate

Synonym: DIOP

Chemical Name:

CAS Registry No: 27554-26-3

Molecular Formula: $C_{24}H_{38}O_4$

Molecular Weight: 390.557

Melting Point ($^{\circ}C$):

−4 (Fishbein & Albro 1972)

−46 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

270 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

524.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.09 (shake flask-GC, Howard et al. 1985)

0.001; 0.00024, 0.00081 (recommended; calculated-QSAR, Staples et al. 1997)

2.49×10^{-3} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.55×10^{-4} (dew-point and tensimeter methods, extrapolated from Clausius-Clapeyron eq., Werner 1952)

$\log(P/\text{micron}) = -4829/(T/K) + 13.262$; temp range 70 – $210^{\circ}C$, (exptl. data fitted to the Clausius-Clapeyron eq., Werner 1952)

7.4×10^{-4} (gas saturation method, Howard et al. 1985)

$\log(P/\text{mmHg}) = 24.8803 - 5.5821 \times 10^3/(T/K) - 1.2116 \cdot \log(T/K) - 1.547 \times 10^{-2} \cdot (T/K) + 6.5101 \times 10^{-6} \cdot (T/K)^2$; temp range 260 – 851 K (vapor pressure eq., Yaw et al. 1994)

1.55×10^{-4} , 7.4×10^{-4} , 4.53×10^{-5} (quoted, Staples et al. 1997)

7.5×10^{-4} ; 1.33×10^{-4} , 2.67×10^{-8} , 1.87×10^{-4} (recommended; calculated-QSAR, Staples 1997)

2.52×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.95 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.0; 8.39 (recommended; calculated-QSAR, Staples et al. 1997)

7.73 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.53 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.3\text{--}3.0$ d (Estimated, Staples et al. 1997).

Hydrolysis: aqueous hydrolysis $t_{1/2} \sim 157$ yr (estimated, Staples et al. 1997).

Biodegradation: primary biodegradation rate constant $k = 0.082\text{ d}^{-1}$ and $t_{1/2} = 8.82$ d in an acclimated shake flask
CO₂ evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.3\text{--}3.0$ d (estimated, Staples et al. 1997).

Surface water: primary biodegradation rate constant $k = 0.082\text{ d}^{-1}$ and $t_{1/2} = 8.82$ d in an acclimated shake flask
CO₂ evolution test (Sugatt et al. 1984);

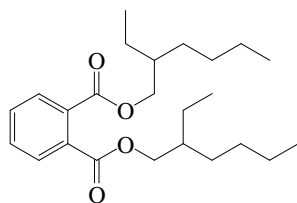
aqueous hydrolysis $t_{1/2} \sim 157$ yr (estimated, Staples et al. 1997).

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.13 *bis*-(2-Ethylhexyl) phthalate (DEHP)

Common Name: Di-(2-ethylhexyl) phthalate

Synonym: DEHP, bis(2-ethylhexyl) phthalate, di-(2-ethylhexyl)orthophthalate, bis(2-ethylhexyl) phthalic acid ester, di-*sec*-octyl phthalate, 2-ethylhexyl phthalate, 1,2-benzenedicarboxylic acid bis(2-ethylhexyl) ester

Chemical Name: bis(2-ethylhexyl) phthalate, di-*sec*-octyl phthalate, 2-ethylhexyl phthalate

CAS Registry No: 117-81-7

Molecular Formula: $C_{24}H_{38}O_4$, $o\text{-C}_6\text{H}_4(\text{COOCH}_2\text{CH}(\text{C}_2\text{H}_5)\text{C}_4\text{H}_9)_2$

Molecular Weight: 390.557

Melting Point ($^{\circ}\text{C}$):

-55.0 (Verschuereen 1983; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

384.0 (Dean 1985; Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at 20°C):

0.9850 (Fishbein & Albro 1972)

0.9843 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

396.1 (20°C , calculated-density, Stephenson & Malanowski 1987)

524.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

107.1, 105.9 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

100 (20°C , Fishbein & Albro 1972)

50.0 (from Monsanto Chemical Co. data sheets, Peakall 1975)

0.60 (Branson 1978; Kenaga & Goring 1980)

0.285 (shake flask-nephelometry on technical grade DEHP, Hollifield 1979)

100 (quoted from Metcalf & Lu 1973, Hollifield 1979; Garten & Trabalka 1983)

2.49 (Neely 1979; quoted, Neely & Blau 1985; Lyman 1985; Elzerman & Coates 1987)

0.40 (shake flask-GC, Wolfe et al. 1979, 1980a, b)

1.16 (solubility in 35 L instant ocean solution, Giam et al. 1980)

0.047 (from OECD 1979/80, Klöpffer et al. 1982)

0.041 (20°C , shake flask-UV, Leyder & Boulanger 1983)

0.34 ± 0.04 (shake flask-HPLC/UV, Howard et al. 1985)

< 100 (quoted, Riddick et al. 1986)

0.27; 0.36 (centrifugation method, turbidity inflection method, DeFoe et al. 1990)

9.8×10^{-6} to 0.633 (lit. values, Sabljic et al. 1990)

0.003 (recommended, Staples et al. 1997)

0.0249 (calculated-QSPR, Cousins & Mackay 2000)

0.017 (22°C , shake flask-surface tension measurement, Thomsen et al. 2001)

0.0019 (20°C , shake flask-GC/MSD, Letinski et al. 2002)

0.00285, 0.00024 (QSAR estimates-SPARC model, WSKOWWIN model, Letinski et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1.45×10^{-5} (20°C, extrapolated, tensimeter, measured range 95–145°C, Hickman et al. 1937)
- $\log(P/\mu\text{mHg}) = 15.116 - 5590/(T/K)$; temp range 95–145°C (Hickman et al. 1937)
- 1.93×10^{-5} (effusion method, extrapolated-Antoine eq., Small et al. 1948)
- $\log(P/\text{mmHg}) = 12.12 - 5590/(T/K)$ (Antoine eq., quoted from Barclay & Butler 1938; Small et al. 1948)
- $\log(P/\text{mmHg}) = 12.47 - 5757/(T/K)$; pressure range 5×10^{-2} to 10^{-4} mmHg (effusion, data presented in graph and Antoine eq., Small et al. 1948)
- 1.51×10^{-5} (20°C, extrapolated, tensimeter, measured range 99–148°C, Perry & Weber 1949)
- $\log(P/\mu\text{mHg}) = 14.62 - 5440/(T/K)$; temp range 99–148°C (pendulum tensimeter method, Perry & Weber 1949)
- $8.26 \times 10^{-6*}$ (measured by dew-point and tensimeter methods, temp range 120–225°C, extrapolated from Antoine eq., Werner 1952)
- $\log(P/\text{micron}) = 12.639 - 3811/(201.2 + t/^{\circ}\text{C})$; temp range 120–225°C (Antoine eq., Dew-Point and Tensimeter methods, data presented in graph, Werner 1952)
- 2.70×10^{-5} (20°C, calculated-Antoine eq., Weast 1972–73)
- 1.73×10^{-5} (submicron droplet evaporation, Chang & Davis 1976)
- 5.81×10^{-5} (36°C, submicron droplet evaporation, Davis & Ray 1977)
- 5.84×10^{-6} (17°C, submicron droplet evaporation, measured range 17–31°C, Ray et al. 1979)
- $\log(P/\text{mmHg}) = 12.729 - 5822/(T/K)$; temp range 17–31°C (submicron droplet evaporation, Ray et al. 1979)
- $6.0 \times 10^{-6*}$, 1.30×10^{-5} (20°C, effusion-vapor pressure balance, gas saturation method, OECD 1981)
- $\log(P/\text{mmHg}) = 10.086 - 5010.357/(T/K)$; temp range 10–50°C (Antoine eq., gas saturation, OECD 1981)
- $\log(P/\text{mmHg}) = 13.243 - 6035.017/(T/K)$; temp range 80–120°C (Antoine eq., effusion, OECD 1981)
- 5.50×10^{-6} (20°C, estimated-evaporation rate, Dobbs & Cull 1982)
- 7.01×10^{-8} (20°C, gas saturation, measured range 120–140°C, Potin-Gauthier et al. 1982)
- $\log(P/\text{mmHg}) = 18.408 - 8112.265/(T/K)$; temp range 120–140°C (Potin-Gauthier et al. 1982)
- 0.00293, 1.87×10^{-6} , 7.47×10^{-4} (estimation-structure based methods, Tucker et al. 1983)
- $8.6 \pm 6.6 \times 10^{-4}$ (gas saturation-HPLC/UV, Howard et al. 1985)
- 70, 700 (literature values, Riddick et al. 1986)
- 5.08×10^{-5} (extrapolation-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 11.8564 - 6416.2/(36.74 + T/K)$; temp range 373–660 K (Antoine eq., Stephenson & Malanowski 1987)
- $(1.20\text{--}2.40) \times 10^{-5}$ (quoted from OECD interlaboratory studies, Hinckley et al. 1990)
- 1.90×10^{-5} (GC-RT correlation, Hinckley et al. 1990)
- $1.2 \times 10^{-4*}$ (40°C, OECD Vapour Pressure Curve Guideline 104, temp range 40–80°C, OECD 1993)
- $\log(P/\text{mmHg}) = -0.7422 - 7.2012 \times 10^3/(T/K) + 9.9887 \cdot \log(T/K) - 2.2697 \times 10^{-2} \cdot (T/K) + 8.2181 \times 10^{-6} \cdot (T/K)^2$; temp range 350–886 K (vapor pressure eq., Yaw et al. 1994)
- $1.50 \times 10^{-4*}$ (40°C, Knudsen effusion with different orifice diameters and variable cell height, measured range 40–80°C, Goodman 1997)
- $\log(P/\text{Pa}) = 14.90 - 5911/(T/K)$; temp range 40–80°C (Knudsen effusion, Goodman 1997)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.0446 (calculated-P/C, Wolfe et al. 1980a)
- 1.1140 (calculated, Lyman et al. 1982)
- 0.0304 (20–25°C, calculated-P/C, Mabey et al. 1982)
- 0.0263, 3.14 (calculated-P/C, calculated-group contribution, Tucker et al. 1983)
- 0.0042 (estimated-P/C, Lyman 1985)
- 0.101 (estimated as per Hine & Mookerjee 1975, Lyman 1985)
- 0.0041 (calculated-P/C, Mackay 1985, Neely & Blau 1985)
- 0.0297 (quoted from WERL Treatability Data, Ryan et al. 1988)
- 1.4940 (calculated-P/C, Meylan & Howard 1991)
- 1.1970 (estimated-bond contribution, Meylan & Howard 1991)
- 1.7324 (selected, Staples et al. 1997)
- 3.95 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW} :

3.58	(Lu & Metcalf 1975)
4.20	(Mayer 1976)
5.30	(Hirzy et al. 1978)
8.73	(calculated, Wolfe et al. 1979)
5.11, 4.66–5.45	(shake flask method: mean, range, OECD 1981)
7.86	(HPLC-extrapolated from alkylbenzenes, Harnish et al. 1983)
5.03	(shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
9.64	(quoted lit. calculated value, Leyder & Boulanger 1983)
7.94	(HPLC-RT correlation, Howard et al. 1985)
7.80, 8.90	(HPLC-RT correlation, TLC-RT, Klein et al. 1988)
7.453 \pm 0.061	(slow-stirring-GC, De Bruijn et al. 1989)
5.22	(shake flask method, Brooke et al. 1990)
7.86, 9.68	(HPLC method, calculated, Brooke et al. 1990)
7.137 \pm 0.153	(stir-flask method by BRE, Brooke et al. 1990)
7.453 \pm 0.061	(stir-flask method by RITOX, Brooke et al. 1990)
7.88	(recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} :

10.53	(calculated-QSPR, Cousins & Mackay 2000)
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Bioconcentration Factor, log BCF:

2.11	(fish, Metcalf et al. 1973)
5.03	(mosquito larvae, Metcalf et al. 1973)
4.13, 3.49, 3.72, 3.36, 2.36	(scud, midge larvae, waterflea, mayfly, sowbug, Sanders et al. 1973)
3.56, 2.54, 2.62, 2.76, 2.66	(scud, midge, waterflea, mayfly, fathead minnow, 14-d exposure, Mayer & Sanders 1973)
3.14	(fathead minnow, 28-d exposure, Mayer & Sanders 1973)
2.76	(fathead minnow, 56-d exposure, Mayer 1976)
2.93	(fathead minnow, Veith et al. 1979)
2.90, 2.15	(fathead minnow, Branson 1978)
2.06	(bluegill sunfish, Barrows et al. 1980)
–1.92	(adipose tissue of female Albino rats, Geyer et al. 1980)
3.95	(bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
0.84–1.05, 1.01–1.22, 1.03–1.13	(oyster, shrimp, fish, Wofford et al. 1981)
1.04	(oyster, Wofford et al. 1981; quoted, Zarogian et al. 1985)
2.93, 2.88	(fish: quoted, calculated- K_{OW} , Mackay 1982)
2.32	(<i>Daphnia magna</i> , Brown & Thompson 1982a)
3.37, 3.42, 3.40	(mussel <i>Mytilus edulis</i> , Brown & Thompson 1982b)
8.36	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
2.49, 2.11	(fish: flowing water, microcosm conditions, Graten & Trabalka 1983)
3.73, 3.57	(alga <i>Chlorella</i> , calculated- K_{OW} , Geyer et al. 1984)
2.80	(sheephead minnows, predicted-pharmacokinetic model, Karara & Hayton 1984)
2.66, 3.73, 3.48	(golden orfe, algae, activated sludge, Freitag et al. 1982)
1.60, 3.73, 3.48	(golden ide, algae, activated sludge, Freitag et al. 1985)
2.96, 2.87	(oyster, estimated values, Zarogian et al. 1985)
2.96, 2.87	(sheephead minnows, estimated values, Zarogian et al. 1985)
2.76	(quoted, Isnard & Lambert 1989)
0.204–1.71	(rainbow trout, BCF to decline as body wt. increased, Tarr et al. 1990)
2.94	(fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

4.0–5.0	(soil, calculated values, Kenaga 1980; Wolfe et al. 1980a)
4.756	(sediment-water, calculated- K_{OW} and S, Wolfe et al. 1980a)
9.301	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)

- 4.31, 5.27, 4.90, 4.98 (estimated- K_{OW} , Karickhoff 1985)
 4.24, 5.06 (estimated-S, Karickhoff 1985)
 5.10 (best estimate, expected at low sediment concn. of $< 10^{-4}$ /mL, Karickhoff 1985)
 5.00 (soil/sediment, Neely & Blau 1985)
 4.94 (Broome County soil in New York, shake flask-GC, Russell & McDuffie 1986;)
 5.22 (soil, calculated- MCI χ and fragment contribution, Meylan et al. 1992)
 2.60 (activated carbon, calculated-MCI χ , Blum et al. 1994)
 7.13 (calculated- K_{OW} , Kolliig 1993)
 4.34, 6.00 (suspended solids, calculated- K_d assuming a 0.1 org. carbon fraction, Staples et al. 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization: calculated evaporation rate $k = 0.00052$ cm/h corresponding to $t_{1/2} = 132600$ h for a pond of 1 m deep (Branson 1978).
- Photolysis: rate constant for direct photolysis $k = 2 \times 10^{-4}$ h $^{-1}$ in natural water (Wolfe et al. 1980a);
 $t_{1/2} \sim 143$ d in water is estimated to be 143 d (Wolfe et al. 1980a; quoted, Howard 1989);
 atmospheric $t_{1/2} = 3500$ –4800 h and aqueous $t_{1/2} = 3500$ –4800 h, based on measured rate of aqueous photolysis for DMP (Howard 1991).
 Aqueous photolysis $k = 0.9$ h $^{-1}$ and $t_{1/2} = 0.75$ h (Jin et al. 1999, quoted, Peterson & Staples 2003)
- Oxidation: the free radical oxidation rate constant $k = 18$ M \cdot s $^{-1}$ (Wolfe et al. 1980b);
 photooxidation $t_{1/2} = 44$ –584 d in water, based on estimated rate constant for the reaction with hydroxyl radicals in water (Wolfe et al. 1980; quoted, Howard et al. 1991);
 rate constant $k \ll 360$ M $^{-1}$ ·h $^{-1}$ for singlet oxygen and $k = 7.2$ M $^{-1}$ ·h $^{-1}$ for peroxy radical (Mabey et al. 1982);
 photooxidation $t_{1/2} = 2.9$ –29 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);
 predicted atmospheric photooxidation $t_{1/2} = 0.2$ –2.0 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997).
 $k_{OH} = 21.955 \times 10^{-12}$ cm 3 molecule $^{-1}$ s $^{-1}$ and $t_{1/2} = 0.38$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm $^{-3}$ in air (Peterson & Staples 2003)
- Hydrolysis: second order alkaline hydrolysis rate constant $k = 1.1 \times 10^{-4}$ M $^{-1}$ ·s $^{-1}$ for pH 10–12 at 30°C in water (Wolfe et al. 1979, 1980b; quoted, Callahan et al. 1979);
 $t_{1/2} = 100$ to 2000 yr for hydrolytic degradation alone in the eutrophic lake ecosystem at steady-state increase (Wolfe et al. 1980a);
 $t_{1/2}(\text{calc}) = 2000$ yr at pH 7 in water (calculated per Radding et al. 1977; quoted, Callahan et al. 1979; Howard 1989; Howard et al. 1991);
 $k(\text{exptl.}) = 9.5 \times 10^{-7}$ d $^{-1}$ at pH 7 and 25°C while estimated rate constant $k = 1.46 \times 10^{-6}$ d $^{-1}$ at pH 7 and 30°C (Neely 1985);
 first-order hydrolysis $t_{1/2} = 2000$ yr at pH 7, based on measured base catalyzed hydrolysis rate constant (Howard et al. 1991; selected, Staples et al. 1997).
- Biodegradation: approximately calculated rate constant $k = 0.091$ d $^{-1}$ in pond water plus sediment incubated under aerobic conditions based on time for 50% degradation (Johnson & Lulves 1975; quoted, Klečka 1985);
 estimated biodegradation $t_{1/2} \sim 4$ –5 wk by naturally occurring, mixed microbial populations in river water (Saeger & Tucker 1976);
 degradation $t_{1/2} = 1.3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977);
 rate constant $k = 0.023$ d $^{-1}$ in river water incubated under aerobic conditions (Klečka 1985);
 rate constant $k(\text{mineralization rate divided by initial substrate concn.}) = 0.028 \pm 0.013$ d $^{-1}$ in lake water incubated under aerobic conditions (Subba-Rao et al. 1982; quoted, Klečka 1985);
 $t_{1/2} = 2.0$ –3.0 wk, based on river die-away test data (Hattori et al. 1975; Saeger & Tucker 1976; Wolfe et al. 1980; estimated, Howard 1989);
 $t_{1/2} = 0.8$ d in activated sludge (Saeger & Tucker 1976; estimated, Howard 1989);
 microbial degradation rate constant $k = 4.2 \times 10^{-12}$ mL·organism $^{-1}$ ·s $^{-1}$ (Wolfe et al. 1980a);
 significant degradation with gradual adaptation from 7 to 21 d in an aerobic environment with a rate $k < 0.5$ d $^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);
 aqueous aerobic $t_{1/2} = 120$ –550 h, based on grab sample die-away test data (Schouten et al. 1979 and Johnson & Lulves 1975; estimated, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 980$ –9336 h, based on anaerobic

die-away test data (Howard et al. 1991) and anaerobic aqueous screening studies (Horowitz et al. 1982 and Shelton et al. 1984; estimated, Howard et al. 1991);
mean rate constant $k = 0.136 \text{ d}^{-1}$ corresponding to $t_{1/2} = 5.25 \text{ d}$ in shake flask biodegradation experiment (Sugatt et al. 1984);

more than 90% of initial 3.3 mg/L will be degraded in activated sludge systems in 2–5 d (O'Grady et al. 1985);

greater than 50% loss in microbial degradation in less than 20 d under aerobic conditions, very low under anaerobic conditions in garden soil (Shanker et al. 1985);

readily metabolized in uninoculated Erie slit loam with the absence of nonaqueous-phase liquids (NAPLs) for about 20 d (Efroymson & Alexander 1994)

biphasic microbial mineralization kinetics: $k = 0.0044 \text{ d}^{-1}$ with $t_{1/2} = 158 \text{ d}$ at 5°C , $k = 0.0081 \text{ d}^{-1}$ with $t_{1/2} = 86 \text{ d}$ at 10°C , and $k = 0.0134 \text{ d}^{-1}$ with $t_{1/2} = 52 \text{ d}$ at 20°C in agriculture soil for phase I; and $t_{1/2} = 224 \text{ d}$ at 5°C , $t_{1/2} = 187 \text{ d}$ at 10°C and $t_{1/2} = 73 \text{ d}$ at 20°C in agriculture soil for phase II. Rate $k = 0.0023 \text{ d}^{-1}$ with $t_{1/2} = 301 \text{ d}$ at 5°C , $k = 0.0055 \text{ d}^{-1}$ with $t_{1/2} = 125 \text{ d}$ at 10°C , and $k = 0.0127 \text{ d}^{-1}$ with $t_{1/2} = 55 \text{ d}$ at 20°C in sludge-amended soil for phase I and $t_{1/2} \geq 365 \text{ d}$ at 5°C , $t_{1/2} = 337 \text{ d}$ at 10°C and $t_{1/2} = 150 \text{ d}$ at 20°C in sludge-amended soil for phase II kinetics in laboratory microcosms. At 20°C , aerobic mineralization rate $k = 0.0182 \text{ d}^{-1}$ with $t_{1/2} = 37 \text{ d}$ for phase I, $t_{1/2} = 51 \text{ d}$ for phase II in well-mixed sludge, $k = 0.0058 \text{ d}^{-1}$ with $t_{1/2} = 120 \text{ d}$ for phase I, $t_{1/2} \geq 365 \text{ d}$ for phase II in aggregate sludge, aerobic $k = 0.0127 \text{ d}^{-1}$ with $t_{1/2} = 55 \text{ d}$ for phase I, $t_{1/2} = 150 \text{ d}$ for phase II and anaerobic $k = 0.0023 \text{ d}^{-1}$ with $t_{1/2} = 301 \text{ d}$ for phase I, $t_{1/2} \geq 365 \text{ d}$ for phase II in sludge-amended soil (Madsen et al. 1999).

aerobic biodegradation in aquatic environments, first order $k = 0.023 \text{ d}^{-1}$ with $t_{1/2} = 30 \text{ d}$ in unstirred river water, $k = 0.2 \text{ d}^{-1}$ with $t_{1/2} = 3.5 \text{ d}$ in shaken river water, $k = 1.73 \text{ d}^{-1}$ with $t_{1/2} = 0.4 \text{ d}$ field data, estuarine sediment (Peterson & Staples 2003)

aerobic soil degradation, pseudo-first-order $k = 0.035 \text{ d}^{-1}$ with $t_{1/2} = 2.0 \text{ d}$ in loam; $k = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 69.3 \text{ d}$ in sand; $k = 0.033 \text{ d}^{-1}$ with $t_{1/2} = 21 \text{ d}$ in outdoor lysimeter, loam; $k = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53.3 \text{ d}$ in outdoor lysimeter, sand; $k = 0.12 \text{ d}^{-1}$ with $t_{1/2} = 5.6 \text{ d}$ in garden soil; $k = 0.040 \text{ d}^{-1}$ with $t_{1/2} = 17.3 \text{ d}$ in soil with 2% OC-organic carbon; $k = 0.019 \text{ d}^{-1}$ with $t_{1/2} = 36.5 \text{ d}$ in soil with 3.3% OC; $k = 0.015 \text{ d}^{-1}$ with $t_{1/2} = 46.2 \text{ d}$ in soil with 1.6% OC and $k = 0.012 \text{ d}^{-1}$ with $t_{1/2} = 58 \text{ d}$ in sludge amended loam. For anaerobic degradation, first order rate $k > 0.3 \text{ d}^{-1}$ with $t_{1/2} < 2.3 \text{ d}$ in undiluted digester sludge, batch incubation; $k = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53.3 \text{ d}$ in flood soil; $k = 0.69 \text{ d}^{-1}$ with $t_{1/2} = 1.0 \text{ d}$ field data, sediment (Peterson & Staples 2003)

Biotransformation: $k = 4.2 \times 10^{-12} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a; quoted, Mabey et al. 1982);

microbial transformation $k = (4.2 \pm 0.7) \times 10^{-15} \text{ L} \cdot \text{organism}^{-1} \cdot \text{h}^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$t_{1/2} = 7 \text{ d}$ for elimination of DEHP from fathead minnows (Mayer & Sanders 1973);

fish elimination $t_{1/2} = 6.2$ to 18.3 d with a mean value of 12.2 d after 56 d exposure period (fathead minnows, Mayer 1976);

$k_1 = 76 \text{ mL g}^{-1} \cdot \text{h}^{-1}$ (fish, Branson 1978);

depuration $t_{1/2} = 72 \text{ h}$ (tissues of bluegill sunfish, Barrows et al. 1980).

$k_2 = 3.69 \times 10^{-5} \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 3.16 \times 10^{-6} \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2}$ = half-life of 2.9–29 h, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

Photodegradation $t_{1/2} = 0.38 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} \sim 4$ to 5 wk in river water by naturally occurring, mixed microbial populations (Saeger & Tucker 1976);

$t_{1/2} = 5 \text{ d}$ in a model ecosystem (Verschuere 1983);

$t_{1/2} = 5.25 \text{ d}$ in an acclimated shake flask CO_2 evolution biodegradation experiment (Sugatt et al. 1984)

$t_{1/2} = 120$ – 550 h , based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2}$ = 0.3–30 d in estuarine river water with sediment and river water (Peterson & Staples 2003)

Ground water: $t_{1/2}$ = 240–9336 h, based on unacclimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: degradation $t_{1/2}$ = 1.3 d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977) biodegradation $t_{1/2}$ < 20 d under anaerobic conditions in a garden soil (Shanker et al. 1985);

$t_{1/2}$ = 10–50 d via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

degradation $t_{1/2}$ = 39 d for initial phase, $t_{1/2}$ = 51 d for the late phase in sludge-amended quartz; $t_{1/2}$ = 58 d for initial phase and $t_{1/2}$ = 147 d for sludge-amended soil, $t_{1/2}$ = 58 d for initial phases and $t_{1/2}$ = 84 d in sludge slurry; $t_{1/2}$ = 9 d for initial phases, $t_{1/2}$ = 35 d for late phase in sludge-amended soil + strain SDE-2 (Roslev et al. 1998)

overall $t_{1/2}$ = 120–550 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

degradation by microorganism in biometer systems, $t_{1/2}$ = 66 d in silty sand standard metabolism experiments, $t_{1/2}$ = 102 d corrected standard conditions, $t_{1/2}$ = 170 d in simulated outdoor conditions; $t_{1/2}$ = 20 d in silty loam standard conditions, $t_{1/2}$ = 30 d corrected standard conditions, $t_{1/2}$ = 31 d in simulated outdoor conditions at constant soil moisture and 20°C; degradation by microorganism in outdoor experiments in small lysimeter systems: $t_{1/2}$ = 54 d outdoor fallow and $t_{1/2}$ = 200 d outdoor barley in silty sand, and $t_{1/2}$ = 21 d outdoor fallow, $t_{1/2}$ = 14 d outdoor barley in silty loam (Rüdel et al. 1993)

microbial mineralization $t_{1/2}$ = 158, 86 and 52 d at 5, 10, and 20°C, respectively, in soil; $t_{1/2}$ = 301, 125 and 55 d at 5, 10 and 20°C in sludge-amended soil in phase I degradation kinetics; $t_{1/2}$ = 224, 187 and 73 d at 5, 10, and 20°C, respectively, in soil; $t_{1/2}$ = 365, 337 and 150 d at 5, 10 and 20°C in sludge-amended soil in phase II degradation kinetics. At 20°C, $t_{1/2}$ varies between 77–89 d and 100–127 d for phase I and II, respectively, in sludge-amended soil with different initial DEHP concns. Aerobic $t_{1/2}$ = 37 d and 51 d for phase I and II in well mixed sludge, $t_{1/2}$ = 120 d and > 365 d for phase I and II in aggregate sludge, $t_{1/2}$ = 55 d and 150 d for phase I and II in sludge-amended soil; anaerobic $t_{1/2}$ = 301 d and > 365 d for phase I and II in sludge-amended soil (laboratory microcosms, Madsen et al. 1999)

biodegradation in aerobic soil: $t_{1/2}$ = 2.0 – 69.3 d in various sand, loam, soils with different organic carbon content and sludge amended loam in laboratory and outdoor experiments (Peterson & Staples 2003)

Biota: elimination and degradation $t_{1/2}$ < 4 d after 7 d for water fleas *Daphnia magna* and $t_{1/2}$ = 7 d for fathead minnows (Mayer & Sanders 1973);

fish elimination $t_{1/2}$ = 12.2 d (fathead minnows *Pimephales promelas*, Mayer 1976);

depuration $t_{1/2}$ = 3 d (in tissues of bluegill sunfish continuously for 42-d exposure, Barrows et al. 1980)

depuration $t_{1/2}$ = 38 d from sheephead minnow (Karara & Hayton 1984).

TABLE 15.1.3.13.1

Reported vapor pressures of *bis*(2-ethylhexyl) phthalate (DEHP) at various temperatures and the coefficients for the vapor pressure equations

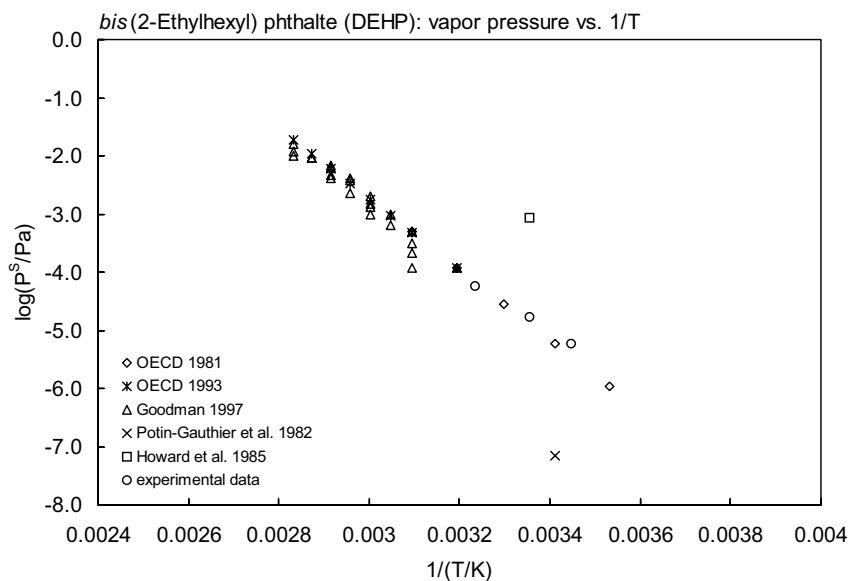
$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

OECD 1981		OECD 1993		Goodman 1997			
effusion/gas saturation		v.p. curve guideline 104		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
effusion-vapor pres. balance				orifice diameter 0.381 mm		orifice diameter 0.0229 mm	
10	1.1×10^{-6}	40	1.2×10^{-4}	50	1.2×10^{-4}	using variable cell height	
20	6.0×10^{-6}	50	4.8×10^{-4}	50	3.1×10^{-4}	50	2.1×10^{-4}
30	2.8×10^{-5}	55	9.3×10^{-4}	55	9.8×10^{-4}	60	9.7×10^{-4}
40	1.2×10^{-4}	60	1.8×10^{-3}	55	6.5×10^{-4}	65	4.1×10^{-3}

(Continued)

TABLE 15.1.3.13.1 (Continued)

OECD 1981		OECD 1993		Goodman 1997			
effusion/gas saturation		v.p. curve guideline 104		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
50	4.9×10^{-4}	65	3.3×10^{-3}	60	2.0×10^{-3}	70	6.8×10^{-3}
		70	5.9×10^{-3}	60	1.3×10^{-3}	75	9.2×10^{-3}
eq. 1	P/Pa	75	0.011	65	3.8×10^{-3}	80	1.0×10^{-2}
A	13.243	80	0.019	65	2.3×10^{-3}	40	1.2×10^{-4}
B	6035.017			70	6.3×10^{-3}	50	4.9×10^{-4}
				70	4.2×10^{-3}	60	1.5×10^{-3}
				75	9.2×10^{-3}	70	4.6×10^{-3}
gas saturation				80	0.012	80	1.6×10^{-2}
10	1.1×10^{-6}	Small et al. 1948					
20	6.0×10^{-6}	effusion method					
30	2.8×10^{-5}	t/°C	P/Pa			eq. 1	P/Pa
40	1.2×10^{-4}					A	14.90
50	4.9×10^{-4}	data presented in graph and				B	5911
		eq. 1	P/mmHg				
eq. 1	P/Pa	A	12.47				
A	10.086	B	5757				
B	5010.357	for pressure range: 0.05 to					
		10^{-4} mmHg					

FIGURE 15.1.3.13.1 Logarithm of vapor pressure versus reciprocal temperature for *bis*(2-ethylhexyl) phthalate.

15.1.3.14 Di(hexyl,octyl,decyl) phthalate

Common Name: Di(hexyl,octyl,decyl) phthalate

Synonym: 610P

Chemical Name:

CAS Registry No: 25724-58-7, 68515-51-5

Molecular Formula: $C_{25}H_{40}O_4$

Molecular Weight: 404.583

Melting Point ($^{\circ}C$):

−4 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

547.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.9 ± 0.5 (shake flask, Howard et al. 1985)

0.05; 0.0004 (recommended; calculated-QSAR, Staples et al. 1997)

8.76×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

6.5×10^{-4} (gas saturation, Howard et al. 1985)

6.5×10^{-4} ; 4.53×10^{-5} , 6.5×10^{-2} (recommended; calculated-QSAR, Staples et al. 1997)

1.31×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.05 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.9–8.61 (HPLC-RT correlation, Howard et al. 1985; quoted, Staples et al. 1997)

7.25; 8.54 (recommended; calculated-QSAR, Staples et al. 1997)

8.17 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.78 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2$ – 4.0 d (estimated, Staples et al. 1997).

Hydrolysis:

Biodegradation: primary biodegradation with a rate constant $k = 0.131$ d^{-1} and $t_{1/2} = 5.30$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}4.0$ d (estimated, Staples et al. 1997).

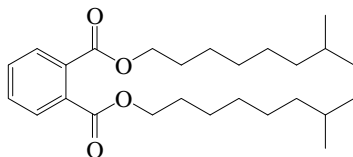
Surface water: primary biodegradation with a rate constant $k = 0.131\text{ d}^{-1}$ and $t_{1/2} = 5.30$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.15 Diisononyl phthalate (DINP)

Common Name: Diisononyl phthalate

Synonym: DINP

Chemical Name:

CAS Registry No: 28553-12-0, 68515-48-0

Molecular Formula: $C_{26}H_{42}O_4$

Molecular Weight: 418.609

Melting Point ($^{\circ}C$):

-48 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

413 (Fishbein & Albro 1972)

Density (g/cm^3 at $20^{\circ}C$):

0.995 (Fishbein & Albro 1972)

Molar Volume (cm^3/mol):

569.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.20 ± 0.1 (shake flask-GC, Howard et al. 1985)

0.20, 0.0006 (quoted, Staples et al. 1997)

< 0.001 ; 7.8×10^{-5} , 2.3×10^{-5} (recommended; calculated-QSAR, Staples et al. 1997)

3.08×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)

6.1×10^{-4} ($20^{\circ}C$, shake flask/slow stirring-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$):

7.2×10^{-5} (gas saturation method, Howard et al. 1985)

6.67×10^{-5} ; 1.33×10^{-8} , 3.07×10^{-5} (recommended; calculated-QSAR, Staples et al. 1997)

6.81×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

9.26 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

> 8.0 ; 9.0, 9.4 (recommended; calculated-QSAR, Staples et al. 1997)

8.60 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

11.03 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

3.27 (*Arca zebra*, Solbakken et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

$k_{OH} = 23.408 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.35$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: primary biodegradation with a rate constant $k = 0.131 \text{ d}^{-1}$ and $t_{1/2} = 5.31$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 848 \text{ mL} \cdot \text{g} \cdot \text{d}^{-1}$ (*Arca zebra*, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)

$k_2 = 0.46 \text{ d}^{-1}$ (*Arca zebra*, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)

$k_2 = 0.02 \text{ d}^{-1}$ (*Diplora strigosa*, 26.5°C, Solbakken et al. 1985; quoted, Staples et al. 1997)

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

Photodegradation $t_{1/2} = 0.35$ h based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: primary biodegradation with a rate constant $k = 0.131 \text{ d}^{-1}$ and $t_{1/2} = 5.31$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

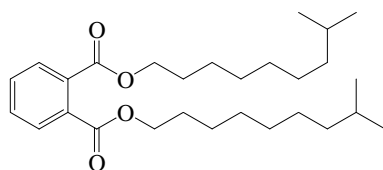
Groundwater:

Sediment:

Soil:

Biota:

15.1.3.16 Di-isodecyl phthalate (DIDP)



Common Name: Di-isodecyl phthalate

Synonym: DIDP

Chemical Name: di-diisodecyl phthalate

CAS Registry No: 26761-40-0, 68515-49-1

Molecular Formula: $C_{28}H_{46}O_4$

Molecular Weight: 446.663

Melting Point ($^{\circ}C$):

- 48 (Stephenson & Malanowski 1987)
- 46 (Staples et al. 1997)
- 50 (Lide 2003)

Boiling Point ($^{\circ}C$):

- 450 (Stephenson & Malanowski 1987)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

- 464.8 (Stephenson & Malanowski 1987)
- 613.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

- < 50 (quoted from Monsanto Chemical Co. data sheets, Peakall 1975)
- 1.19 ± 0.19 (shake flask-GC, Howard et al. 1985)
- 0.28 (shake flask-nephelometry, Hollifield 1979)
- 0.19, 0.28, < 0.00013 (quoted, Staples et al. 1997)
- < 0.001; 2.2×10^{-6} , 7.4×10^{-6} (recommended, calculated-QSAR, Staples et al. 1997)
- 3.81×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)
- 1.7×10^{-4} ($20^{\circ}C$, shake flask/slow stirring-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

- $\log (P_L/kPa) = 14.0158 - 10984/(242.24 + T/K)$, temp range: 371–496 K, (Antoine eq., Stephenson & Malanowski 1987)
- $\log (P/mmHg) = 81.7895 - 7.4225 \times 10^3/(T/K) - 26.916 \cdot \log (T/K) + 1.1502 \times 10^{-2} \cdot (T/K) - 4.353 \times 10^{-14} \cdot (T/K)^2$; temp range 233–723 K (vapor pressure eq., Yaw et al. 1994)
- 6.67×10^{-5} , 7.47×10^{-5} (quoted, Staples et al. 1997)
- 6.67×10^{-5} ; 6.67×10^{-6} , 4.93×10^{-6} , 1.33×10^{-8} (recommended, calculated-QSAR, Staples et al. 1997)
- 1.84×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

- 21.6 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 7.70 (estimated, Williams et al. 1995)
- > 8.0; 10.0, 1.0.3 (recommended; calculated-QSAR, Staples et al. 1997)
- 9.46 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

11.52 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

1.95–2.1, 2.06 (*Daphnia magna*, 20°C, range, mean, Brown & Thompson 1982a)

3.48, 3.60; 3.54 (*Mytilus edulis*, 15°C, exposure concn: 4.4, 4.17 µg/L; mean value, Brown & Thompson 1982b)

Sorption Partition Coefficient, $\log K_{OC}$:

5.04, 5.78, 5.16 (soil/sediment, exptl. data, Williams et al. 1995)

5.46, 7.60 (soil/sediment: mean value, calculated- K_{OW} , Williams et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2$ – 2.0 d (estimated, Staples et al. 1997).

$k_{OH} = 26.217 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.32$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 4.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);

primary biodegradation with a rate constant $k = 0.088 \text{ d}^{-1}$ and $t_{1/2} = 9.6$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 795, 539 \text{ mL} \cdot \text{g} \cdot \text{d}^{-1}$ (*Mytilus edulis*, for exposure concn: 4.4, 41.7 µg/L, 15°C, Brown & Thompson 1982b; quoted, Staples et al. 1997).

$k_2 = 0.20, 0.18 \text{ d}^{-1}$ (*Mytilus edulis*, for exposure concn: 4.4, 41.7 µg/L, 15°C, Brown & Thompson 1982b; quoted, Staples et al. 1997).

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2$ – 2.0 d (estimated, Staples et al. 1997).

photodegradation $t_{1/2} = 0.32$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

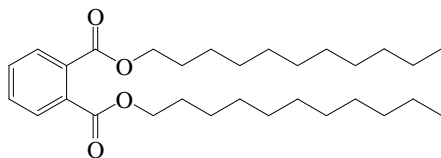
Surface water: primary biodegradation with a rate constant $k = 0.088 \text{ d}^{-1}$ and $t_{1/2} = 9.6$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 4.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota: depuration $t_{1/2} = 3.5$ and 3.8 d DIDP concn at 5 and 50 µg/L for *Mytilus edulis* at 15°C (Brown & Thompson 1982b).

15.1.3.17 Diundecyl phthalate (DUP)

Common Name Diundecyl phthalate

Synonym: DUP

Chemical Name: diundecyl phthalate

CAS Registry No: 3648-20-2

Molecular Formula: $C_{30}H_{50}O_4$

Molecular Weight: 474.716

Melting Point ($^{\circ}C$):

-9 (Staples et al. 1997)

35.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

0.96 (Staples et al. 1997)

Molar Volume (cm^3/mol):

658.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.789 (mp at $35.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.11 ± 0.28 (shake flask, Howard et al. 1985)

< 0.001 ; 1.6×10^{-7} , 4.2×10^{-7} (recommended; calculated-QSAR, Staples et al. 1997)

2.14×10^{-8} (calculated-UNIFAC, Thomsen et al. 1999)

4.41×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

6.67×10^{-5} , 7.07×10^{-5} (quoted, Staples et al. 1997)

6.67×10^{-5} ; 1.33×10^{-8} , 1.6×10^{-7} (recommended; calculated-QSAR, Staples et al. 1997)

4.97×10^{-7} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

50.5 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

> 8.0 ; 11.2, 11.5 (recommended; calculated-QSAR, Staples et al. 1997)

10.54 (calculated-UNIFAC, Thomsen et al. 1999)

10.33 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

12.02 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

$k_{\text{OH}} = 31.847 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.26$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: primary biodegradation rate constant $k = 0.115 \text{ d}^{-1}$ and $t_{1/2} = 6.17$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

aerobic biodegradation in aquatic environments, first order $k = 0.03 \text{ d}^{-1}$ with $t_{1/2} = 23$ d in unstirred river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997)

Photodegradation $t_{1/2} = 0.26$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: primary biodegradation rate constant $k = 0.115 \text{ d}^{-1}$ and $t_{1/2} = 6.17$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

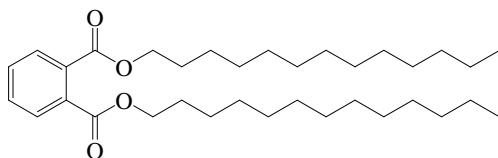
biodegradation $t_{1/2} = 23$ d in aerobic aquatic environments (Peterson & Staples 2003)

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.18 Ditridecyl phthalate (DTDP)

Common Name: Ditridecyl phthalate

Synonym: DTDP

Chemical Name:

CAS Registry No: 119-06-2. 68515-47-9

Molecular Formula: $C_{34}H_{58}O_4$

Molecular Weight: 530.823

Melting Point ($^{\circ}C$):

-37 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

0.953 (Staples et al. 1997)

Molar Volume (cm^3/mol):

746.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.34 (shake flask-nephelometry, Hollifield 1979)

< 0.30 (shake flask, Howard et al. 1985; quoted, Adams et al. 1995)

0.34, < 0.30 (quoted, Staples et al. 1997)

< 0.001; 1.5×10^{-9} , 4.2×10^{-9} (recommended, calculated-QSAR, Staples et al. 1997)

4.07×10^{-10} (calculated-UNIFAC, Thomsen et al. 1999)

7.0×10^{-8} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

< 6.67×10^{-5} (quoted, Staples et al. 1997)

< 6.67×10^{-5} ; 1.33×10^{-9} , 3.33×10^{-9} (recommended; calculated-QSAR, Staples et al. 1997)

3.63×10^{-8} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

275 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.40 (estimated, Williams et al. 1995)

> 8.0; 13.1, 13.4 (recommended; calculated-QSAR, Staples et al. 1997)

12.28 (calculated-UNIFAC, Thomsen et al. 1999)

12.06 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

13.01 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

6.08 (soil/sediment, Williams et al. 1995; quoted, Staples et al. 1997)

5.87, 6.45, 6.28; 6.08 (soil/sediment: exptl. data; mean value, Williams et al. 1995)

6.26, 8.30 (soil/sediment: exptl. mean, calculated- K_{OW} , Williams et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 10.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);

primary biodegradation rate constant $k = 0.029\text{ d}^{-1}$ and $t_{1/2} = 27.6$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

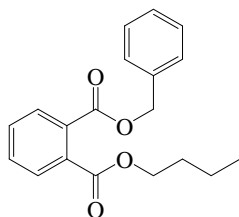
Surface water: primary biodegradation rate constant $k = 0.029\text{ d}^{-1}$ and $t_{1/2} = 27.6$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 10.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

15.1.3.19 Butyl benzyl phthalate (BBP)

Common Name: Butyl benzyl phthalate

Synonym: BBP, benzyl butyl phthalate

Chemical Name: butyl benzyl phthalate, benzyl butyl phthalate

CAS Registry No: 85-68-7

Molecular Formula: $C_{19}H_{20}O_4$, $C_6H_5COOCH_2C_6H_4COOC_4H_9$

Molecular Weight: 312.360

Melting Point ($^{\circ}C$):

–35.0 (Callahan et al. 1979; Mabey et al. 1982; Howard 1989)

Boiling Point ($^{\circ}C$):

370.0 (Verschuereen 1983; Howard 1989; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.111 (Staples et al. 1997)

Molar Volume (cm^3/mol):

369.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.90 (Hirzy et al. 1978)

0.71 (shake flask-nephelometry, practical grade, Hollifield 1979)

2.9 ± 1.2 (shake flask-GC, Gledhill et al. 1980)

40.2 (shake flask-LSC, Veith et al. 1980)

2.82 ($20^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)

2.90 ± 1.2 (Verschuereen 1983)

2.69 ± 0.15 (shake flask-HPLC/UV, Howard et al. 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00115 ($20^{\circ}C$, Gledhill et al. 1980)

0.00799 (calculated using Trouton's rule, Mabey et al. 1982)

0.00115 (Petrasek et al. 1983)

0.00115 ($20^{\circ}C$, Verschuereen 1983)

$\log(P_L/kPa) = 9.1472 - 4647.5/(T/K)$, temp range: 416–516 K, (Antoine eq., Stephenson & Malanowski 1987)

0.0011, 0.00133 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

0.00067 (recommended, Staples et al. 1997)

0.0249 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.132 (calculated-P/C, Wolfe et al. 1980a)

0.132 (calculated, Lyman et al. 1982)

0.841 (calculated-P/C, Mabey et al. 1982)

0.104 (quoted from WERL Treatability Data, Ryan et al. 1988)

0.077 (selected, Staples et al. 1997)

0.205 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.80	(Hirzy et al. 1978)
5.80	(calculated as per Leo et al. 1971)
4.77	(shake flask-GC analysis of both phases, Gledhill et al. 1980)
4.05	(shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982)
4.75	(RPHPLC-RT correlation, Veith et al. 1980)
3.97	(HPLC- k' correlation, McDuffie 1981)
4.11, 3.23–4.45	(shake flask method: mean, range, OECD 1981)
4.91	(20°C, shake flask-UV, Leyder & Boulanger 1983)
4.78	(Verschuere 1983)
3.57	(HPLC-RT correlation, Howard et al. 1985)
4.91	(calculated, Hansch & Leo 1985)
4.87	(calculated-CLOGP, Müller & Klein 1992)
4.59	(recommended, Staples et al. 1997)
4.70	(calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.78	(calculated-QSPR, Cousins & Mackay 2000)
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Bioconcentration Factor, $\log BCF$:

2.74–3.34	(calculated- K_{OW} , Veith et al. 1979, 1980)
2.82	(bluegill sunfish, Barrows et al. 1980;)
2.71	(calculated- K_{OW} , Gledhill et al. 1980)
2.82	(bluegill sunfish, quoted, Gledhill et al. 1980)
2.19–2.95	(fathead minnows, quoted, Gledhill et al. 1980)
2.89	(bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
3.90	(calculated- K_{OW} , Wolfe et al. 1980a)
4.67	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
3.57	(sediment, calculated- K_{OW} , Pavlou & Weston 1983, 1984)
2.89	(quoted, Isnard & Lambert 1988; quoted, Banerjee & Baughman 1991)
2.72	(calculated- K_{OW} and $S_{octanol}$, Banerjee & Baughman 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

1.83–2.54	(soil, batch equilibration-GC, Gledhill et al. 1980;)
3.95	(soil/sediment, Gledhill et al. 1980)
3.81	(calculated- K_{OW} , Wolfe et al. 1980a)
5.23	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)
4.23	(Broome County soil in New York, Russell & McDuffie)
4.23, 3.97	(soil, quoted, calculated-MCI and fragment contribution, Meylan et al. 1992)
2.60	(activated carbon, calculated-MCI, Blum et al. 1994)
3.21	(quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
5.00	(suspended solids, calculated- K_d assuming a 0.1 org. carbon fraction, Staples et al. 1997)
3.21, 3.88; 3.11, 3.07, 3.21, 3.32, 3.15	(soil: quoted lit., calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photolysis (near surface) rate constant $k = 2 \times 10^{-4} \text{ h}^{-1}$ in natural water (Wolfe et al 1980a); photodegradation $t_{1/2} > 100 \text{ d}$ (Gledhill et al. 1980; quoted, Verschuere 1983; Howard 1989).

Oxidation: the free radical oxidation rate constant $k = 18 \text{ M}^{-1}\text{s}^{-1}$ for reaction with peroxy radical (Wolfe et al. 1980a);

rate constant $k \ll 360 \text{ M}^{-1}\text{h}^{-1}$ for singlet oxygen and $k = 280 \text{ M}^{-1}\text{h}^{-1}$ for peroxy radical (Mabey et al. 1982); photooxidation $t_{1/2} = 6\text{--}60 \text{ h}$, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

predicted atmospheric photooxidation $t_{1/2} = 0.5\text{--}5.0$ d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997).

$k_{\text{OH}} = 11.049 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.75$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis: the alkaline hydrolysis rate constant $k \sim 38 \text{ M}^{-1}\cdot\text{h}^{-1}$; hydrolytic $t_{1/2} = 80$ to 4000 d at pH 8 and 30°C (Wolfe et al. 1980a; quoted, Gledhill et al. 1980);

chemical degradation (hydrolysis) $t_{1/2} > 100$ d (Gledhill et al. 1980; quoted, Verschuere 1983; Howard 1989; selected, Staples et al. 1997).

Biodegradation: degradation $t_{1/2} \sim 2$ d in river water and $t_{1/2} = 2$ h in activated sludge (Saeger & Tucker 1976)

degradation $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

microbial degradation rate constant $k = 2.9 \times 10^{-8} \text{ mL}\cdot\text{organism}^{-1}\cdot\text{s}^{-1}$ (Wolfe et al. 1981a);

0–24% mineralization in > 8 wk in municipal digested sludge (Horowitz et al. 1982);

primary degradation accounted for > 95% loss in 7 d with an initial concentration of 1.0 mg/L in a lake water microcosm with $t_{1/2} < 4$ d and 100% primary degradation was observed after 9 d while $t_{1/2} = 2.0$ d (Gledhill et al. 1980; quoted, Verschuere 1983; Howard 1989);

significant degradation with rapid adaptation within 7 d in an aerobic environment with $k > 0.5 \text{ d}^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);

degradation rate constant $k = 0.043 \text{ d}^{-1}$ corresponding to $t_{1/2} = 19.4$ d in a shake flask biodegradation experiment (Sugatt et al. 1984);

greater than 90% degraded within 40 d in digested sludge (Shelton et al. 1984);

99% degraded in activated sludge systems in 48 h (O'Grady et al. 1985);

anaerobic digestion of sludge with first-order rate constant $k = 6.5 \times 10^{-3} \text{ h}^{-1}$ and $t_{1/2} = 107$ h (Ziogou et al. 1989);

aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated river die-away test and aqueous anaerobic $t_{1/2} = 672\text{--}4320$ h, based on unacclimated anaerobic screening test data (Howard et al. 1991)

Aerobic biodegradation in aquatic environments, first order $k = 0.46 \text{ d}^{-1}$ with $t_{1/2} = 1.5$ d in unstirred river water, $k = 0.50 \text{ d}^{-1}$ with $t_{1/2} = 1.4$ d in microcosm, lake, $k = 0.35 \text{ d}^{-1}$ with $t_{1/2} = 2.0$ d in river water, $k = 0.14 \text{ d}^{-1}$ with $t_{1/2} = 5.0$ d in microcosm, un-impacted, $k > 0.023 \text{ d}^{-1}$ with $t_{1/2} < 3.0$ d in microcosm, Illinois river, and $k = 2.2 \text{ d}^{-1}$ with $t_{1/2} = 0.32$ d in shake river water (Peterson & Staples 2003)

Anaerobic biodegradation $k = 0.056 \text{ d}^{-1}$ with $t_{1/2} = 12.4$ d in undiluted sludge, batch incubation, $k = 0.19 \text{ d}^{-1}$ with $t_{1/2} = 3.7$ d in undiluted sludge, $k = 0.096 \text{ d}^{-1}$ with $t_{1/2} = 7.2$ d in 10% dilute sludge; $k = 0.076 \text{ d}^{-1}$ with $t_{1/2} = 9.1$ d in 10% freshwater sediment and $k = 0.051 \text{ d}^{-1}$ with $t_{1/2} = 13.6$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: estimated rate constant $k = 3 \times 10^{-9} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982);

microbial transformation $k = (3.1 \pm 0.8) \times 10^{-11} \text{ L}\cdot\text{organism}^{-1}\cdot\text{h}^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

depuration $t_{1/2} < 24$ and > 48 h from tissues of bluegill sunfish (Barrows et al. 1980).

$k_2 = 0.0464 \text{ d}^{-1}$ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.00397 \text{ d}^{-1}$ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} = 1.5$ d in the atmosphere (GEMS 1984; quoted, Howard 1989);

$t_{1/2} = 6\text{--}60$ h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

photodegradation $t_{1/2} = 0.75$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} \sim 2$ h by naturally occurring, mixed microbial populations in river water (Saeger & Tucker 1976);

hydrolytic $t_{1/2} = 80$ to 4000 d at pH 8 and 30°C (Wolfe et al. 1980a; quoted, Gledhill et al. 1980);

$t_{1/2} = 2$ d for river water, $t_{1/2} < 4$ d for lake water-sediment microcosm, and $t_{1/2} < 100$ d for chemical degradation (hydrolysis) (Gledhill et al. 1980);

biodegradation $t_{1/2} = 19.4$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984);

overall $t_{1/2} = 24\text{--}168$ h, based on unacclimated river die-away test (Howard et al. 1991)

biodegradation $t_{1/2} = 0.32\text{--}3$ d in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 48\text{--}4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: anaerobic biodegradation $t_{1/2} = 9.1$ h in 10% freshwater sediment, and $t_{1/2} = 13.6$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Soil: degradation $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

$t_{1/2} = 10\text{--}50$ d via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

$t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

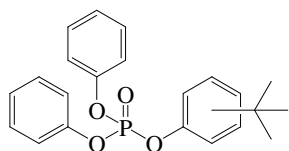
Biota: depuration $t_{1/2} < 24$ and > 48 h (tissues of bluegill sunfish in 21-d exposure, Barrows et al. 1980)

$t_{1/2} < 2$ d from bluegill sunfish (Gledhill et al. 1980; quoted, Verschueren 1983).

15.1.4 PHOSPHATE ESTERS

15.1.4.1 Triaryl phosphates

15.1.4.1.1 *t*-Butylphenyl diphenyl phosphate (tBPDP, BPDP)



Common Name: *t*-Butylphenyl diphenyl phosphate

Synonym: TBPDP, BPDP

Chemical Name:

CAS Registry No: 56803-37-3

o-*tert*-butylphenyl diphenyl phosphate (*o*-TBPDP) 83242-23-2

m-*tert*-butylphenyl diphenyl phosphate (*m*-TBPDP) 83242-22-2

p-*tert*-butylphenyl diphenyl phosphate (*p*-TBPDP) 981-40-8

Molecular Formula: C₂₂H₂₃O₄P, (CH₃)C₆H₄(C₆H₅)₂O₄P

Molecular Weight: 382.389

Melting Point (°C):

−21 (Muir 1984)

Boiling Point (°C):

195/0.20 mmHg, 200/0.2 mmHg, 200/0.20 mmHg (*o*-, *m*-, *p*-TBPDP, Wightman & Malaiyanki 1983)

261/6 mmHg (Muir 1984)

420 (Boethling & Cooper 1985)

Density (g/cm³):

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

3.2 (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at 25°C):

180 (200°C, Muir 1984)

1.87 × 10^{−4} (quoted measured value, Boethling & Cooper 1985)

6.13 × 10^{−5} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.086 (estimated-P/C, Muir 1984, Muir et al. 1985)

0.0223, 0.0073 (calculated-P/C, Boethling & Cooper 1985)

2.18 (gas stripping, Muir et al. 1985)

Octanol/Water Partition Coefficient, log K_{OW}:

5.12 (shake flask-concn ratio, Saeger et al. 1979;)

3.23, 4.76, 6.44; 5.97 (RP-HPLC-*k'* correlation; mean value, Renberg et al. 1980)

Bioconcentration Factor, log BCF:

2.89 (calculated, Saeger et al. 1979)

3.36, 3.04, 3.13 (rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)

2.89 (rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)

3.52, 2.89, 2.70 (fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)

2.76 (fathead minnow, calculated with hexane extract, Muir et al. 1983b)

- 3.94, 2.89 (rainbow trout, fathead minnow, static expt., quoted, Boethling & Cooper 1985)
 3.64 (calculated- K_{OW} , Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.16 (calculated- K_{OW} , Muir 1984)
 3.36 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 128$ d from 1 m deep water system was estimated to be 128 d (calculated, Muir 1984)
 moderate rate of volatilization from water, $t_{1/2} = 152$ d at 0.5-m depth (Muir et al. 1985).

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 1.92$ h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b).

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 22.8 \text{ h}^{-1}$, 29.3 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).

$k_1 = 17.7 \text{ h}^{-1}$, 18.0 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).

$k_2 = 0.0137 \text{ h}^{-1}$, 0.0113 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).

$k_2 = 0.0106 \text{ h}^{-1}$, 0.0111 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b).

$k_2 = 0.0088 \text{ h}^{-1}$, 0.0074 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).

$k_2 = 0.0078 \text{ h}^{-1}$, 0.0070 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b).

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

hydrolysis $t_{1/2} = 1.92$ h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b);

$t_{1/2} = 128$ d, volatilization from 1 m deep water system (Muir 1984);

pseudo-first-order $t_{1/2} = 0.44$ d in pond water; moderate rate of volatilization from water column with $t_{1/2} = 152$ d at 0.5-m depth (Muir et al. 1985).

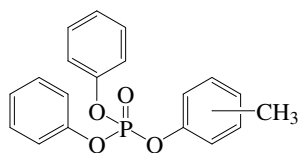
Groundwater:

Sediment: pseudo-first-order $t_{1/2} = 39$ d in pond bottom sediment during a 49-d period (Muir et al. 1985).

Soil:

Biota: depuration $t_{1/2} = 42$ h in chironomid larvae (Muir et al. 1985).

15.1.4.1.2 Cresyl diphenyl phosphate (CDP)



Common Name: Cresyl diphenyl phosphate

Synonym: CDP

Chemical Name:

CAS Registry No: 78-31-9

o-CDP 5254-12-6

m-CDP 69500-28-3

p-CDP 78-31-9

Molecular Formula: C₁₉H₁₇O₄P

Molecular Weight: 340.309

Melting Point (°C):

−40 (*p*-CDP, Lide 2003)

Boiling Point (°C):

180/0.60 mmHg, 190/0.60 mmHg, 200/0.70 mmHg (*o*-, *m*-, *p*-CDP, Wightman & Malaiyandi 1983)

368, 390 (at 1 atm, Boethling & Cooper 1985)

235–255/4 mmHg, 255/5 mmHg (Boethling & Cooper 1985)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

2.60 (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at 25°C):

5.47 × 10^{−3}, 1.21 × 10^{−3}, 3.87 × 10^{−4}, 2.80 × 10^{−4} (estimated from reported boiling points, Boethling & Cooper 1985)

6.27 × 10^{−4} (quoted measured value, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.470 (calculated-P/C, Muir 1984)

0.798, 0.162, 0.0820, 0.0507, 0.0355 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:

4.505 (shake flask-concn ratio, Saeger et al. 1979)

3.23, 3.63, 4.06; 3.77 (RP-HPLC-*k'* correlation; mean value, Renberg 1980)

4.40 (Bengtsson et al. 1986)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.56 (calculated, Saeger et al. 1979)

2.99 (calculated-K_{OW}, Boethling & Cooper 1985)

2.002.34 (bleak, 280-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.83 (calculated- K_{OW} , Muir 1984)
- 3.41 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 22$ d for 1 m deep water system (estimated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

volatilization $t_{1/2} = 22$ d for 1 m deep water system (estimated, Muir 1984).

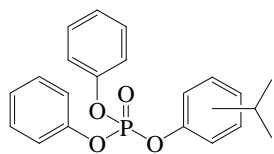
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 4$ d or less (beak, 28-d exposure, Bengtsson 1986).

15.1.4.1.3 Isopropylphenyl diphenyl phosphate (IPDP)



Common Name: Isopropylphenyl diphenyl phosphate

Synonym: IPPDP, IPDP

Chemical Name:

CAS Registry No: 28108-99-8

o-IPPDP 64532-94-1

m-IPPDP 69515-46-4

p-IPPDP 55864-04-5

Molecular Formula: $C_{21}H_{21}O_4P$, $(CH_3)_2CHC_6H_4O_4P$

Molecular Weight: 368.362

Melting Point ($^{\circ}C$):

-26 (Muir 1984)

Boiling Point ($^{\circ}C$):

175/0.05 mmHg, 180/0.02 mmHg, 185/0.05 mmHg (Wightman & Malaiyandi 1983)

220–230/1 mmHg (Muir 1984, Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.20 (room temp, shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at $25^{\circ}C$):

1.47×10^{-4} (estimated from boiling point, Boethling & Cooper 1985)

3.73×10^{-5} (quoted measured value, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.243, 0.0628 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.305 (shake flask-concn ratio, Saeger et al. 1979; quoted, Muir 1984)

3.23, 4.30, 5.40, 6.57; 5.99 (RP-HPLC- k' correlation; mean, Renberg et al. 1980)

5.70 (quoted measured value, Boethling & Cooper 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.99 (calculated, Saeger et al. 1979)

3.88 (estimated from solubility, Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

4.26 (calculated- K_{OW} , Muir 1984)

3.45 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 21 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2} = 28\text{--}48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} = 28\text{--}48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

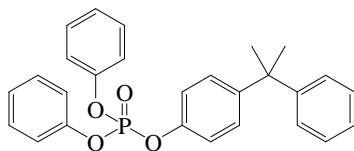
Groundwater:

Sediment:

Soil:

Biota:

15.1.4.1.4 4-Cumylphenyl diphenyl phosphate (CPDPP)



Common Name: 4-Cumylphenyl diphenyl phosphate

Synonym: CPDPP

Chemical Name:

CAS Registry No: 84602-56-2

Molecular Formula: $C_{27}H_{25}O_4P$, $C_6H_5C(CH_3)_2(C_6H_5)_2O_4P$

Molecular Weight: 444.458

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

230–235/0.15 mmHg (Wightman & Malaiyandi 1983)

494 (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.063 ± 0.025 (Mayer et al. 1981)

0.060 (Boethling & Cooper 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

1.726×10^{-9} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

8.62×10^{-4} (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.08 (Mayer et al. 1981)

6.10 (quoted, Boethling & Cooper 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.40 (calculated- K_{ow} , Mayer et al. 1981)

3.45, 3.10–3.66 (mean value, range, rainbow trout 90-d exposure, Mayer et al. 1981)

4.40 (calculated- K_{ow} , Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{oc}$:

4.53 (soil, calculated-S and K_{ow} , Mayer et al. 1981)

4.30 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: hydrolyzed in alkaline solutions, $t_{1/2} = 5$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).

Biodegradation: $t_{1/2} > 21$ d in river die-away procedure; the half-lives of the disappearance by sediment adsorption and degradation of CPDFF for microcosm core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d, sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolyzed in alkaline solutions, $t_{1/2} = 5$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7; biodegradation $t_{1/2} > 21$ d in river die-away procedure (Mayer et al. 1981).

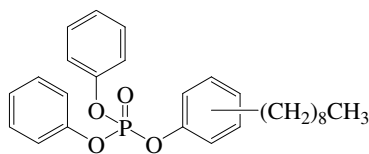
Groundwater:

Sediment: rapidly disappeared from the active core-water columns, 90% in < 3 d in the microcosm-lake simulation study, the half-lives of the disappearance of CPDFF by sediment adsorption and degradation are, for microcosm core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d; sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

Soil:

Biota:

15.1.4.1.5 Nonylphenyl diphenyl phosphate (NPDPP)



Common Name: Nonylphenyl diphenyl phosphate

Synonym: NPDPP, Pydral 50E

Chemical Name:

CAS Registry No: 38638-05-0

m-NPDPP 84602-55-1

p-NPDPP 64532-97-4

Molecular Formula: $C_{27}H_{33}O_4P$, $C_9H_{19}(C_6H_5)_3O_4P$

Molecular Weight: 452.522

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

220–225/0.07 mmHg (*m*-NPDPP, Wightman & Malaiyandi 1983)

215–220/0.07 mmHg (*p*-NPDPP, Wightman & Malaiyandi 1983)

471 (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.77 ± 0.25 (Mayer et al. 1981)

0.80 (Boethling & Cooper 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

6.13×10^{-5} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.00142 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.93 (Mayer et al. 1981; quoted, Muir 1984)

5.90 (quoted, Boethling & Cooper 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.32 (estimated, Mayer et al. 1981)

2.84, 2.49–2.96 (mean value and range, rainbow trout 90-d exposure, Mayer et al. 1981)

4.26 (calculated- K_{ow} , Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

4.36 (soil, calculated-solubility and K_{ow} , Mayer et al. 1981)

4.61 (calculated- K_{ow} , Muir 1984)

3.69 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, Half-Lives, $t_{1/2}$

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 6$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).

Biodegradation: primary biodegradation $t_{1/2} > 21$ d in river die-away procedure; half-life for disappearance by sediment adsorption and degradation in microcosms-lake simulation study, for core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d; sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolyzed in alkaline solutions, $t_{1/2} = 6$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).

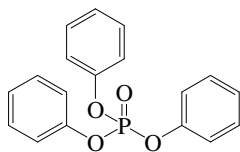
Groundwater:

Sediment: rapidly disappeared from the active core-water column, 90% in < 3 d. Time to 50% disappearance by sediment adsorption and degradation in microcosms-lake simulation study, for microcosm core conditions: active, aerated or nitrogen-purge, light or dark – $t_{1/2} < 3$ d; sterile, aerated, light – $t_{1/2} = 7$ d and sterile, nitrogen-purge, light – $t_{1/2} > 28$ d (Mayer et al. 1981).

Soil:

Biota:

15.1.4.1.6 Triphenyl phosphate (TPP)



Common Name: Triphenyl phosphate

Synonym: TPP

Chemical Name: triphenyl phosphate

CAS Registry No: 115-86-6

Molecular Formula: $C_{18}H_{15}O_4P$

Molecular Weight: 326.283

Melting Point ($^{\circ}C$):

50.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

245/11 mmHg (Verschuereen 1983; Budavari 1989; Lide 2003)

377 (Stephenson & Malanowski 1987)

Density (g/cm^3):

Molar Volume (cm^3/mol):

270.7 ($50^{\circ}C$, Stephenson & Malanowski 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.27, 0.292

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.90 (shake flask-GC, Saeger et al. 1979)

1.9 ± 0.2 (Mayer et al. 1981)

0.73 (shake flask-nephelometry, Hollifield 1979)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

< 13.3 ($30^{\circ}C$, Verschuereen 1983)

2.0×10^{-4} , 1.6×10^{-4} , 1.07×10^{-4} (estimated from reported boiling points, Boethling & Cooper 1985)

$\log(P/kPa) = 8.195 - 4253/(T/K)$; temp range 275 – $410^{\circ}C$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 28.0972 - 5.6684 \times 10^3/(T/K) - 5.9768 \cdot \log(T/K) - 3.1567 \times 10^{-9} \cdot (T/K) + 1.0751 \times 10^{-12} \cdot (T/K)^2$;
temp range 323 – $687 K$ (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.168 (calculated-P/C, Muir 1984)

0.0265, 0.0284, 0.018 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.63 (shake flask-concn ratio, Saeger et al. 1979)

4.62 (Mayer et al. 1981)

4.78 (shake flask-concn ratio, Sasaki et al. 1981)

3.15 (RP-HPTLC- k' correlation, Renberg et al. 1980)

3.63–3.61 (literature average, Muir 1984)

4.60, 4.70 (Boethling & Cooper 1985)

3.90 (Bengtsson et al. 1986)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.45, 2.62 (quoted-rainbow trout data, calculated- K_{ow} , Saeger et al. 1979)

2.22 (fathead minnow, mixed isomers, Veith et al. 1979)

3.41	(rainbow trout, rate constant ratio k_1/k_2 , Muir et al. 1980)
3.29, 2.63, 2.58	(rainbow trout, calculated- K_{OW} , Muir et al. 1980)
3.02, 2.92, 2.00	(rainbow trout, calculated-S, Muir et al. 1980)
2.62	(rainbow trout, estimated from K_{OW} , Mayer et al. 1981)
2.43, 2.12–2.56	(mean value, range, rainbow trout in 90-d exposure, Mayer et al. 1981)
2.40–2.79	(killifish, whole fish basis, 72-h exposure, static system, Sasaki et al. 1981)
2.04–2.18	(goldfish, static system, Sasaki et al. 1981; quoted, Boethling & Cooper 1985)
2.20–2.79	(killifish, flow through system, Sasaki et al. 1982; quoted, Boethling & Cooper 1985)
2.28–2.29	(killifish, 32–35 d exposure, flow through system, Sasaki et al. 1983)
3.14, 2.76, 2.96	(rainbow trout: “initial rate” method, static test, Biofac, Muir et al. 1983b)
2.51	(rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
3.24, 2.75, 2.34	(fathead minnow: “initial rate” method, static test, Biofac, Muir et al. 1983b)
2.62	(fathead minnow, calculated with hexane extract, Muir et al. 1983b)
2.76, 2.51	(rainbow trout in static test expt., quoted from Muir et al. 1983b, Boethling & Cooper 1985)
2.75, 2.62 1985)	(fathead minnow in static test expt., quoted from Muir et al. 1983b, Boethling & Cooper 1985)
3.26	(estimated- K_{OW} , Boethling & Cooper 1985)
2.60	(bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log K_{OC} :

3.74	(soil, calculated-S, K_{OW} , Mayer et al. 1981)
3.89	(calculated- K_{OW} , Muir 1984)
3.49	(calculated-solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 60$ d (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

$k = 0.0253$ and 0.0227 L mol⁻¹ s⁻¹ for the colorimetric and acid-base method, respectively, in dioxan-water (3:1 v/v) at 35°C; the mean second order rate constants: $10^3 k_2$ at 0°C, 10.1°C, 24.7°C, and 35°C were 0.235, 0.477, 1.06, and 2.32 L mol⁻¹ s⁻¹, respectively, in 60% dioxan-water (Barnard et al. 1961);

$t_{1/2} = 1.3$ yr under neutral conditions from kinetic data in the environment (estimated, Saeger et al. 1979)

$k = 6.0 \times 10^{-8}$ s⁻¹, with $t_{1/2} = 130$ d, the pseudo-first-order rate constant in dioxan-water (3:1 v/v) at 100°C; while the second-order rate constant $k = 0.0106$ L mol⁻¹ s⁻¹ with $t_{1/2} = 23$ d at pH 9.5 and $t_{1/2} = 474$ d at pH 8.2 under alkaline conditions at 24.7°C (quoted, Howard & Deo 1979);

$k(\text{second order alkaline}) = 0.027$ M⁻¹ s⁻¹, with an estimated $t_{1/2} \sim 1000$ yr (Wolfe 1980)

$t_{1/2} = 19$ d at pH 7 but $t_{1/2} = 3$ d at pH 9 at 25°C, the most important process for abiotic transformation of aryl phosphates in the environment, much more rapid at alkaline than at neutral pH (Mayer et al. 1981, quoted, Boethling & Cooper 1985)

$t_{1/2} = 7.5$ d at pH 8.2, $t_{1/2} = 1.3$ d at pH 9.5, $t_{1/2} = 20$ –25 d at pH 7 and 21°C (Howard & Deo 1979; quoted, Boethling & Cooper 1985)

$t_{1/2} = 0.49$ h at pH 13.0 in acetone/water 1:1 solution (Muir et al. 1983b)

Biodegradation: complete primary degradation in less than 7 d in the river die-away studies exposed to the natural microbial population of the river water; $t_{1/2} < 7$ d for primary biodegradation rate for from semicontinuous activated sludge studies (Saeger et al. 1979);

readily biodegraded, in the semicontinuous activated sludge test, degradation of TPP exceeding 95% was observed over a 24-h cycle, and river die-away tests showed $t_{1/2} = 2$ –4 d; time to 50% from the active core water-column disappearance for TPP in microcosms simulating lake conditions was 3–10 d (Mayer et al. 1981).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 46.36$ h⁻¹ (rainbow trout, Muir et al. 1980).

$k_2 = 0.0197$ h⁻¹ (rainbow trout, 0–9 d, fast clearance, Muir et al. 1980).

$k_2 = 0.00245$ h⁻¹ (rainbow trout, 9–31 d, slow clearance, Muir et al. 1980)

- $k_1 = 0.4\text{--}0.6\text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
- $k_1 = 2.1\text{--}4.2\text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
- $k_1 = 3.3\text{--}10.4\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
- $k_1 = 3.3\text{--}16.9\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)
- $k_2 = 0.023\text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, calculated by concn decay curve, Muir et al. 1983)
- $k_2 = 0.039\text{ h}^{-1}$ (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)
- $k_2 = 0.011\text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)
- $k_2 = 0.016\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983).
- $k_1 = 22.7\text{ h}^{-1}$, 20.7 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).
- $k_1 = 16.5\text{ h}^{-1}$, 14.5 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).
- $k_2 = 0.0116\text{ h}^{-1}$, 0.0144 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b)
- $k_2 = 0.0121\text{ h}^{-1}$, 0.0140 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).
- $k_2 = 0.0076\text{ h}^{-1}$, 0.0107 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7\text{ d}$ for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

$t_{1/2} = 5\text{ h}$ in the water containing killifish and over 100 h for goldfish (Sasaki et al. 1981);

hydrolysis $t_{1/2} = 19\text{ d}$ at pH 7 but $t_{1/2} = 3\text{ d}$ at pH 9; $t_{1/2} = 2\text{--}4\text{ d}$ in river die-away test at 25°C, (Mayer et al. 1981, quoted, Boethling & Cooper 1985);

$t_{1/2} = 7.5\text{ d}$ at pH 8.2 and $t_{1/2} = 1.3\text{ d}$ at pH 9.5, $t_{1/2} = 20\text{--}25\text{ d}$ at pH 7 at 21°C (Howard & Deo 1979; quoted, Boethling & Cooper 1985);

estimated hydrolysis $t_{1/2} \sim 10^3\text{ yr}$ (Wolfe 1980);

volatilization $t_{1/2}(\text{calc}) = 60\text{ d}$ for 1 m deep water (Muir 1984).

Ground water:

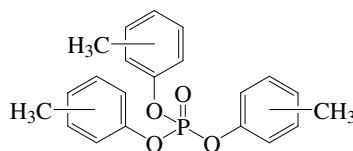
Sediment: water-column disappearance $t_{1/2} \sim 3\text{ d}$ of TPP by both adsorption and degradation from microcosms-lake simulation study, for the microcosm core conditions: active, aerated, light or dark – $t_{1/2} = 3\text{ d}$; active, nitrogen-purge, light – $t_{1/2} = 3\text{ d}$; sterile, aerated, light – $t_{1/2} = 7\text{ d}$ and sterile, nitrogen-purge, light – $t_{1/2} = 10\text{ d}$ (Mayer et al. 1981).

Soil:

Biota: elimination $t_{1/2} = 30.4\text{ h}$ in pond sediment-water, $t_{1/2} = 17.6\text{ h}$ in river water, $t_{1/2} = 62.7\text{ h}$ in river sediment-water, $t_{1/2} = 44.4$ in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983a);

elimination $t_{1/2} = 4\text{ d}$ or less (bleak, 28-d exposure, Bengtsson et al. 1986).

15.1.4.1.7 Tricresyl phosphate (TCP)



Common Name: Tricresyl phosphate

Synonym: TCP, tritolyl phosphate, tris(methylphenyl) phosphate

Chemical Name: phosphoric acid tris(methylphenyl) ester

o-TCP:- tris(2-methylphenyl) phosphate; phosphoric acid tri(2-tolyl) ester

m-TCP:- tris(3-methylphenyl) phosphate; phosphoric acid tri(3-tolyl) ester

p-TCP:- tris(4-methylphenyl) phosphate; phosphoric acid tri(4-tolyl) ester

CAS Registry No:

o-TCP [78-30-8]; *m*-TCP[563-04-2]; *p*-TCP [78-32-0]

mixed isomers - tris(methylphenyl) phosphate [1330-78-5]

Molecular Formula: $C_{21}H_{21}O_4P$, $(CH_3C_6H_4)_3O_4P$

Molecular Weight: 368.362

Melting Point ($^{\circ}C$):

-25/-30	(<i>o</i> -TCP, Verschueren 1983)
-33	(mixed isomers, Riddick et al. 1986)
11, 25-26, 77-8	(<i>o</i> -TCP, <i>m</i> -TCP, <i>p</i> -TCP, Muir 1984)
11, 25, 77.5	(<i>o</i> -TCP, <i>m</i> -TCP, <i>p</i> -TCP, Stephenson & Malanowski 1987)
11, 25.5, 77.5	(<i>o</i> -TCP, <i>m</i> -TCP, <i>p</i> -TCP, Lide 2003)

Boiling Point ($^{\circ}C$):

201/1 mmHg (commercial quality, Burrow 1946)	
420	(<i>o</i> -TCP, Verschueren 1983)
410	(<i>o</i> -TCP, Muir 1984; Lide 2003)
313, 206, 216/0.5 mmHg (mixed isomers, <i>o</i> -, <i>m</i> -TCP, Riddick et al. 1986)	
241-255/4 mmHg, 265/5 mmHg (Boethling & Cooper 1985)	

Density (g/cm^3 at $20^{\circ}C$):

1.159, 1.1718	($25^{\circ}C$, mixture of isomers, <i>o</i> -TCP, Riddick et al. 1986)
1.16	(<i>o</i> -TCP, Verschueren 1983; Riddick et al. 1987; Budavari 1989)

Molar Volume (cm^3/mol):

308.1	($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)
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Enthalpy of Vaporization, ΔH_v (kJ/mol):

116.3, 102.9, 113	(<i>m</i> -TCP, Small et al. 1948)
113.4	(<i>p</i> -TCP, Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.40	(shake flask-GC, Saeger et al. 1979)
0.074	(<i>p</i> -TCP practical grade, shake flask-nephelometry; Hollifield 1979)
0.36	(mixed isomers, Muir 1984)
< 0.10	(Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00516-0.00612* (*m*-TCP, Celluloid Corporation samples at $80^{\circ}C$, static and dynamic methods, measured range $80-136^{\circ}C$, Verhoek & Marshall 1939)

$\log(P/\mu mHg) = 15.886 - 6088/(T/K)$; temp range $80-136^{\circ}C$ (*m*-TCP, Celluloid Corporation samples, static and dynamic methods, Verhoek & Marshall 1939)

- 0.0132* (*m*-TCP, Eastman Kodak Co. samples at 85.2°C, static and dynamic methods, measured range 85.2–126°C, Verhoek & Marshall 1939)
 $\log(P/\mu\text{mHg}) = 13.982 - 5373/(T/K)$; temp range 85.2–126°C (*m*-TCP, Eastman Kodak Co. samples, static and dynamic methods, Verhoek & Marshall 1939)
 0.0113* (*p*-TCP, 92°C, static and dynamic methods, measured range 92–145°C, Verhoek & Marshall 1939)
 $\log(P/\mu\text{mHg}) = 15.223 - 5926/(T/K)$; temp range 92–145°C (*p*-TCP, static and dynamic methods, Verhoek & Marshall 1939)
 4.13×10^{-4} (extrapolated from exptl. data, measured range 140–156°C, commercial quality, ebulliometry, Burrows 1946)
 $\log(P/\text{mmHg}) = 12.69 - 5925/(T/K)$; temp range: ~100–150°C (Antoine eq. from exptl., effusion, technical grade, Small et al. 1948)
 $\log(P/\text{mmHg}) = 12.89 - 6088/(T/K)$ (*m*-TCP, Antoine eq. from literature, Small et al. 1948)
 $\log(P/\text{mmHg}) = 10.98 - 5373/(T/K)$ (*m*-TCP, Antoine eq. from literature, Small et al. 1948)
 $\log(P/\text{mmHg}) = 12.22 - 5895/(T/K)$; temp range: 100–150°C (*m*-TCP, Antoine eq., effusion method, data presented in graph and Antoine eq., Small et al. 1948)
 $\log(P/\text{mmHg}) = 12.22 - 5926/(T/K)$ (*p*-TCP, effusion, Antoine eq., Small et al. 1948)
 $\log(P/\mu\text{mHg}) = 14.12 - 5480/(T/K)$; temp range 115–168°C (*p*-TCP, pendulum-tensimeter method, Perry & Weber 1949)
 $\log(P/\text{mmHg}) = [-0.2185 \times 20835.9/(T/K)] + 10.654252$; temp range 154.6–313°C (tritoyl phosphate, Antoine eq., Weast 1972–73)
 $\log(P/\text{kPa}) = 11.81 - 5925/(T/K)$ (mixed isomers, Antoine eq., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 8.56 - 4535/(T/K)$ (*o*-TCP, Antoine eq., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 10.67 - 5787/(T/K)$ (*m*-TCP, Antoine eq., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 13.24 - 5480/(T/K)$ (*p*-TCP, Antoine eq., Riddick et al. 1986)
 2.26×10^{-4} (*o*-TCP, Antoine eq., interpolated, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 8.565 - 4535/(T/K)$; temp range 293–700 K (*o*-TCP, Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 11.8856 - 6104.5/[(T/K) - 10.81]$; temp range 398–530 K (*m*-TCP, Antoine eq. for liquid state, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 10.245 - 5480/(T/K)$; temp range 388–530 K (*p*-TCP, Antoine eq. for liquid state, Stephenson & Malanowski 1987)
 3.07×10^{-4} , 1.25×10^{-4} (estimated from reported boiling points, Boethling & Cooper 1985)
 1.87×10^{-4} (quoted measured value, Boethling & Cooper 1985)
 6.10×10^{-6} (liquid P_L , GC-RT correlation, Hinckley et al. 1990)
 $\log(P/\text{mmHg}) = 21.1624 - 5.2756 \times 10^3/(T/K) - 3.3565 \cdot \log(T/K) + 8.666 \times 10^{-6} \cdot (T/K) - 2.9202 \times 10^{-9} \cdot (T/K)^2$;
 temp range 428–566 K (*o*-TCP, vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

- 0.0218 (calculated-P/C, Muir 1984, Muir et al. 1985)
 0.283, 0.172, 0.111 (calculated-P/C, Boethling & Cooper 1985)
 8.38 (*m*-TCP, gas stripping, Muir et al. 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.42 (HPLC-RT correlation, Veith 1979)
 5.11 (shake flask-concn ratio, Saeger et al. 1979)
 4.30, 4.65; 4.50 (RP-HPTLC- k' correlation, Renberg et al. 1980)
 5.107–5.12 (Muir 1984)
 5.10–5.30 (Bengtsson et al. 1986)

Bioconcentration Factor, $\log BCF$:

- 5.505, 4.45, 3.57, 3.57, 3.46 (*p*-TCP, ecological magnification factors for alga, snail, mosquito, fish and *Daphnia*, Metcalf 1976)
 2.88 (calculated for rainbow trout, Saeger et al. 1979)
 2.22 (fathead minnow, 32-d exposure, Veith et al. 1979)
 3.44, 3.15, 3.17 (*p*-TCP for rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)

- 2.89 (*p*-TCP for rainbow trout, calculated with hexane extract, Muir et al. 1983b)
 3.34, 2.97, 2.77 (*p*-TCP for fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)
 2.85 (*p*-TCP, fathead minnow, calculated with hexane extractable radioactivity, Muir et al. 1983b)
 3.07, 2.89, 3.04 (*m*-TCP for rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)
 2.49 (*m*-TCP for rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
 3.22, 2.77, 2.59 (*m*-TCP for fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)
 2.66 (*m*-TCP, fathead minnow, calculated with hexane extract, Muir et al. 1983b)
 3.15, 2.89; 3.64 (rainbow trout: *p*-, *m*-TCP, static expt.; estimated- K_{OW} , Boethling & Cooper 1985)
 2.60 (bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log K_{OC} :

- 4.44 (calculated- K_{OW} , Muir 1984)
 3.86 (estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 496$ d (estimated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 73$ d and 52 d at 22°C for aryl phosphates (75% TCP and 18% TXP) in demineralized and river water (Wagemann et al. 1974; quoted, Boethling & Cooper 1985);
 degradation $t_{1/2} = 3$ –4 d for *o*-, *m*-TCP and 5 d for *p*-TCP in Lake Ontario water (Howard & Dao 1979)
 second order alkaline hydrolysis rate constant $k = 0.025$ M⁻¹ s⁻¹ (estimated, *p*-TCP, Wolfe 1980)
 $t_{1/2} = 1.31$ h, 1.66 h for *m*-TCP and *p*-TCP, respectively, at pH 13.0 in acetone/water 1:1 solution (Muir et al. 1983b).

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

For *p*-TCP:

- $k_1 = 25.8$ h⁻¹, 21.8 h⁻¹ (rainbow trout, exposure concn 5, 50 µg/L, Muir et al. 1983b).
 $k_1 = 15.9$ h⁻¹, 7.80 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L, Muir et al. 1983b).
 $k_2 = 0.0104$ h⁻¹, 0.00963 h⁻¹ (rainbow trout, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
 $k_2 = 0.0106$ h⁻¹, 0.0133 h⁻¹ (rainbow trout, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b).
 $k_2 = 0.0096$ h⁻¹, 0.0077 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
 $k_2 = 0.0070$ h⁻¹, 0.0095 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b).

For *m*-TCP:

- $k_1 = 28.8$ h⁻¹, 24.0 h⁻¹ (rainbow trout, exposure concn 5, 50 µg/L, Muir et al. 1983b).
 $k_1 = 18.2$ h⁻¹, 12.2 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L, Muir et al. 1983b).
 $k_2 = 0.0242$ h⁻¹, 0.0229 h⁻¹ (rainbow trout, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
 $k_2 = 0.0115$ h⁻¹, 0.0149 h⁻¹ (rainbow trout, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b).
 $k_2 = 0.0147$ h⁻¹, 0.0117 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L for 0–144 h interval, Muir et al. 1983b).
 $k_2 = 0.0085$ h⁻¹, 0.0101 h⁻¹ (fathead minnow, exposure concn 5, 50 µg/L for 0–432 h interval, Muir et al. 1983b).

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
 degradation $t_{1/2} = 3$ –4 d for *o*-, *m*-TCP and $t_{1/2} = 5$ d for *p*-TCP in Lake Ontario water (Howard & Dao 1979);
 $t_{1/2} = 1.66$ h and 1.31 h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b);
 volatilization $t_{1/2}(\text{calc}) = 296$ d in 1 m deep water system (Muir 1984);

pseudo-first-order $t_{1/2} = 0.57$ d in pond water; moderate volatilization from water column with $t_{1/2} = 84$ d at 0.5-m depth (Muir et al. 1985).

Groundwater:

Sediment: $t_{1/2} = 39$ d in bottom sediment of a small pond (Muir et al. 1985).

Soil:

Biota: depuration $t_{1/2} = 135$ h in chironomid larvae (Muir et al. 1985);

elimination $t_{1/2} = 4$ d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

TABLE 15.1.4.1.7.1

Reported vapor pressures of tricresyl phosphate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
tri- <i>m</i> -cresyl phosphate				tri- <i>p</i> -cresyl phosphate	
Verhoek & Marshall 1939				Verhoek & Marshall 1939	
static and dynamic methods				static and dynamic methods	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
Celluloid Corp. samples		Eastman Kodak samples			
80	0.00612	85.2	0.0132	92.0	0.0113
80	0.00604	95.4	0.0333	100.0	0.0267
80	0.00516	105.6	0.0749	110.0	0.0653
90	0.0177	115.8	0.1773	119.0	0.180
100.2	0.0461	126.0	0.448	119.0	0.189
109.9	0.1233			123.5	0.281
110.5	0.1276	eq. 1	P/ μmHg	124.0	0.283
114.0	0.212	A	13.982	125.0	0.249
114.0	0.208	B	5373	129.0	0.441
114.0	0.213			129.0	0.448
119.0	0.323	$\Delta H_v = 102.84$ kJ/mol		134.0	0.668
120.0	0.315			134.5	0.696
120.7	0.316			135.0	0.600
124.0	0.492			145.0	1.560
124.0	0.504				
125.9	0.509			eq. 1	P/ μmHg
128.8	0.739			A	15.223
129.0	0.785			B	5926
130.0	0.777				
131.0	0.809			$\Delta H_v = 113.43$ kJ/mol	
136.2	1.352				
eq. 1	P/ μmHg				
A	15.886				
B	6088				
$\Delta H_v = 116.54$ kJ/mol					

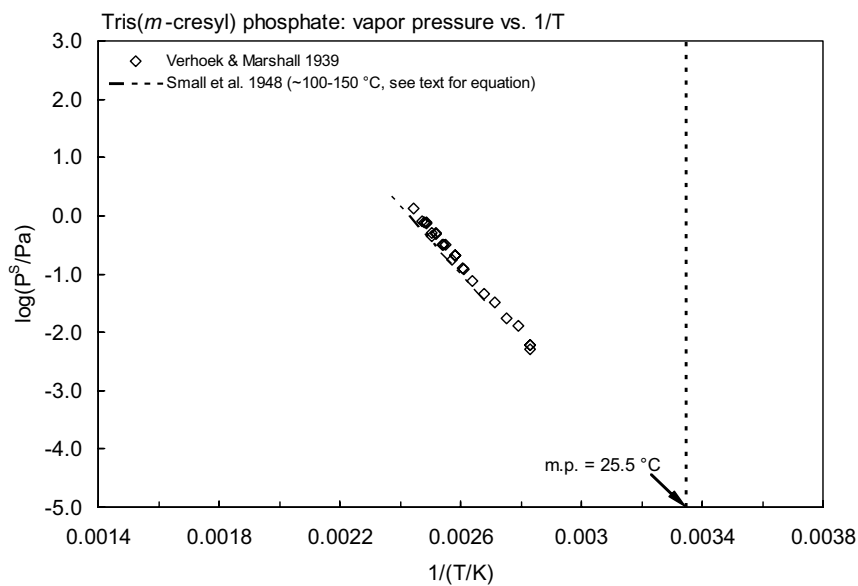


FIGURE 15.1.4.1.7.1a Logarithm of vapor pressure versus reciprocal temperature for *tris(m-cresyl)* phosphate.

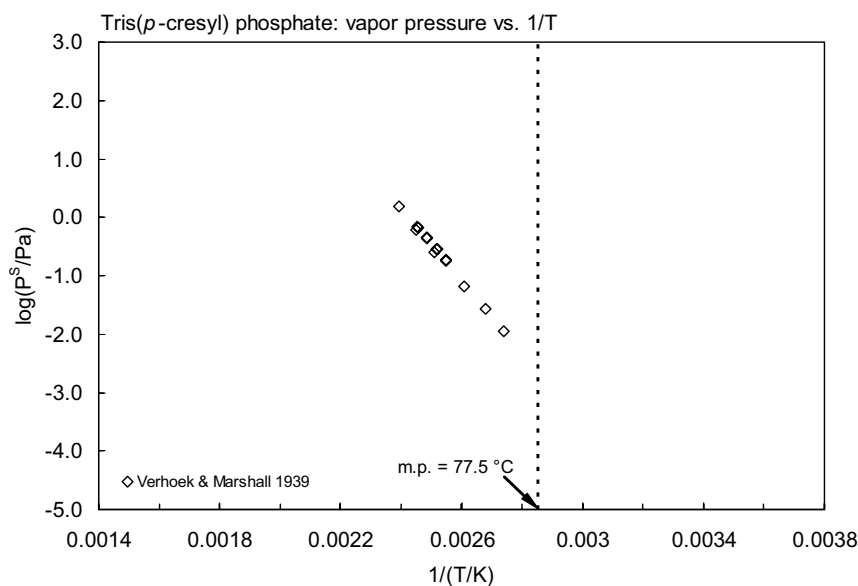
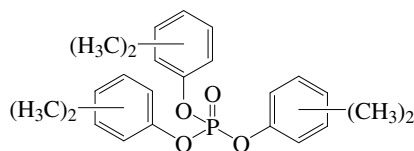


FIGURE 15.1.4.1.7.1b Logarithm of vapor pressure versus reciprocal temperature for *tris(p-cresyl)* phosphate.

15.1.4.1.8 Trixylenyl phosphate (TXP)



Common Name: Trixylenyl phosphate

Synonym: TXP

Chemical Name:

CAS Registry No: 25155-23-1

Molecular Formula: $C_{24}H_{27}O_4P$, $[(CH_3)_2C_6H_3]_3O_4P$

Molecular Weight: 410.442

Melting Point ($^{\circ}C$):

-20 (mixed isomers, Muir 1984)

Boiling Point ($^{\circ}C$):

261 (at 6 mmHg, Muir 1984)

225–295/6 mmHg, 248–265/4 mmHg, 270/3 mmHg (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.89 (shake flask-GC, Saeger et al. 1979)

0.89 (mixed isomers, Muir 1984)

Vapor Pressure (Pa at $25^{\circ}C$):

7.20×10^{-4} , 1.47×10^{-4} , 3.067×10^{-5} (estimated from reported boiling points, Boethling & Cooper 1985)

6.93×10^{-6} ($30^{\circ}C$, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.334, 0.0689, 0.0142, 0.00314 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.63 (shake flask-concn ratio, Saeger et al. 1979)

5.26 (RP-HPTLC- k' correlation, Renberg et al. 1980)

5.63 (Muir 1984)

5.70 (Boethling & Cooper 1985)

6.40–6.60 (Bengtsson et al. 1986)

Bioconcentration Factor, $\log BCF$:

3.15 (calculated for rainbow trout, Saeger et al. 1979)

4.04 (estimated from K_{OW} , Boethling & Cooper 1985)

3.11, 3.24, 3.28 (bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

4.44 (calculated- K_{OW} , Muir 1984)

3.67 (estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: 65% primary biodegradation in 14 weeks test duration for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} = 28\text{--}48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: 65% primary biodegradation in 14 weeks test duration for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} = 28\text{--}48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Groundwater:

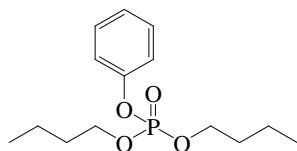
Sediment:

Soil:

Biota: eliminated $t_{1/2} = 4$ d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

15.1.4.2 Triaryl/alkyl phosphates

15.1.4.2.1 Dibutyl phenyl phosphate (DBPP)



Common Name: Dibutyl phenyl phosphate

Synonym: DBPP

Chemical Name:

CAS Registry No: 2528-26-1

Molecular Formula: $C_{14}H_{23}O_4P$, $(C_4H_9)_2C_6H_5O_4P$

Molecular Weight: 286.303

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

200/20 mmHg (Muir 1984)

155/2 mmHg, 155/1 mmHg (quoted, Boethling & Cooper 1985)

Density (g/cm^3):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

96 (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

66.7 (200 $^{\circ}C$, Muir 1984)

0.084, 0.0307 (estimated from boiling points, Boethling & Cooper 1985)

746* (170 $^{\circ}C$, GC-RT correlation, measured range 170–200 $^{\circ}C$, Skene & Krzymien 1995)

Henry's Law Constant (Pa $\cdot m^3/mol$ at $25^{\circ}C$):

0.253, 0.089 (estimated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{ow} :

4.27 (shake flask-concn ratio, Saeger et al. 1979)

3.23 (RP-HPTLC- k' correlation, Renberg et al. 1980)

Bioconcentration Factor, log BCF:

2.43 (calculated, Saeger et al. 1979)

3.04 (calculated- K_{ow} , Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{oc} :

3.70 (calculated- K_{ow} , Muir 1984)

2.56 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 0.4$ d (calculated, Muir 1984)

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

volatilization $t_{1/2} \sim 0.4$ d from 1 m deep water (Muir 1984).

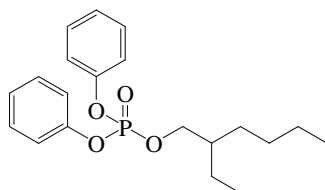
Groundwater:

Sediment:

Soil:

Biota:

15.1.4.2.2 2-Ethylhexyl diphenyl phosphate (EHDP)



Common Name: 2-Ethylhexyl diphenyl phosphate

Synonym: EHDP

Chemical Name:

CAS Registry No: 1241-94-7

Molecular Formula: $C_{20}H_{27}O_4P$, $C_8H_{17}(C_6H_5)_2O_4P$

Molecular Weight: 362.399

Melting Point ($^{\circ}C$):

-80 (Muir 1984)

Boiling Point ($^{\circ}C$):

181/0.6 mmHg (Wightman & Malaiyandi 1983)

239/1 mmHg (Muir 1984)

150/0.2 mmHg, 375/760 mmHg, 230/5 mmHg (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.9 (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at $25^{\circ}C$):

4.0×10^{-3} , 3.47×10^{-3} , 1.87×10^{-3} (estimated from reported boiling points, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.60 (calculated-P/C, Muir 1982, 1984)

0.77, 0.648, 0.345 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.73 (shake flask-concn ratio, Saeger et al. 1979)

5.00 (RP-HPLC- k' correlation, Renberg et al. 1980)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.20 (calculated, Saeger et al. 1979)

3.17, 3.06; 3.12 (rainbow trout: calculated from rate constant ratio k_1/k_2 for exposure concn 5 and 50 $\mu g/L$; mean, Muir & Grift 1981)

3.52 (calculated- K_{ow} , Muir & Grift 1981)

4.11 (calculated- K_{ow} , Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{oc}$:

4.49 (calculated- K_{ow} , Muir 1984)

3.49 (estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: half-life for 1 m deep water was estimated to be 7 d (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

rapid biodegradation $t_{1/2} = 2$ d in river water (quoted, Muir & Grift 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 48.5 \text{ h}^{-1}$, 33.0 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir & Grift 1981)

$k_2 = 0.0298 \text{ h}^{-1}$, 0.0294 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir & Grift 1981)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

rapid biodegradation $t_{1/2} = 2$ d in river water (quoted, Muir & Grift 1981);

volatilization $t_{1/2} \sim 7$ d for 1 m deep water (estimated, Muir 1984).

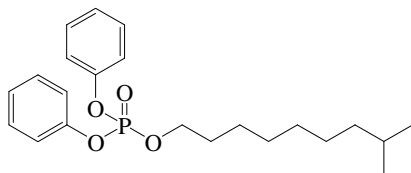
Groundwater:

Sediment:

Soil:

Biota:

15.1.4.2.3 Isodecyl diphenyl phosphate (IDDP)



Common Name: Isodecyl diphenyl phosphate

Synonym: IDDP

Chemical Name:

CAS Registry No: 29761-21-5

Molecular Formula: $C_{22}H_{31}O_4P$, $C_{10}H_{21}(C_6H_5)_2O_4P$

Molecular Weight: 390.452

Melting Point ($^{\circ}C$):

< -50 (Muir 1984)

Boiling Point ($^{\circ}C$):

245/10 mmHg (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.75 (room temp, shake flask-GC, Saeger et al. 1979)

0.80 (Boethling & Cooper 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

< 13.33, 66.7 (100, $150^{\circ}C$, Muir 1984)

2.133×10^{-3} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

12.97 (calculated-P/C, Muir 1984)

1.013 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.44 (shake flask-concn ratio, Saeger et al. 1979)

3.31, 5.72; 5.42 (RP-HPTLC- k' correlation; mean, Renberg et al. 1980)

5.70 (quoted measured value, Boethling & Cooper 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.04 (calculated, Saeger et al. 1979)

3.88 (estimated from solubility, Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

4.33 (calculated- K_{ow} , Muir 1984)

3.69 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 1.3$ d for 1 m deep water system (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
volatilization $t_{1/2} \sim 1.3$ d for 1 m deep water system (Muir 1984).

Groundwater:

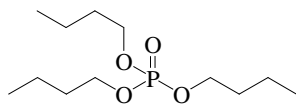
Sediment:

Soil:

Biota:

15.1.4.3 Trialkyl phosphate

15.1.4.3.1 Tributyl phosphate (TBP)



Common Name: Tributyl phosphate

Synonym: TBP, butyl phosphate

Chemical Name: tri-*n*-butyl phosphate

CAS Registry No: 126-73-8

Molecular Formula: $C_{12}H_{27}O_4P$; $(C_4H_9)_3O_4P$

Molecular Weight: 266.314

Melting Point ($^{\circ}C$):

< -80 (Dean 1985, Stephenson & Malanowski 1987)

Boiling Point ($^{\circ}C$):

289 (Lide 2003)

Density (g/cm^3):

0.972 ($25^{\circ}C$, Dean 1992)

0.976 (Riddick et al. 1986; Budavari 1989)

Molar Volume (cm^3/mol):

273.8 (Stephenson & Malanowski 1987)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

14.67 (Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

422* (shake flask-electrometric titration, measured range 3.4 – $50^{\circ}C$, Higgins et al. 1959)

280 (shake flask-GC, Saeger et al. 1979)

390 (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.89 (extrapolated, Evans et al. 1930)

0.10, 2.0 (114, $160.2^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 7.7110 - 3206.5/(t/^{\circ}C + 273)$ (Antoine eq., Riddick et al. 1986)

$\log(P/kPa) = 7.7110 - 3206.5/(T/K)$ (Antoine eq., liquid phase, temp range 500 – 562 K, Stephenson & Malanowski 1987)

0.0202 (estimated from average air-borne concn, Skene & Krzymien 1995)

0.031, 0.015, 0.026, 0.030, 0.022 (extrapolated values from various reported Antoine equations, Skene & Krzymien 1995)

0.149* (gas saturation-GC, measured range 0 – $80^{\circ}C$; Skene & Krzymien 1995)

$\log(P/Pa) = 8.85629 - 1690.26/(T/K - 123.431)$; temp range 0 – $80^{\circ}C$, (Antoine eq. derived from exptl. data, gas saturation-GC, Skene & Krzymien 1995)

0.015 (TBP in Skydrol 500B-4 hydraulic fluid, gas saturation-GC, Skene & Krzymien 1995)

927 – $1060^{\circ}C$ ($170^{\circ}C$, GC-RT correlation, measured range 170 – $200^{\circ}C$. Skene & Krzymien 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2513 (estimated-P/C, Muir 1984)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.004 (shake flask-concn ratio, Saeger et al. 1979)
- 3.99 (Sasaki et al. 1981)
- 4.004, 4.01 (quoted, Muir 1984)

Bioconcentration Factor, $\log BCF$:

- 2.28 (calculated, Saeger et al. 1979)
- 1.49–1.54 (killifish, 90-h exposure, static water system, Sasaki et al. 1981)
- 0.78–1.04 (goldfish, 90-h exposure, static water system, Sasaki et al. 1981)
- 0.602–1.43 (killifish, static water system, Sasaki et al. 1982)
- 1.20–1.43 (killifish, 4–38 d exposure, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.56 (calculated- K_{OW} , Muir 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 0.4$ d for 1 m deep water system (calculated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

hydrolysis $t_{1/2} \sim 1$ yr for trialkyl phosphates (Wolfe 1980);

$t_{1/2} = 58$ h in the water containing killifish and more than 100 h for goldfish (Sasaki et al. 1981)

volatilization $t_{1/2} \sim 0.4$ d from 1 m deep water (estimated, Muir 1984).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.4.3.1.1

Reported aqueous solubilities and vapor pressures of tributyl phosphate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Aqueous solubility		Vapor pressure					
Higgins et al. 1959		Skene & Krzymien 1995					
shake flask-titration		gas saturation-GC		GC-RT correlation			
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
3.4	1075	0	0.004	different reference standards			
4.0	1012	5	0.01	170	1042	170	1060
5.0	957	15	0.04	185	1646	185	1849
13.0	640	25	0.15	200	4442	200	4102
25	422	35	0.39	Linear extrapolation eq.*		Linear extrapolation eq.*	
50	285	50	1.59	eq. 1	P/Pa	eq. 1	P/Pa
		65	7.17	A	12.336	A	12.333
		80	31.9	B	4124.2	B	4127.8
				170	927	170	993
		eq. 3	P/Pa	185	2179	185	1849
		A	8.85629	200	3030	200	3559
		B	1690.26	Linear extrapolation eq.*		Linear extrapolation eq.*	
		C	-123.431	eq. 1	P/Pa	eq. 1	P/Pa
				A	12.633	A	12.480
				B	4306.7	B	4215.3
				170	1109		
				185	2080		
				200	4408		
				Linear extrapolation eq.*			
				eq. 1	P/Pa		
				A	12.253		
				B	4080.7		
*regression eq. for extrapolation to temp range of gas saturation measurements 0–50°C							

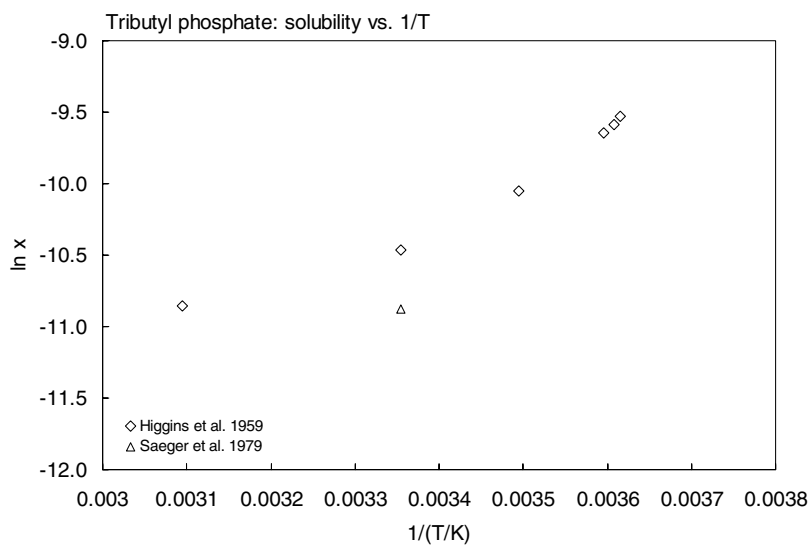


FIGURE 15.1.4.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tributyl phosphate.

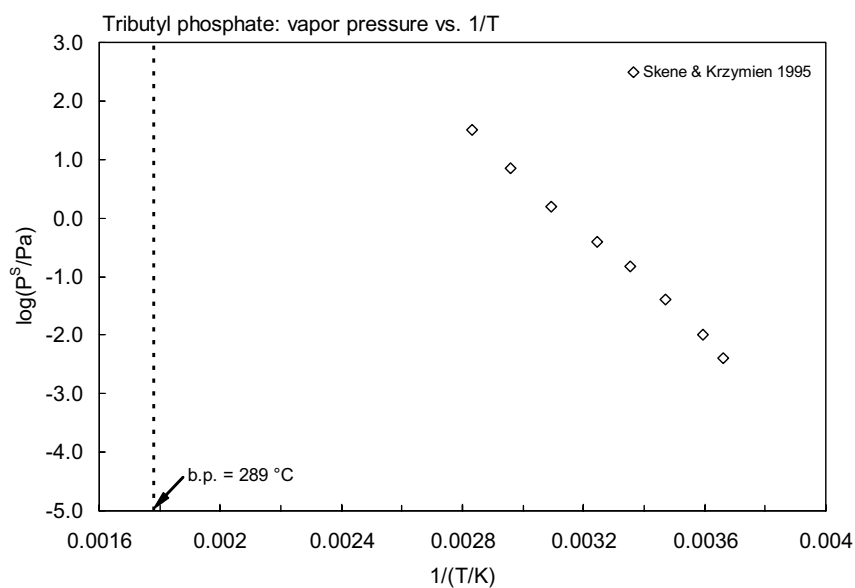
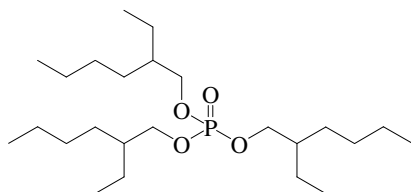


FIGURE 15.1.4.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for tributyl phosphate.

15.1.4.3.2 *Tris(2-ethylhexyl) phosphate (TEHP)*

Common Name: Tris(2-ethylhexyl) phosphate

Synonym: TEHP

Chemical Name:

CAS Registry No: 78-42-2

Molecular Formula: $C_{24}H_{51}O_4P$, $(C_8H_{17})_3O_4P$

Molecular Weight: 434.633

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

215 $^{\circ}C$ /4 mmHg (Aldrich Catalog 1989–99)

Density (g/cm³ at 20 $^{\circ}C$): 0.924 (Aldrich catalog 1998–99)

Molar Volume (cm³/mol):

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25 $^{\circ}C$):

< 1000 (room temp, shake flask-GC, Saeger et al. 1979)

600 (practical grade, shake flask-nephelometry, Hollifield 1979)

Vapor Pressure (Pa at 25 $^{\circ}C$):

$\log(P/\text{mmHg}) = 12.85 - 5812/(T/K)$; exptl. data presented in graph and Antoine eq. (effusion, Small et al. 1948)
(See figure at the end of this section.)

1.10×10^{-5} (liquid P_L , GC-RT correlation, Hinckley et al. 1990)

Henry's Law Constant (Pa·m³/mol at 25 $^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.23 (shake flask-concn ratio, Saeger et al. 1979)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.40 (calculated, Saeger et al. 1979)

Sorption Partition Coefficient, $\log K_{oc}$:

3.68 (soil, calculated- K_{ow} , Muir 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water (Saeger et al. 1979).

Groundwater:

Sediment:

Soil:

Biota:

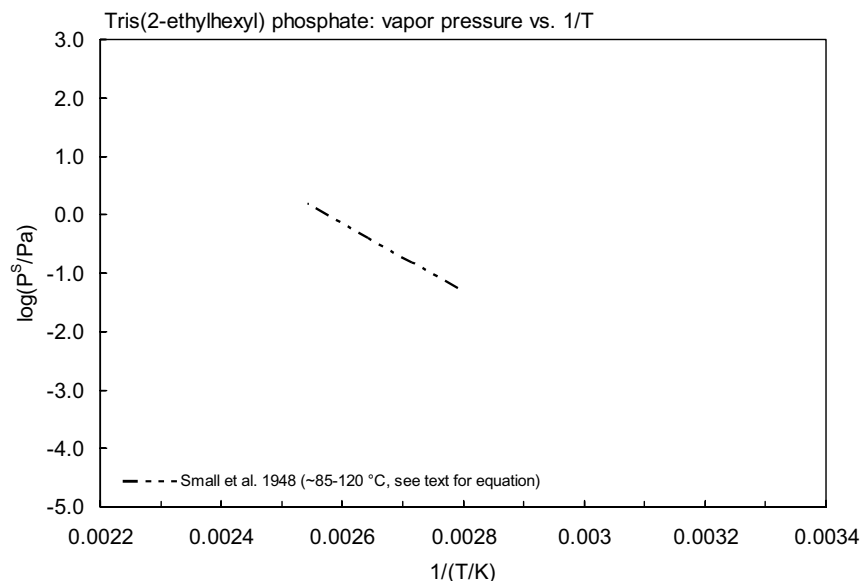
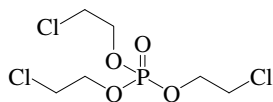


FIGURE 15.1.4.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for *tris*(2-ethylhexyl) phosphate.

15.1.4.4 Trihaloalkyl phosphates

15.1.4.4.1 Tris(2-chloroethyl) phosphate (TCEP)



Common Name: Tris(2-chloroethyl) phosphate

Synonym: TCEP

Chemical Name:

CAS Registry No: 115-96-8

Molecular Formula: $C_6H_{12}Cl_3O_4P$, $(C_2H_4Cl)_3O_4P$

Molecular Weight: 285.490

Melting Point ($^{\circ}C$): -55

Boiling Point ($^{\circ}C$):

214/25 mmHg (Muir 1984)

330 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.390 (Aldrich catalog 1989–99)

Molar Volume (cm^3/mol):

205.4 ($20^{\circ}C$, Stephenson & Malanowski 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

7000 (Eldefrawi et al. 1977; quoted, Sasaki et al. 1981)

7000 (quoted, Muir 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

8.23 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 4.346 - 1917/(T/K)$ (Antoine eq., temp range: 293–546 K, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.00241 (calculated-P/C, Muir 1984)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.43 (shake flask, Sasaki et al. 1981)

1.48 (quoted, Muir 1984)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.40 (calculated, Saeger et al. 1979)

0.34 (killifish, 90-h exposure, static water system, Sasaki et al. 1981)

$-0.155, -0.046$ (goldfish, 90-h exposure, static water system, Sasaki et al. 1981)

0.36–1.10 (killifish, static water system, Sasaki et al. 1982)

0.041–1.10 (killifish, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

2.18 (calculated- K_{ow} , Muir 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 536$ d from 1 m deep water system (estimated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

biological $t_{1/2} = 1.65$ h and elimination $t_{1/2} = 0.7$ h for killifish (Sasaki et al. 1982).

Half-Lives in the Environment:

Air:

Surface water: first order reduction process in river water, an estimated $t_{1/2} \sim 2.3$ d in Rhine River (Zoeteman et al. 1980);

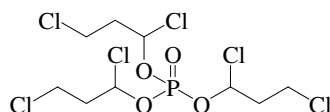
volatilization $t_{1/2}(\text{calc}) = 536$ d from 1 m deep water system (Muir 1984).

Groundwater:

Sediment:

Soil:

Biota: biological $t_{1/2} = 1.65$ h for accumulation, $t_{1/2} = 0.7$ h for elimination in killifish (Sasaki et al. 1982).

15.1.4.4.2 *Tris(1,3-dichloropropyl) phosphate (TDCPP)*

Common Name: Tris(1,3-dichloropropyl) phosphate

Synonym: TDCPP, TCPP, Fyrol FR-2, 1,3-dichloro-2-propanol phosphate (3:1), phosphoric acid tris(1,3-dichloro-2-propyl)ester, tris[2-chloro-1-(chloromethyl)ethyl]phosphate

Chemical Name:

Use: flame retardant

CAS Registry No: 40120-74-9

Molecular Formula: $C_9H_{15}Cl_6O_4P$, $(C_3H_5Cl_2)_3O_4P$

Molecular Weight: 430.906

Melting Point ($^{\circ}C$):

26.7 (Muir 1984)

viscous liquid (Budavari 1989)

Boiling Point ($^{\circ}C$):

236–237/5 mmHg (Muir 1984)

Density (g/cm^3 at $20^{\circ}C$):

1.5022 (Budavari 1989)

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.966

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

19.2 (Metcalf 1976)

7.0 (practical grade, shake flask-nephelometry, Hollifield 1979)

100 (Eldefrawi et al. 1977; quoted, Sasaki et al. 1981, Muir 1984)

~ 100 (Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.76 (shake flask-concn ratio, Sasaki et al. 1981)

3.74 (quoted, Muir 1984)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.89–2.05 (killifish, 100-h exposure, static system, Sasaki et al. 1981)

0.48–0.70 (goldfish, 90-h exposure, static system, Sasaki et al. 1981)

1.67–2.03 (killifish, static system, Sasaki et al. 1982)

1.49–1.69 (killifish, 32-d exposure, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

3.41 (calculated- K_{OW} , Muir 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$t_{1/2} = 31$ h in the water containing killifish and $t_{1/2} = 42$ h for goldfish, so that absorption occurred at similar rates in both fishes (Sasaki et al. 1981).

Half-Lives in the Environment:

Air:

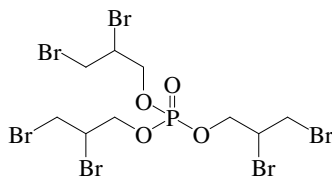
Surface water: $t_{1/2} = 31$ h in the water containing killifish and $t_{1/2} = 42$ h for goldfish, so that absorption occurred at similar rates in both fishes (Sasaki et al. 1981).

Groundwater:

Sediment:

Soil:

Biota: biological $t_{1/2} = 1.65$ h (killifish, Sasaki et al. 1982).

15.1.4.4.3 *Tris(2,3-dibromopropyl) phosphate (TDBPP)*

Common Name: Tris(2,3-dibromopropyl) phosphate

Synonym: TDBPP, Tris-BP, 2,3-dibromo-1-propanol phosphate(3:1), phosphoric acid tris(2,3-dibromopropyl) ester, Apex 462-3, Flammex AP, Firemaster: V-T 23P, Fyrol HB 32

Chemical Name:

Use: flame retardant

CAS Registry No: 126-72-7

Molecular Formula: $C_9H_{15}Br_6O_4P$, $(C_3H_5Br_2)_3O_4P$

Molecular Weight: 697.610

Melting Point ($^{\circ}C$):

5.5 (Muir 1984)

viscous liquid (Budavari 1989)

Boiling Point ($^{\circ}C$):

65/0.005 mmHg (Muir 1984)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

8.0 (practical grade, shake flask-nephelometry, Hollifield 1979)

1.60 (Muir 1984)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0108 (calculated-P/C, Muir 1984)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.98 (HPLC-RT correlation, Veith et al. 1979)

4.39 (Muir 1984)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

0.44 (calculated- K_{OW} , Veith et al. 1979)

Sorption Partition Coefficient, $\log K_{OC}$:

3.76 (calculated- K_{OW} , Muir 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ (calc) = 1.9 d in 1 m deep water system (Muir 1984).

Half-Lives in the Environment:

Surface water: volatilization $t_{1/2}$ (calc) = 1.9 d in 1 m deep water system (Muir 1984).

15.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 15.2.1

Summary of physical properties of esters and phthalate esters

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M	
							cm ³ /mol	
							MW/ρ at 20°C	Le Bas
Aliphatic esters:								
Methyl formate	107-31-3	HCO ₂ CH ₃	60.052	−99	31.7	1	61.64	62.6
Ethyl formate	109-94-4	HCO ₂ C ₂ H ₅	74.079	−79.6	54.4	1	80.35	86.4
Propyl formate	110-74-7	C ₄ H ₈ O ₂	88.106	−92.9	80.9	1	97.30	110.8
Butyl formate	592-84-7	C ₅ H ₁₀ O ₂	102.132	−91.9	106.1	1		133
Isobutyl formate	542-55-2	C ₅ H ₁₀ O ₂	102.132	−95.8	98.2	1		133
Methyl acetate	79-20-9	(CH ₃) ₂ CO ₂	74.079	−98.25	56.87	1	79.30	84.8
Vinyl acetate	108-05-4	C ₄ H ₆ O ₂	86.09	−93.2	72.8	1	92.40	101.2
Allyl acetate	591-87-7	C ₅ H ₈ O ₂	100.117		103.5	1		125.6
Ethyl acetate	141-78-6	C ₄ H ₈ O ₂	88.106	−83.8	77.11	1	97.83	108.6
Propyl acetate	109-60-4	C ₅ H ₁₀ O ₂	102.132	−93	101.54	1	115.04	133
Butyl acetate	123-86-4	C ₆ H ₁₂ O ₂	116.158	−78	126.1	1	132.54	155.2
Isobutyl acetate	110-19-0	C ₆ H ₁₂ O ₂	116.158	−98.8	116.5	1		155.2
Pentyl acetate	628-63-7	C ₇ H ₁₄ O ₂	130.185	−70.8	149.2	1	148.51	177.4
Isopentyl acetate	123-92-2	C ₇ H ₁₄ O ₂	130.185	−78.5	142.5	1		177.4
Hexyl acetate	142-92-7	C ₈ H ₁₆ O ₂	144.212	−80.9	171.5	1		199.6
Cyclohexyl acetate	622-45-7	C ₈ H ₁₄ O ₂	142.196		173			177.2
2-Ethylhexyl acetate	103-09-3	C ₁₀ H ₂₀ O ₂	172.265	−80	199	1		244
Benzyl acetate	140-11-4	C ₉ H ₁₀ O ₂	150.174	−51.3	213	1		177.2
Ethyl propionate	105-37-3	C ₅ H ₁₀ O ₂	102.132	−73.9	99.1	1		130.8
Ethyl butyrate	105-54-4	C ₆ H ₁₂ O ₂	116.158	−98	121.3	1		153
Methyl acrylate	96-33-3	C ₄ H ₆ O ₂	86.09	< −75	80.7	1	90.29	99.6
Ethyl acrylate	140-88-5	C ₅ H ₈ O ₂	100.117	−71.2	99.4	1	108.42	123.8
Methyl methacrylate	80-62-6	C ₅ H ₈ O ₂	100.117	−47.55	100.5	1	106.06	121.8
Ethyl methacrylate	97-63-2	C ₆ H ₁₀ O ₂	114.142		117			145.6
Aromatic esters:								
Methyl benzoate	93-58-3	C ₈ H ₈ O ₂	136.149	−12.4	199	1	125.07	151.2
Ethyl benzoate	93-89-0	C ₉ H ₁₀ O ₂	150.174	−34	212	1	142.87	175
Propyl benzoate	2315-68-6	C ₁₀ H ₁₂ O ₂	164.201	−51.6	211	1	160.48	199.4
Phenyl benzoate	93-99-2	C ₁₃ H ₁₀ O ₂	198.217	71	314	0.354		221.4
Benzyl benzoate	120-51-4	C ₁₄ H ₁₂ O ₂	212.244	21	323.5	1		243.6

Phthalate esters:

Dimethyl phthalate (DMP)	131-11-3	C ₁₀ H ₁₀ O ₄	194.184	5.5	283.7	1	163.11	206.4
Diethyl phthalate (DEP)	84-66-2	C ₁₂ H ₁₄ O ₄	222.237	-40.5	295	1	198.87	254
Diallyl phthalate (DAP)	131-17-9	C ₁₄ H ₁₄ O ₄	246.259	-77	290		219.68	288
Di- <i>n</i> -propyl phthalate (DnPP)	131-16-8	C ₁₄ H ₁₈ O ₄	250.291	-31.0	304.5	1		302.8
Di-isopropyl phthalate (DIPP)	605-45-8	C ₁₄ H ₁₈ O ₄	250.291	liquid		1		302.8
Di- <i>n</i> -butyl phthalate (DBP)	84-74-2	C ₁₆ H ₂₂ O ₄	278.344	-35	340	1	265.85	347.2
Di-isobutyl phthalate (DIBP)	84-69-5	C ₁₆ H ₂₂ O ₄	278.344		296.5	1		347.2
Dipentyl phthalate (DPP)	131-18-0	C ₁₈ H ₂₆ O ₄	306.397	< -54.5	342	1		391.6
Dihexyl phthalate (ΔHP)	84-75-3	C ₂₀ H ₃₀ O ₄	334.45	-27.4		1	337.83	436
Butyl 2-ethylhexyl phthalate (BOP)	85-69-8	C ₂₀ H ₃₀ O ₄	334.45	-37		1		436
Di- <i>n</i> -octyl phthalate (DOP)	117-84-0	C ₂₄ H ₃₈ O ₄	390.557	25		1	399.34	524.8
Di-isooctyl phthalate (DIOP)	27554-26-3	C ₂₄ H ₃₈ O ₄	390.557		370	1		524.8
<i>bis</i> (2-Ethylhexyl) phthalate (DEHP)	117-81-7	C ₂₄ H ₃₈ O ₄	390.557	-55	384	1	396.79	524.8
Di (hexyl, octyl, decyl) phthalate	39289-94-6	C ₂₅ H ₄₀ O ₄	404.583	-4		1		547.0
Di-isononyl phthalate (DINP)	9727830	C ₂₆ H ₄₂ O ₄	418.609	-48		1	420.71	569.2
Di-isodecyl phthalate (DIDP)	26761-40-0	C ₂₈ H ₄₆ O ₄	446.663	-50		1		613.6
Diundecyl phthalate (DUP)	3648-20-2	C ₃₀ H ₅₀ O ₄	474.716	35.5		0.789		658.0
Ditridecyl phthalate (DTDP)	43617	C ₃₄ H ₅₈ O ₄	530.823	-37		1		746.8
Butyl benzyl phthalate (BBP)	85-68-7	C ₁₉ H ₂₀ O ₄	312.360	-35	370	1		369.2

Phosphate esters:

<i>t</i> -Butylphenyl diphenyl phosphate	56803-37-3	C ₂₂ H ₂₃ O ₄ P	382.389	-21		1		
Cresyl diphenyl phosphate (CDP)	26444-49-5	C ₁₉ H ₁₇ O ₄ P	340.309					
Isopropylphenyl diphenyl phosphate (IPDP)	28108-99-8	C ₂₁ H ₂₁ O ₄ P	368.362	-26		1		
4-Cumylphenyl diphenyl phosphate	84602-56-2	C ₂₇ H ₂₅ O ₄ P	444.458					
Nonylphenyl diphenyl phosphate	13418387	C ₂₇ H ₃₃ O ₄ P	452.522					
Triphenyl phosphate (TPP)	115-86-6	C ₁₈ H ₁₅ O ₄ P	326.283	50.5		0.562		
Tricresyl phosphate (TCP)	1330-78-5	C ₂₁ H ₂₁ O ₄ P	368.362					
Trixylenyl phosphate (TXP)	25155-23-1	C ₂₄ H ₂₇ O ₄ P	410.442					
Dibutyl phenyl phosphate (DBPP)	2528-26-1	C ₁₄ H ₂₃ O ₄ P	286.303					
2-Ethylhexyl diphenyl phosphate	1241-94-7	C ₂₀ H ₂₇ O ₄ P	362.399	-80		1		
Isodecyl diphenyl phosphate (IDDP)	29761-21-5	C ₂₂ H ₃₁ O ₄ P	390.452	< -50		1		
Tributylphosphate (TBP)	126-73-8	C ₁₂ H ₂₇ O ₄ P	266.314	< -80		1		
Tris(2-ethylhexyl) phosphate	78-42-2	C ₂₄ H ₅₁ O ₄ P	434.633					
Tris(2-chloroethyl) phosphate	115-96-8	C ₆ H ₁₂ Cl ₃ O ₄ P	285.49			1		
Tris(1,3-dichloropropyl) phosphate	40120-74-9	C ₉ H ₁₅ Cl ₆ O ₄ P	430.906	26.7		0.962		
Tris(2,3-dibromopropyl) phosphate	126-72-7	C ₉ H ₁₅ Br ₆ O ₄ P	697.61	5.5		1		

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 15.2.2
Summary of selected physical-chemical properties of esters and phthalate esters at 25°C

Compound	Selected properties						Henry's law constant		
	Vapor pressure		Solubility			log K _{OW}	H/(Pa·m ³ /mol)		
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		calcd P/C	exptl (a)	exptl (b)
Aliphatic esters:									
Methyl formate	78060	78060	230000	3830	3830	−0.26	20.38		
Ethyl formate	32370	32600	118000	1593	1593	0.23	20.32		
Propyl formate	11030	11030	20500	232.7	232.7	0.73	47.40		
Butyl formate	3840	3840							
Isobutyl formate	5343	5400	10000	97.91	97.91		54.57		
Methyl acetate	28800	28800	245000	3307	3307	0.23	8.708	0.65	13.06
Vinyl acetate	14100	14100	20000	232.3	232.3	0.73	60.69		
Allyl acetate	6130	6130							
Ethyl acetate	12600	12600	80800	917.1	917.1		13.74		17.2
Propyl acetate	4500	4500	21000	205.6	205.6	1.24	21.88		22.09
Butyl acetate	1600	1600	6000	51.65	51.65	1.82	30.98		29.506
Isobutyl acetate	2860	2860	6300	54.24	54.24	1.6	52.73		
Pentyl acetate	550	550	1700	13.06	13.06	2.42	42.12		35.94
Isopentyl acetate	600	600	2000	15.36	15.36	2.13	39.06		
Hexyl acetate	670	670	500	3.446	3.467		193.2		
2-Ethylhexyl acetate	53	53	98.4	0.5712	0.5712	3.72	92.79		
Phenyl acetate						1.49			
Benzyl acetate	189	189	sl. sol.	sl. sol.		1.96			
Methyl propionate	11600	11600	62370	707.9	707.9		16.39	17.6	
Ethyl propionate	4966	4966	19200	188.0	188.0	1.21	26.42		
Methyl butyrate								20.82	
Ethyl butyrate	2300	2300	6500	55.96	55.96	1.73	41.10		
Methyl pentanoate								32.22	
Methyl hexanoate								37.18	
Methyl octanoate								79.32	
Methyl acrylate	11000	11000	49400	573.8	573.8	0.8	19.17		
Ethyl acrylate	5100	5100	15000	149.82	149.82	1.33	34.041		
Methyl methacrylate	5100	5100	15600	155.8	155.8	1.38	32.73		
Ethyl methacrylate						1.94			

Aromatic esters:

Methyl benzoate	52.58	52.28	2100	15.42	15.42	2.2	3.389
Ethyl benzoate	24	24	350	2.331	2.331	2.64	10.30
Propyl benzoate	100	100				3.18	
Phenyl benzoate		0.416				3.59	
Benzyl benzoate	0.043	0.043	16	0.0754	0.0754	3.97	0.5704

Phthalate esters:

Dimethyl phthalate (DMP)	0.22	0.22	4000	20.60	20.60	2.12	0.0107
Diethyl phthalate (DEP)	0.22	0.22	1080	4.859	4.859	2.47	0.0453
Di- <i>n</i> -butyl phthalate (DBP)	0.00187	0.00187	11.2	0.0402	0.0402	4.72	0.0465
Di- <i>n</i> -octyl phthalate (DOP)	1.33×10^{-5}	1.33×10^{-5}	0.0005	1.28×10^{-6}	1.28×10^{-6}	8.06	10.39
<i>bis</i> (2-Ethylhexyl)-phthalate	1.33×10^{-5}	1.33×10^{-5}	0.003	7.68×10^{-6}	7.68×10^{-6}	7.5	1.731
Butyl benzyl phthalate	0.00115	0.00115	2.69	0.0086	0.0086	4.60	0.1335

(a) Buttery et al. 1969

(b) Kieckbusch & King 1979

TABLE 15.2.3

Suggested half-life classes for esters and phthalate esters in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aliphatic esters:				
Methyl formate	3	3	4	5
Ethyl formate	3	3	4	5
Butyl formate	3	3	4	5
Methyl acetate	3	3	4	5
Vinyl acetate	3	3	4	5
Allyl acetate	3	3	4	5
Ethyl acetate	3	3	4	5
Propyl acetate	3	3	4	5
Butyl acetate	3	3	4	5
Pentyl acetate	3	3	4	5
Methyl methacrylate	2	3	4	5
Phthalate esters:				
Dimethyl phthalate (DMP)	4	5	6	7
Diethyl phthalate (DEP)	4	5	6	7
Di- <i>n</i> -butyl phthalate (DBP)	3	5	6	7
<i>bis</i> (2-Ethylhexyl)-phthalate (DEHP)	3	5	6	7
Butyl benzyl phthalate (BBP)	3	5	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

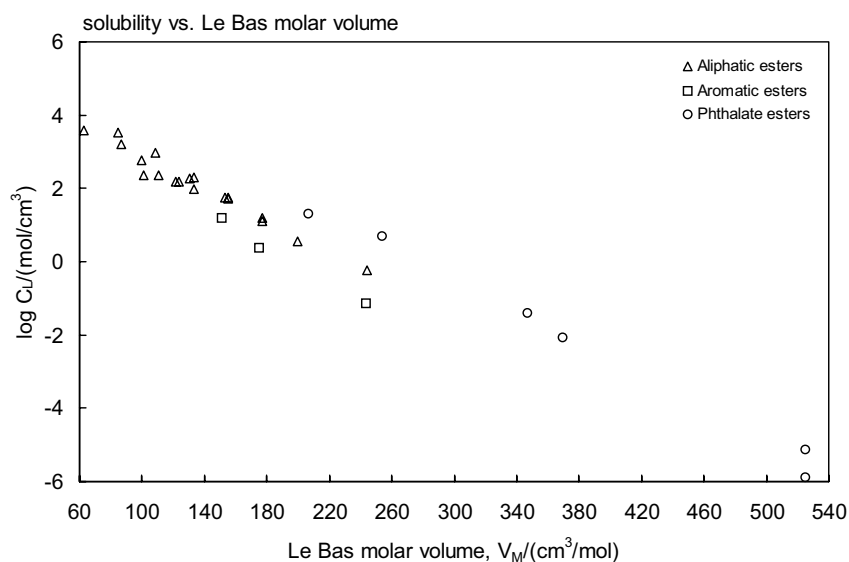


FIGURE 15.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for esters.

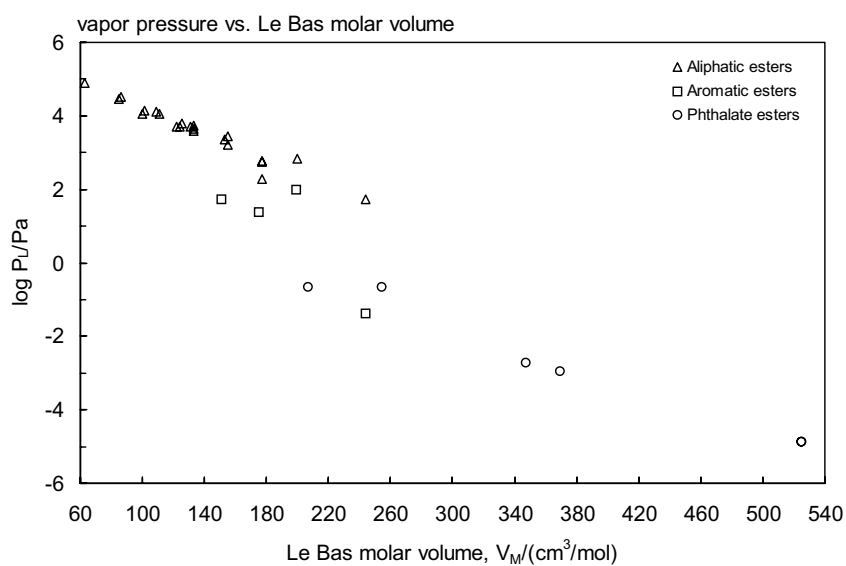


FIGURE 15.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for esters.

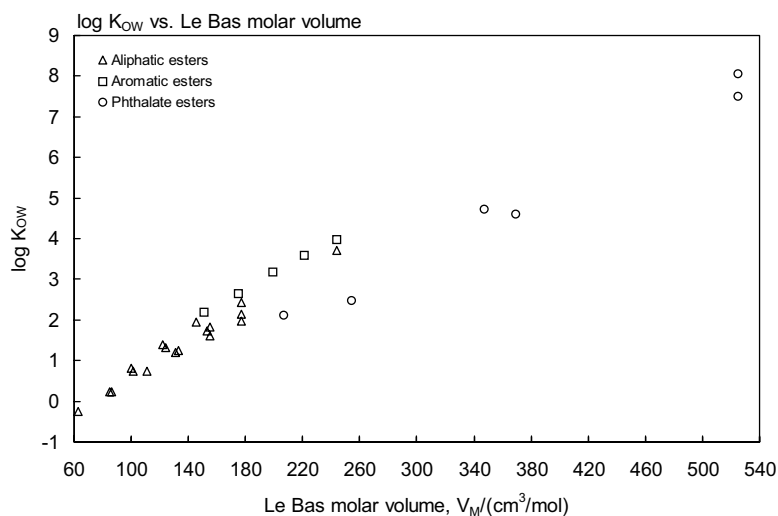


FIGURE 15.2.3 Octanol-water partition coefficient versus Le Bas molar volume for esters.

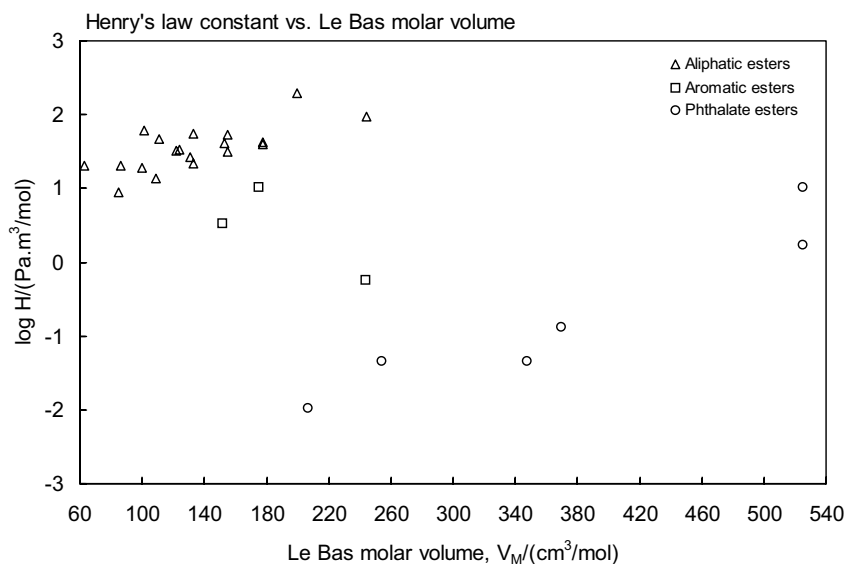


FIGURE 15.2.4 Henry's law constant versus Le Bas molar volume for esters.

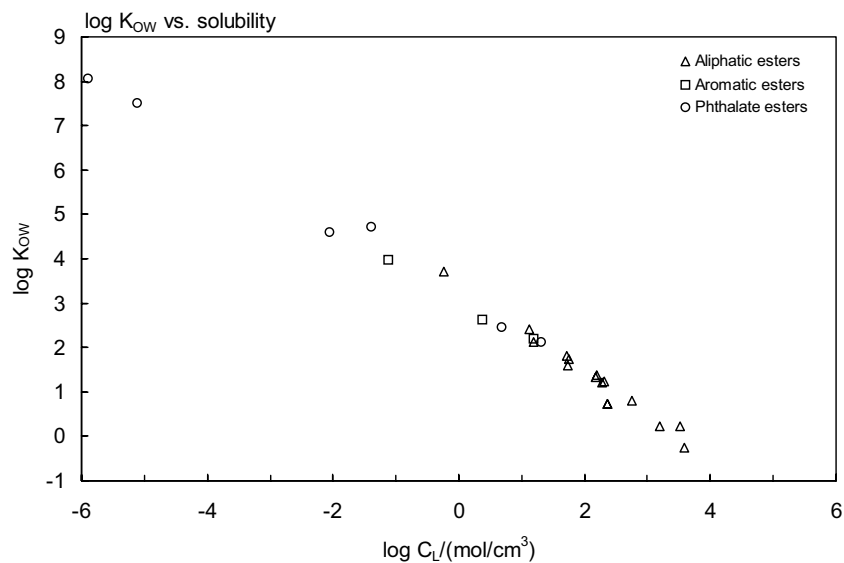


FIGURE 15.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for esters.

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16.1 LIST OF CHEMICALS AND DATA COMPILATIONS

16.1.1 NITRILES (ORGANIC CYANIDES)

16.1.1.1 Acetonitrile



Common Name: Acetonitrile

Synonym: cyanomethane, ethanenitrile, methyl cyanide

Chemical Name: acetonitrile

CAS Registry No: 75-05-8

Molecular Formula: $\text{C}_2\text{H}_3\text{N}$, CH_3CN

Molecular Weight: 41.052

Melting Point ($^{\circ}\text{C}$):

−43.82 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

81.65 (Lide 2003)

Density (g/cm^3 at 20°C):

0.7857 (Dreisbach 1961; Weast 1982–83; Dean 1985)

0.7803 (25°C , Dreisbach 1961)

Molar Volume (cm^3/mol):

52.7 (calculated-density, Rohrschneider 1973)

57.4 (exptl. at normal bp, Lee et al. 1972)

56.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:

29.1 (pK_a , Riddick et al. 1986; Howard 1993)

32.2 (pK_s , Riddick et al. 1986)

−10.12 (pK_{BH^+} , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.01, 31.51 (25°C , bp, Dreisbach 1961)

32.94, 29.82 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.167 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

$> 3.1 \times 10^6$ (Booth & Everson 1948)

miscible (Dean 1985; Riddick et al. 1986; Yaws et al. 1990; Howard 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11870* (interpolated-regression of tabulated data, temp range -47 – 81.8°C , Stull 1947)

$\log (P/\text{mmHg}) = 7.12257 - 1315.2/(230 + t/^{\circ}\text{C})$, (Antoine eq., Dreisbach & Martin 1949)

11240 (calculated by formula, Dreisbach 1961)

$\log (P/\text{mmHg}) = 7.07354 - 1279.2/(224.0 + t/^{\circ}\text{C})$, temp range 5 – 119°C , (Antoine eq. for liquid state, Dreisbach 1961)

12156* (25.56°C , measured range 7.3 – 27.38°C , Putnam et al. 1965)

$\log (P/\text{mmHg}) = 7.89511 - 1773.06/(T/\text{K})$; temp range 280 – 300.5 K (Antoine eq., Putnam et al. 1965)

11510 (Hoy 1970)

24459* (41.82°C , ebulliometry, measured range 41 – 82°C , Meyer et al. 1971)

$\log (P/\text{mmHg}) = 6.23655 - 1397.9228/(239.275 + t/^{\circ}\text{C})$; temp range 41 – 82°C (ebulliometry, Meyer et al. 1971)

$\log (P/\text{mmHg}) = [-0.2185 \times 8173.2/(T/\text{K})] + 7.938662$; temp range: -47.0 to 81.8°C , (Antoine eq., Weast 1972–73)

11919* (25.3°C , measured range 15.1 – 89.2°C , Dojcanske & Heinrich 1974)

- 8306* (saturated-vapor volume, extrapolated from fitted Antoine eq., Mousa 1981)
 $\log(P/\text{kPa}) = 6.4914 - 1420.8649/(T/K - 42.15)$; temp range 438.9–530.1 K (ebulliometry, Mousa 1981)
 9864, 15330 (20°C, 30°C, Verschueren 1983)
 11790, 11830 (interpolated values-Antoine equations, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.39532 - 1420.682/(241.852 + t/^\circ\text{C})$, temp range: 15.1–89.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 7.54606 - 2093.145/(298.369 + t/^\circ\text{C})$, temp range: 7.26–27.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 12310 (calculated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 7.11988 - 1314.4/(230 + t/^\circ\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
 11840 (Riddick et al. 1986; Howard et al. 1986; quoted, Banerjee et al. 1990; Howard 1993)
 $\log(P/\text{kPa}) = 6.24747 - 1315.2/(230.0 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 11800 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.34522 - 1388.446/(-34.856 + T/K)$, temp range: 314–355 K, (Antoine eq., Stephenson & Malanowski 1987)
 11840 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.24724 - 1315.2/(230 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P/\text{mmHg}) = 23.1953 - 2.3389 \times 10^3/(T/K) - 5.4954 \cdot \log(T/K) + 7.9894 \times 10^{-10} \cdot (T/K) + 2.3293 \times 10^{-6} \cdot (T/K)^2$; temp range 229–546 K (vapor pressure eq., Yaws 1994)
 10604* (22.634°C, comparative ebulliometry, measured range 278–373 K, Ewing & Sanchez Ochoa 2004)
 $\ln(P/\text{kPa}) = 14.7340 - 3268.53/(T/K - 31.615)$, for temp range 290–362 K (comparative ebulliometry, Ewing & Sanchez Ochoa 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):

- 3.50, 2.78 (exptl., calculated-bond contribution, Hine & Mookerjee 1975)
 2.07* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 2.033 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 1.474* (20°C, headspace-GC, measured range 6.0–30°C, Benkelberg et al. 1995)
 1.474, 1.477, 1.685 (20°C, headspace-GC, deionized water, rain water, artificial seawater, Benkelberg et al. 1995)
 $\ln(k_H/\text{atm}) = (13.8 \pm 0.3) - (4106 \pm 101)/T/K$, temp range: 6–30°C (headspace-GC measurement, Benkelberg et al. 1995)
 1.55 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 2.353 - 1627/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 2.05 (Ostwald concentration coefficient-concn ratio-GC/FID, Bebahani et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.34 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1969, 1971; Hansch & Leo 1985)
 –0.54 (shake flask-GC, Tani & Hashimoto 1984)
 –0.34 (recommended, Sangster 1989, 1993)
 –0.34 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 2.31 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 0.523 (estimated- K_{OW} as per regression eq of Bysshe 1982, Howard 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.523 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)
 –0.714 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2} \sim 21$ h from a model river of 1-m deep flowing at 1 m/s with a wind velocity of 3 m/s based on Henry's law constant (Lyman et al. 1982; quoted, Howard 1993)

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 314 - 12559$ yr in water, based on measured rate data for reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991)

$k_{\text{OH}}^* = (4.94 \pm 0.6) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297.2 K, measured range 297–424 K (flash photolysis-resonance fluorescence, Harris et al. 1981; quoted, Howard 1993)

$k_{\text{OH}}^* = (1.94 \pm 0.37) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 250–363 K (flash photolysis-resonance fluorescence, Kurylo & Knable 1984)

$k_{\text{OH}}^* = (2.1 \pm 0.3) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–393 K (discharge flow-EPR, Poulet et al. 1984)

$k_{\text{OH}}(\text{exptl}) = 2.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 2.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985)

$k_{\text{OH}} = 3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1985; quoted, Howard et al. 1991; Howard 1993)

$k_{\text{OH}} = 1.90 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k(\text{soln}) = 3.70 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}}^* = 2.14 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

$k = 5.8 \times 10^{-3} \text{ M}^{-1} \text{ h}^{-1}$ at pH 7 and 25°C with $t_{1/2} > 150000$ yr (Ellington et al. 1987)

$k_{\text{O}_3}(\text{aq.}) \leq 6 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C, with $t_{1/2} \geq 18$ yr at pH 7 (Yao & Haag 1991).

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 168 - 672$ h, based on aerobic river die-away test data (Ludzack et al. 1958; quoted, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 672 - 2688$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 1299 - 12991$ h, based on measured rate constant $k = 3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991; Howard 1993);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 168 - 672$ h, based on aerobic river die-away test data (Howard et al. 1991);

photooxidation $t_{1/2} = 314 - 12559$ yr, based on measured rate data for reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991);

$t_{1/2} \geq 18$ yr for direct reaction with ozone in water at pH 7 and 22°C (Yao & Haag 1991).

Groundwater: $t_{1/2} = 336 - 8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168 - 672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.1.1

Reported vapor pressures of acetonitrile at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

(Continued)

TABLE 16.1.1.1.1 (Continued)

1.

Stull 1947		Putnam et al. 1965		Meyer et al. 1971		Dojcanske & Heinrich 1974	
summary of literature data		manometer		ebulliometry		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−47.0	133.3	7.259	4997	41.82	24459	15.1	7359
−26.6	666.6	10.47	5861	46.09	29026	20.1	9413
−16.3	1333	13.791	6914	46.11	29032	25.3	11919
−5.0	2666	18.701	8809	50.36	34288	30.7	15252
7.7	5333	21.905	10244	55.37	41393	35	18292
15.9	7999	23.401	11031	60.64	50155	39.95	22465
27	13332	25.563	12156	65.91	60390	40	22625
43.7	26664	27.38	13187	70.74	71145	44.9	27638
62.5	53329			76.31	85512	50.1	33797
81.8	101325	eq. 1	P/mmHg	81.87	101990	54.9	40517
		A	7.89511	81.89	102010	60	49022
mp/°C	−41.0	B	1773.06			64.4	57182
				bp/°C	81.66	64.95	58102
				eq. 2	P/mmHg	70	68967
				A	6.23655	73.05	76713
				B	1397.923	75.1	81380
				C	239.275	77.2	87952
						81.1	99431
						85.2	112364
						88.2	123189
						89.2	124776

2.

Mousa 1981		Ewing & Sanchez Ochoa 2004			
ebulliometry-pressure gauge		comparative ebulliometry			
T/K	P/kPa	t/°C	P/Pa	t/°C	P/kPa
		set A		set B	
438.9	784.4	4.772	4323#	81.4	100.745
440.9	842.8	5.475	4490#	87.792	122.631
442.6	862.3	8.417	5247#	98.589	168.122
444.5	876.9	12.226	6385#	105.665	204.592
447.9	960.3	14.517	7165#	110.961	235.792
450.5	999.2	17.497	8296	121.144	306.279
455.7	1116.5	19.596	9182	132.086	399.5
460.2	1234.6	22.634	10604	142.063	502.665
505.3	2604.9	27.674	13366	150.533	605.601
508.1	1704.6	30.661	15271	157.974	708.993
512.1	1924.0	36.486	19639	164.152	804.861
519.7	3243.3	42.283	24972	170.346	910.819
521.6	3303.1	47.968	31311	176.446	1025.47
524.8	3482.8	51.872	36387	182.586	1151.97
530.1	3722.1	58.125	45907	188.724	1290.2
		63.263	55169	195.22	1450.28
bp/K	354.8	68.029	65092	200.902	1602.63
		72.425	75440	206.004	1749.88

TABLE 16.1.1.1.1 (Continued)

Mousa 1981		Ewing & Sanchez Ochoa 2004			
ebulliometry-pressure gauge		comparative ebulliometry			
T/K	P/kPa	t/°C	P/Pa	t/°C	P/kPa
eq.3	P/kPa	76.178	85311	211.619	2110.77
A	6.4914	79.929	95589	217.22	2303.51
B	1420.8649	81.515	101120	222.602	2523.66
C	−42.15	84.406	110614	228.33	2747.95
		88.462	125129	233.771	2999.22
		95.816	155329	339.66	3254.08
		100.02	175036	244.858	3512.89
				254.64	3760.37
		for temp range 290–373 K		258.929	4001.46
		eq. 2a	P/mmHg	261.882	4174.61
		A	14.734		
		B	3268.53	data fitted to Wagner eq.	
		C	−31.615	for temp range 354.5–535 K	
		# data not used in regression			

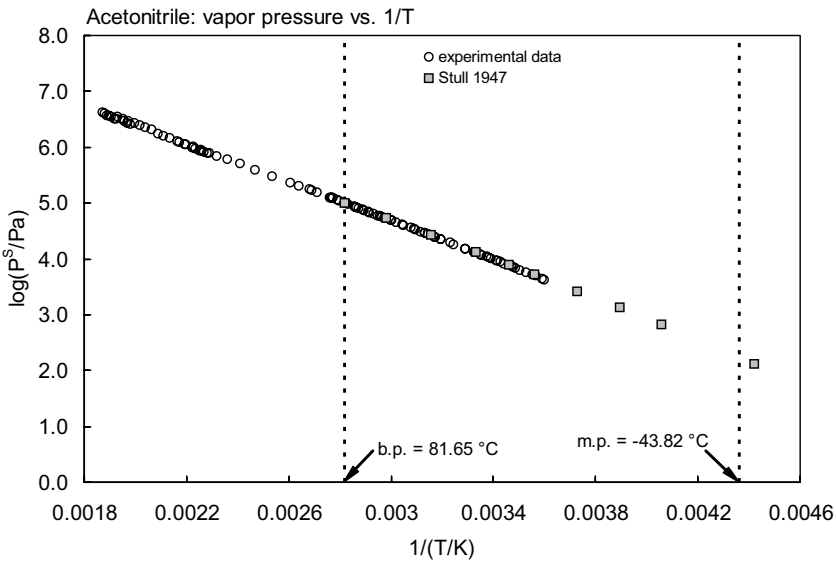


FIGURE 16.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for acetonitrile.

TABLE 16.1.1.2

Reported Henry's law constants of acetonitrile at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

Snider & Dawson 1985		Benkelberg et al. 1995	
gas stripping-GC		equil. vapor phase concn-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
			deionized water
0	0.614	6	0.72
25	2.066	10	1.0706
		20	1.474
		30	2.356
enthalpy of transfer:			rain water
$\Delta H/(\text{kJ mol}^{-1}) = 30.54$		20	1.477
			artificial
		20	1.685
		eq. 3	H/atm
		A	13.8 ± 0.3
		B	4106 ± 101

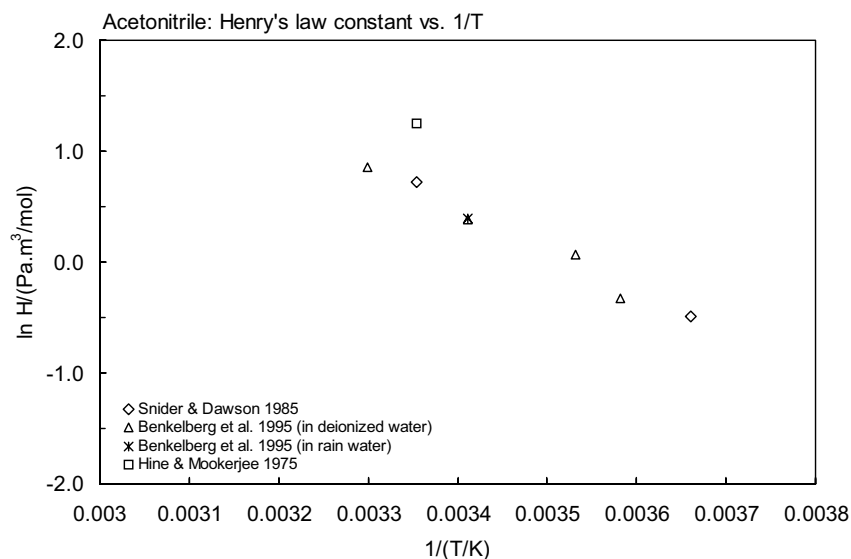
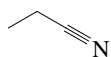


FIGURE 16.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for acetonitrile.

16.1.1.2 Propionitrile



Common Name: Propionitrile

Synonym: propanenitrile, ethyl cyanide, cyanoethane, propyl nitrile

Chemical Name: propionitrile

CAS Registry No: 107-12-0

Molecular Formula: C_3H_5N , CH_3CH_2CN

Molecular Weight: 55.079

Melting Point ($^{\circ}C$):

−92.78 (Lide 2003)

Boiling Point ($^{\circ}C$):

97.14 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7818 (Weast 1982–83; Dean 1985)

0.78182, 0.77682 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

70.4 (calculated-density, Taft et al. 1985; Leahy 1986; Kamlet et al. 1986, 1987)

78.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

33.54 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_{vap} (kJ/mol):

37.41, 32.77 ($25^{\circ}C$, bp, Dreisbach 1961)

36.03, 30.96 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.045 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

104950 (Seidell 1941)

105200 (Hansch et al. 1968)

103000 (Dean 1985; Riddick et al. 1986; Howard 1990)

55000, 65000 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC, measured range 0 – $90^{\circ}C$, Stephenson 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6005* (interpolated-regression of tabulated data, temp range -35 – $97.1^{\circ}C$, Stull 1947)

10114* ($35.5^{\circ}C$, ebulliometry, measured range 35.5 – $97.35^{\circ}C$, Dreisbach & Shrader 1949)

$\log (P/mmHg) = 7.15217 - 1398.2/(230 + t/^{\circ}C)$; temp range 35.5 – $97.35^{\circ}C$, (Antoine eq., Dreisbach & Martin 1949)

5333* ($22.05^{\circ}C$, measured range -84.66 – $22.05^{\circ}C$, Milazzo 1956)

5950 (calculated by formula, Dreisbach 1961)

$\log (P/mmHg) = 7.05846 - 1327.9/(221.0 + t/^{\circ}C)$, temp range: 17 – $137^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = [-0.2185 \times 8769.0/(T/K)] + 8.079473$; temp range: -35 to $97.1^{\circ}C$, (Antoine eq., Weast 1972–73)

6140 ($22.05^{\circ}C$, quoted exptl., Boublik et al. 1973, 1984)

6163, 6143 (extrapolated values-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.89149 - 1181.562/(206.603 + t/^{\circ}C)$, temp range: 35.5 – $97.39^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 4.43918 - 677.415/(160.551 + t/^{\circ}C)$, temp range: -84.7 to $22.05^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6140 (extrapolated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 5.2782 - 665.52/(159.0 + t/^{\circ}\text{C})$, temp range: -84 to 22°C (Antoine eq., Dean 1985, 1992)
 5950 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.27702 - 1398.2/(230 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 7.15190 - 1894.10/(T/\text{K})$; temp range: 9 – 25°C , (Antoine eq., Riddick et al. 1986)
 6306 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.395 - 3213/(T/\text{K})$, temp range: 357 – 413 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 10.31055 - 3994.667/(T/\text{K})$, temp range: 373 – 413 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 33.7908 - 2.9113 \times 10^3/(T/\text{K}) - 9.1506 \cdot \log(T/\text{K}) + 1.1173 \times 10^{-11} \cdot (T/\text{K}) + 3.2756 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 180 – 564 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

3.800 (partial pressure, Butler & Ramchandani 1935)
 3.748 (partial vapor pressure-GC, Buttery et al. 1969)
 3.752, 3.752, 4.114 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 5.947 (Howard 1990)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.041 (shake flask, Collander 1951)
 0.16 (shake flask-GC, Hansch & Anderson 1967; Hansch et al. 1968)
 -0.10 (shake flask-GC, Tani & Hashimoto 1984)
 0.16 (recommended, Sangster 1989, 1993)
 0.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.69 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

-0.108 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

0.079 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 13.3$ h was estimated for a model river 1 m deep flowing 1 m/s with wind speed 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}^* = (1.94 \pm 0.20) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.2 K, measured range 298 – 423 K (flash photolysis-resonance fluorescence, Harris et al. 1981)

$k_{\text{OH}} = 1.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985)

$k_{\text{OH}} = 1.94 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.2 K, $k(\text{soln}) = 1.60 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

photooxidation $t_{1/2} = 83$ d in air, based on experimental rate constant assuming $t_{1/2} = 12$ h of sunlight for the vapor-phase reaction with hydroxyl radical in air and $t_{1/2} > 100$ d for the reaction with ozone in the atmosphere (Howard 1990)

$k_{\text{OH}} = 0.194 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.2 K (review, Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

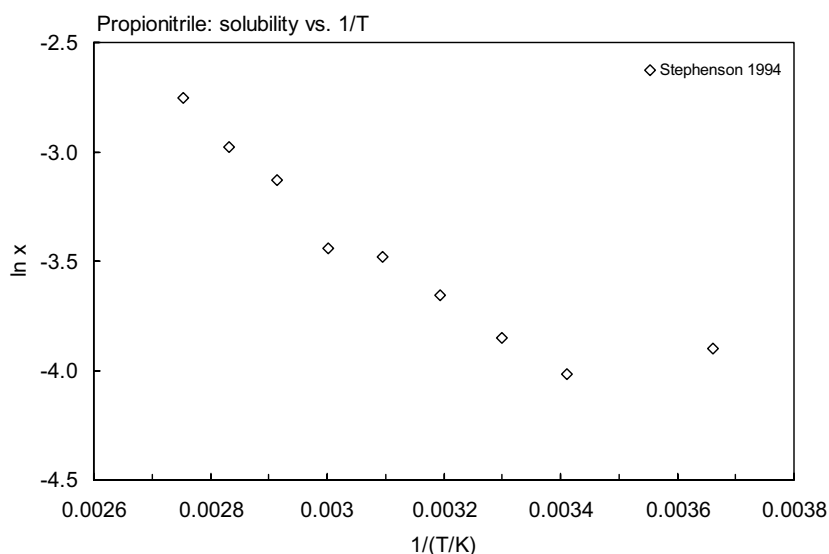
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 83$ d, based on experimental rate constant assuming 12 h of sunlight for the vapor-phase reaction with hydroxyl radical in air and $t_{1/2} > 100$ d for the reaction with ozone in the atmosphere (Harris et al. 1981; quoted, Howard 1990).

TABLE 16.1.1.2.1**Reported aqueous solubilities and vapor pressures of propionitrile at various temperatures**

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Aqueous solubility	Vapor pressure						
Stephenson 1994	Stull 1947	Dreisbach & Shrader 1949	Milazzo 1956				
shake flask-GC	summary of literature data	ebulliometry					
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	62000	-35.0	133.3	35.5	10114	-84.66	1
20	55000	-13.8	666.6	43.76	16500	-77.01	2
30	65000	-3.0	1333	70.45	42066	-67.42	6
40	79000	8.8	2666	84.44	67661	-65.49	7
50	94000	22	5333	97.35	101325	-59.72	13
60	98000	30.1	7999			-52.96	17
70	134000	41.4	13332			-46.19	49
80	156000	58.2	26664			-34.95	133
90	195000	77.7	53329			-22.85	356
		97.1	101325			-13.08	707
						-2.95	1347
		mp/°C	-91.9			6.36	2400
						16.42	4146
						22.05	5333

**FIGURE 16.1.1.2.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for propionitrile.

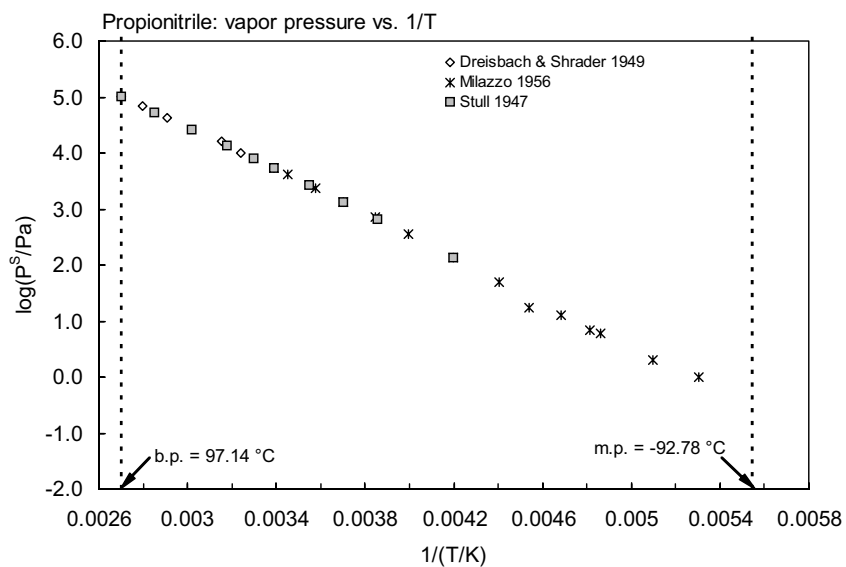
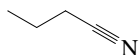


FIGURE 16.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for propionitrile.

16.1.1.3 Butyronitrile



Common Name: *n*-Butyronitrile

Synonym: butanenitrile

Chemical Name: butyronitrile

CAS Registry No: 109-74-0

Molecular Formula: C_4H_7N , $CH_3CH_2CH_2CN$

Molecular Weight: 69.106

Melting Point ($^{\circ}C$):

−111.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

117.6 (Lide 2003)

Density (g/cm^3):

0.7911, 0.7865 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

88.4 ($30^{\circ}C$, Stephenson & Malanowski 1987)

100.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.33, 34.43 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.021 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Other data at other temperatures designated * are compiled at the end of this section):

33000 (selected, Riddick et al. 1986)

33500* ($20^{\circ}C$, shake flask-GC/TC, measured range 0 – $90^{\circ}C$, Stephenson 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1333* ($25.7^{\circ}C$, summary of literature data, temp range -20 to $117.5^{\circ}C$, Stull 1947)

3592* ($30.64^{\circ}C$, ebulliometry, measured range 30.64 – $120.223^{\circ}C$, Meyer et al. 1971)

$\log (P/mmHg) = 6.771124 - 1444.5851/(t/^{\circ}C + 223.275)$; temp range 30.64 – $120.223^{\circ}C$ (Antoine eq., ebulliometric measurements, Meyer et al. 1971)

13831* ($59.807^{\circ}C$, ebulliometry, measured range 59.807 – $127.707^{\circ}C$, Meyer & Hotz 1976)

2546 (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.25390 - 1452.076/(t/^{\circ}C + 224.1855)$; temp range not specified (Riddick et al. 1986)

$\log (P_L/kPa) = 6.25397 - 1452.076/(-46.9645 + T/K)$; temp range 332 – $401\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 4.8780 - 2.5505 \times 10^3/(T/K) + 3.6306 \cdot \log (T/K) - 1.663 \times 10^{-2} \cdot (T/K) + 1.0604 \times 10^{-5} \cdot (T/K)^2$; temp range 161 – $582\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.53 (shake flask-GC, Tani & Hashimoto 1984)

0.53 (recommended, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

TABLE 16.1.1.3.1

Reported aqueous solubilities and vapor pressures of butyronitrile at various temperatures

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Aqueous solubility		Vapor pressure					
Stephenson 1994		Stull 1947		Meyer et al. 1971		Meyer & Hotz 1976	
shake flask-GC		summary of literature data		ebulliometry		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	37500	–20.0	133.3	30.64	3592	59.807	13831
20	33500	2.10	666.6	39.03	5459	65.615	17513
30	33100	13.4	1333	49.913	9041	71.638	22151
40	32500	25.7	2666	59.226	13527	77.023	27111
50	32300	38.4	5333	67.536	18888	83.599	34366
60	32100	47.3	7999	77.313	27448	89.462	42109
70	31900	59.0	13332	86.71	39316	96.022	52382
80	34000	76.7	26664	93.675	48525	102.279	63984
90	36100	96.8	53329	100.638	60811	109.175	79081
		117.5	101325	100.701	60928	115.651	95737
		mp/°C		107.041	74214	121.838	114148
				112.04	88451	127.707	134135
				117.254	100344		
				120.223	109170		
				bp/°C	117.583		
			log P = A – B/(C + t/°C)				
				P/mmHg			
				A	6.771124		
				B	1444.5851		
				C	223.275		

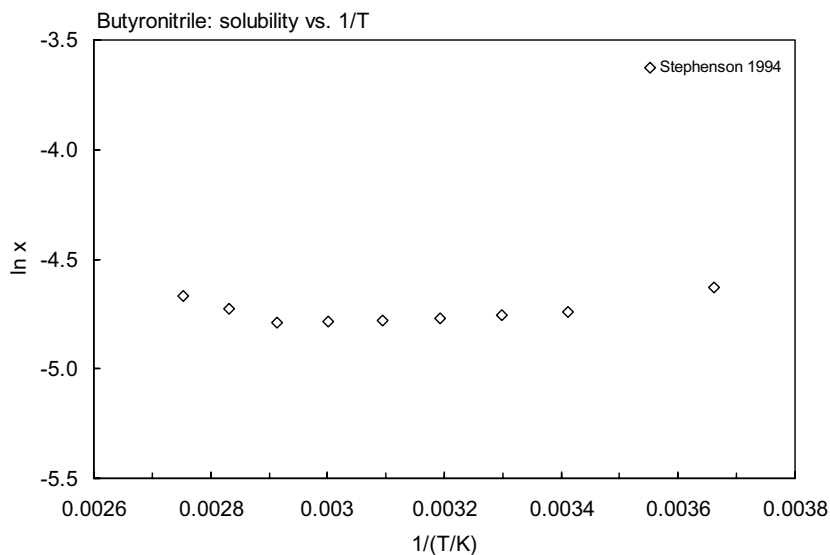


FIGURE 16.1.1.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for butyronitrile.

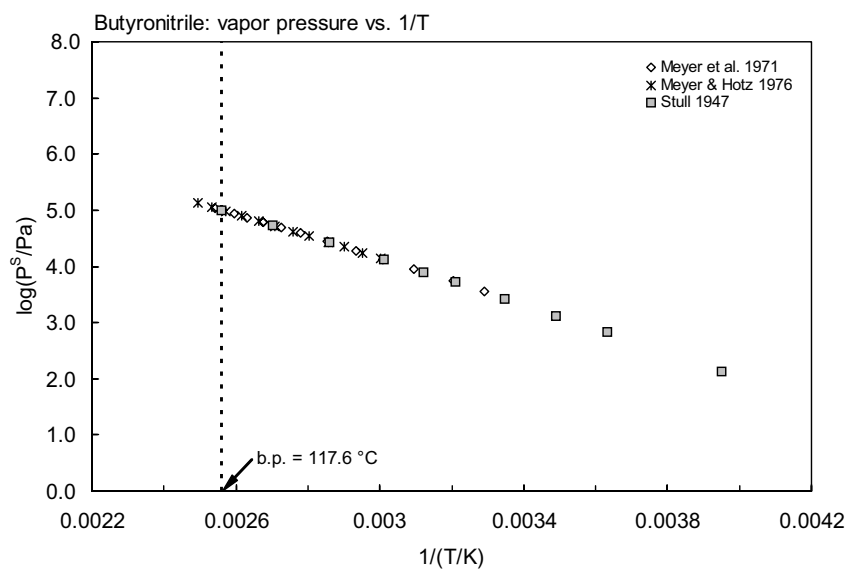
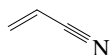


FIGURE 16.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for butyronitrile.

16.1.1.4 Acrylonitrile (2-Propenenitrile)



Common Name: Acrylonitrile

Synonym: cyanoethylene, propenenitrile, 2-propenenitrile, vinyl cyanide

Chemical Name: acrylonitrile, cyanoethylene

CAS Registry No: 107-13-1

Molecular Formula: C_3H_3N , $CH_2=CHCN$

Molecular Weight: 53.063

Melting Point ($^{\circ}C$):

-83.48 (Lide 2003)

Boiling Point ($^{\circ}C$):

77.30 (Riddick et al. 1986; Howard 1989; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8060, 0.8004 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

65.8 ($20^{\circ}C$, calculated-density)

71.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.230 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

79000 (Klein et al. 1957)

75000 (Günther et al. 1968)

73500 ($20^{\circ}C$, Windholz 1976)

73240 (shake flask-LSC, Veith et al. 1980)

7.35 wt%* ($20^{\circ}C$, Kirk-Othmer Encyclopedia 3rd ed., measured range 0 – $60^{\circ}C$, quoted, Basu et al. 1983)

73500 ($20^{\circ}C$, Riddick et al. 1986)

69000*, 66400 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC, measured range 0 – $70^{\circ}C$, Stephenson 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

14340* (interpolated-regression of tabulated data, temp range -51 to $78.5^{\circ}C$, Stull 1947)

11732* ($20^{\circ}C$, temp range 20 – $77^{\circ}C$, Gudkov et al. 1964; quoted, Boublik et al. 1984)

14100 (Hoy 1970)

$\log(P/mmHg) = [-0.2185 \times 7941.4/(T/K)] + 7.851016$; temp range: -51 to $78.5^{\circ}C$, (Antoine eq., Weast 1972–73)

14720 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 4.77668 - 649.583/(155.006 + t/^{\circ}C)$, temp range 20 – $70^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

14370 (Daubert & Danner 1985)

15240 (calculated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.03855 - 1232.53/(222.47 + t/^{\circ}C)$, temp range -20 to $140^{\circ}C$ (Antoine eq., Dean 1985, 1992)

11000 ($20^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 6.643 - 11644.7/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

14560 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.12021 - 1288.9/(-38.74 + T/K)$; temp range 257 – 352 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.4811 - 1518.381/(-12.003 + T/K)$; temp range 283 – 343 K (Antoine eq.-II, Stephenson & Malanowski 1987)

15600 (calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 35.921 - 2.7763 \times 10^3/(T/K) - 10.101 \cdot \log (T/K) - 3.1547 \times 10^{-10} \cdot (T/K) + 4.7299 \times 10^{-6} \cdot (T/K)^2$;
temp range 190–535 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

11.14 (Bocek 1976; quoted, Basu et al. 1983; Howard 1989)

8.918 (calculated-P/C, Mabey et al. 1982)

9.420 (quoted, WERL Treatability Database, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.25 (shake flask-HPLC, Pratesi et al. 1979)

0.00 (shake flask, Fujisawa & Masuhara 1980, 1981)

0.09 (shake flask-GC, Tani & Hashimoto 1984)

0.25 (Hansch & Leo 1985)

0.25 (recommended, Sangster 1989)

0.25 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.68 (bluegill sunfish, Barrows et al. 1978)

0.00 (estimated-S, Kenaga 1980)

1.68, 0.32 (bluegill sunfish, calculated- K_{OW} , Veith et al. 1980)

0.017 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

0.954 (soil, calculated-S, Kenaga 1980)

−0.071 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.101, 1.006; 1.09 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

−0.0899 (calculated- K_{OW} , Walton et al. 1992)

−0.0890 (calculated- K_{OW} , Kolig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 6, 1.2, 4.8$ d in a typical pond, river and lake are 6, 1.2, and 4.8 d, respectively, with the reaeration for oxygen in typical bodies of water (Lyman et al. 1982; quoted, Howard 1989)

evaporation $t_{1/2} = 795$ min from water with an assumed 1-m depth (Basu et al. 1983).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k < 1 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, and $36 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$t_{1/2} = 4.0$ h for photooxidation in the troposphere (Callahan et al. 1979)

$k_{OH} = (40.6 \pm 4.1) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (flash photolysis-resonance fluorescence technique, Harris et al. 1981)

$k_{O_3} < 1 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K, and tropospheric lifetimes, $\tau > 115$ d and $\tau = 3$ d due to reactions with O_3 and OH radical, respectively (Atkinson et al. 1982)

$k_{O_3} < 1 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Atkinson et al. 1983; quoted, Atkinson & Carter 1984)

$t_{1/2} = 3.5$ d for the reaction with photochemically produced hydroxyl radical by the sunlight (Edney et al. 1983; quoted, Howard 1989)

$k_{OH} = 4.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.7 K, and $k_{OH} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (review, flash photolysis-resonance fluorescence technique Atkinson 1985)

photooxidation $t_{1/2} = 3.4\text{--}189$ h, based on measured rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991)

$k_{OH} = (3.4 - 4.80) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296–298.2 K (review, Atkinson 1989)

Hydrolysis: $k(\text{acid}) = 4.2 \times 10^{-2} \text{ M}^{-1} \text{ h}^{-1}$ at pH 5.0 with $t_{1/2} = 188 \text{ yr}$ and $k(\text{base}) = 6.1 \times 10^{-2} \text{ M}^{-1} \text{ h}^{-1}$ at pH 9.0 with $t_{1/2} = 13 \text{ yr}$ (Ellington et al. 1987; quoted, Howard et al. 1991, Kollig 1993);
 $t_{1/2} = 1210 \text{ yr}$ at pH 7.0, based on measured acid and base catalyzed hydrolysis constants (Ellington et al. 1987; quoted, Howard et al. 1991)
 $t_{1/2} = 69 \text{ d}$ at pH 2, $t_{1/2} = 440000 \text{ d}$ at pH 7 and $t_{1/2} = 4.7 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995).
 Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 30\text{--}552 \text{ h}$, based on river die-away test data (Going et al. 1979; Ludzack et al. 1958; quoted, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 120\text{--}2208 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
 ^{14}C labeled acrylonitrile at concentrations up to 100 ppm was completely degraded within 2.0 d in a London soil under aerobic conditions (Donberg et al. 1992)
 $t_{1/2}(\text{aerobic}) = 1.3 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 5 \text{ d}$ in natural waters (Capel & Larson 1995)
 Biotransformation: $k = \text{of } 3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982).
 Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 4.0 \text{ h}$ for photooxidation in the troposphere (Callahan et al. 1979);
 $t_{1/2} = 3.5 \text{ d}$ for the reaction with photochemically produced hydroxyl radical by the sunlight (Edney et al. 1983; quoted, Howard 1989);
 photooxidation $t_{1/2} = 13.4\text{--}189 \text{ h}$, based on measured rate constant for the reaction with hydroxyl radicals in air (Atkinson 1985; quoted, Howard et al. 1991);
 atmospheric transformation lifetime was estimated to be 1 – 5 to > 5 d (Kelly et al. 1994).
 Surface water: $t_{1/2} = 30\text{--}552 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
 Biodegradation $t_{1/2}(\text{aerobic}) = 100 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 400 \text{ d}$; hydrolysis $t_{1/2} = 69 \text{ d}$ at pH 2, $t_{1/2} = 440000 \text{ d}$ at pH 7 and $t_{1/2} = 4.7 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995).
 Groundwater: $t_{1/2} = 60\text{--}1104 \text{ h}$ based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
 Sediment:
 Soil: $t_{1/2} < 10 \text{ d}$ in soil (USEPA 1979; quoted, Ryan et al. 1988);
 $t_{1/2} = 30\text{--}552 \text{ h}$ based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
 Biota:

TABLE 16.1.1.4.1

Reported aqueous solubilities and vapor pressures of acrylonitrile at various temperatures

Aqueous solubility				Vapor pressure			
Othmer Encyclopedia		Stephenson 1994		Stull 1947		Gudkov et al. 1964	
Basu et al. 1983		shake flask-GC		summary of literature data		in Boublik et al. 1984	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
0	72000	0	65800	–51.0	133.3	20	11732
20	73500	10	66800	–30.7	666.6	30	18932
40	79000	20	69000	–20.3	1333	40	27998
60	91000	30	66400	–9.0	2666	50	38530
		40	68800	3.8	5333	60	57328
		50	73600	11.8	7999	70	78660
		60	73900	22.8	13332		
		70	85600	38.7	26664		
				58.3	53329		
				78.5	101325		
				mp/°C	–82.0		

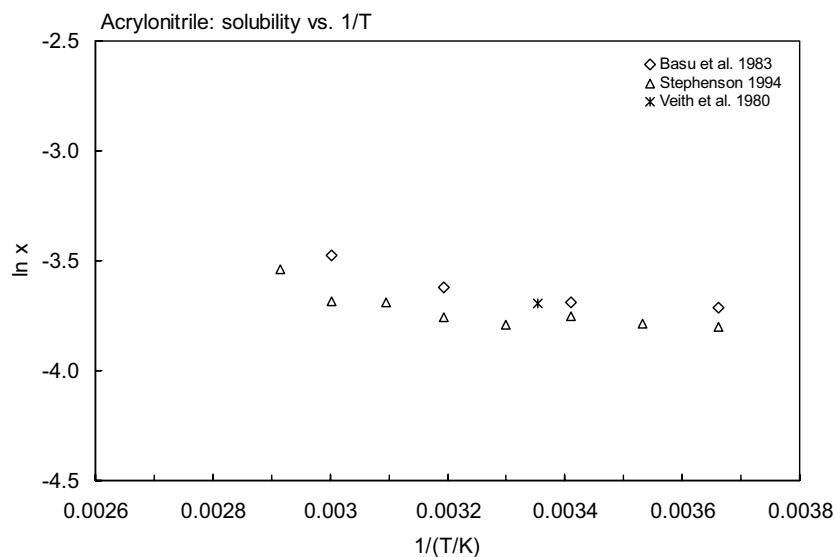


FIGURE 16.1.1.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for acrylonitrile.

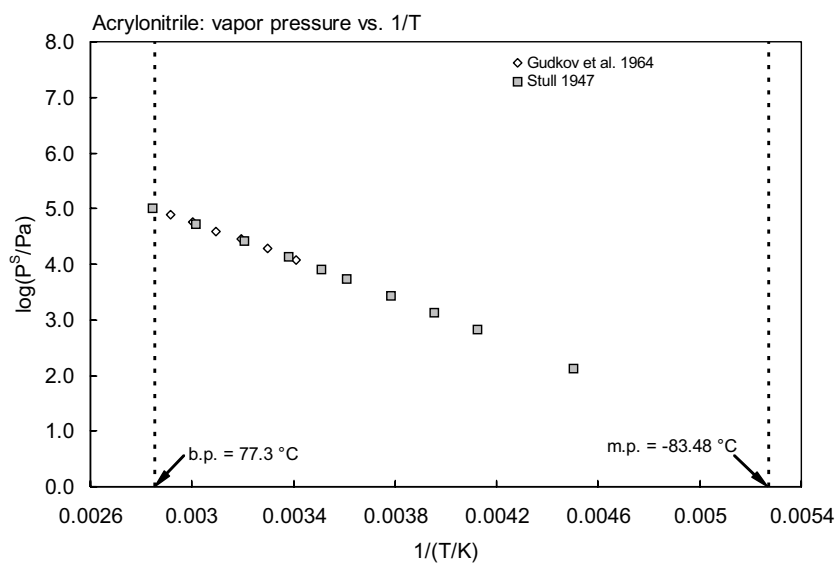
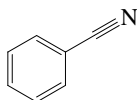


FIGURE 16.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for acrylonitrile.

16.1.1.5 Benzonitrile



Common Name: Benzonitrile

Synonym: benzenecarbonitrile, cyanobenzene, phenyl cyanide

Chemical Name: benzonitrile, benzoic acid nitrile

CAS Registry No: 100-47-0

Molecular Formula: C_6H_5CN

Molecular Weight: 103.122

Melting Point ($^{\circ}C$):

-13.99 (Lide 2003)

Boiling Point ($^{\circ}C$):

191.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0006 ($25^{\circ}C$, Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

103.1 ($25^{\circ}C$, calculated-density)

107.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

55.48, 45.94 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.88 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

4330 (shake flask-UV, McGowan et al. 1966)

2000 (Dean 1985; Riddick et al. 1986)

10000 (selected, Yaws et al. 1990)

4000* (shake flask-GC/TC, measured range $0-90^{\circ}C$, Stephenson 1994)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($38.4^{\circ}C$, static method, measured range $38.4-190.6^{\circ}C$, Kahlbaum 1898)

133.3* ($28.2^{\circ}C$, summary of literature data, temp range $28.2-190.6^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11341.0/(T/K)] + 8.239760$; temp range: $28.2-190.6^{\circ}C$ (Antoine eq., Weast 1972-73)

78.86 (calculated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.74631 - 1436.72/(181 + t/^{\circ}C)$, temp range: liquid (Antoine eq., Dean 1985, 1992)

100.0 (Riddick et al. 1986)

$\log(P/kPa) = 5.87121 - 1436.72/(181.0 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

106.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.79506 - 2066.71/(-32.19 + T/K)$, temp range $301-464 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

55.32 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.56 (shake flask-UV spectrophotometry, Fujita et al. 1964; quoted, Leo et al. 1969; Hansch & Leo 1979)

1.56 (shake flask-UV, Holmes & Lough 1976)

1.67	(calculated-fragment const., Rekker 1977)
1.56	(shake flask at pH 7, Unger et al. 1978)
1.66	(RP-HPLC- k' correlation, Miyake & Terada 1982)
1.65 \pm 0.01	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.50	(HPLC- k' correlation, Haky & Young 1984)
1.56	(shake flask-GC, Tanii & Hashimoto 1984)
1.56	(RP-HPLC-capacity ratio, Minick et al. 1988)
1.45	(RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
1.56	(recommended, Sangster 1989, 1993)
1.56	(shake flask-GC, Alcorn et al. 1993)
1.56	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

4.46	(head-space GC, Abraham et al. 2001)
------	--------------------------------------

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k ; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Zetzsch 1982; Atkinson 1989)

$k_{OH}(\text{calc}) = 4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{OH}(\text{calc}) = 3.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1985)

$k_{OH}(\text{calc}) = 3.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs}) = 3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}(\text{calc}) = 4.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: an estimated $t_{1/2} = 1.3 \text{ d}$ in Rhine River in case of first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.1.5.1

Reported aqueous solubilities and vapor pressures of butyronitrile at various temperatures

Aqueous solubility		Vapor pressure					
Stephenson 1994		Kahlbaum 1898*				Stull 1947	
shake flask-GC		static-manometer				summary of literature data	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
0	3500	38.4	133.3	141.4	26664	28.2	133.3
10	3300	45.3	266.6	155.8	39997	55.3	666.6
20	4000	50.0	400.0	165.8	53329	69.2	1333
40	4500	53.8	533.3	174.4	66661	83.4	2666
50	3800	56.9	666.6	181.6	79993	99.6	5333
60	4200	69.1	1333.2	187.7	93326	109.8	7999

(Continued)

TABLE 16.1.1.5.1 (Continued)

Aqueous solubility		Vapor pressure					
Stephenson 1994		Stull 1947		Meyer et al. 1971		Meyer & Hotz 1976	
shake flask-GC		summary of literature data		ebulliometry		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70	6000	83.0	2666.4	190.6	101325	123.5	13332
80	9500	92.1	3999.7			144.1	26664
90	9100	98.5	5332.9	*complete list see ref.		156.7	53329
		103.9	6666.1			190.6	101325
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$		113.7	9999.2				
25 °C		121.3	13332			mp/°C	-12.9

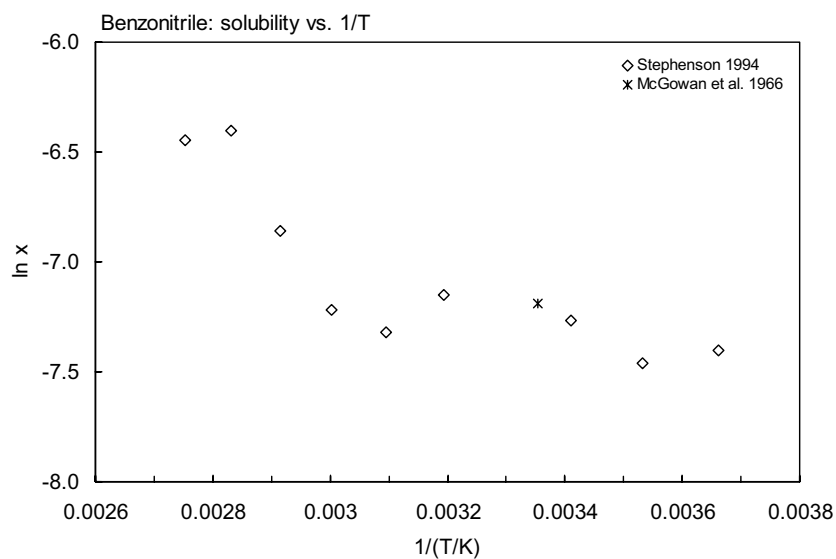


FIGURE 16.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzonitrile.

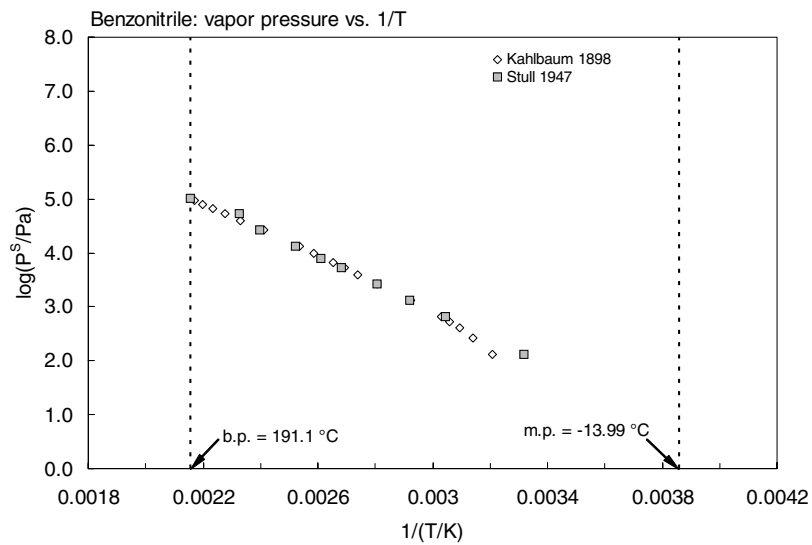


FIGURE 16.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for benzonitrile.

16.1.2 ALIPHATIC AMINES

16.1.2.1 Dimethylamine



Common Name: Dimethylamine

Synonym: aminomethylmethane, N-methylmethanamine

Chemical Name: aminomethylmethane, dimethylamine

CAS Registry No: 124-40-3

Molecular Formula: C_2H_7N , CH_3NHCH_3

Molecular Weight: 45.084

Melting Point ($^{\circ}C$):

-92.18 (Lide 2003)

Boiling Point ($^{\circ}C$):

6.88 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6804 ($0^{\circ}C$, Weast 1982-83)

0.6556, 0.6496 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

68.8 ($20^{\circ}C$, calculated-density)

67.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

10.732 (Perrin 1965; Weast 1982-83; Howard 1990)

10.77 (protonated cation + 1, Dean 1985)

10.77 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

23.84, 24.61 ($25^{\circ}C$, bp, Dreisbach 1961)

23.65, 24.61 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.941 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

very soluble (Dean 1985)

620000 (selected, Yaws et al. 1990)

miscible (Stephenson 1993b)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

101141* ($280.018 K$, static method, measured range $201.387-280.018 K$, Ashton et al. 1939)

236420* (extrapolated-regression of tabulated data, temp range -87.2 to $+7.4^{\circ}C$, Stull 1947)

196800 (calculated by formula, Dreisbach 1961)

$\log (P/mmHg) = 7.06396 - 1024.4/(238.0 + t/^{\circ}C)$, temp range -55 to $37^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = [-0.2185 \times 6660.0/(T/K)] + 7.995166$; temp range -87.7 to $162.6^{\circ}C$, (Antoine eq., Weast 1972-73)

172220 ($20^{\circ}C$, Verschueren 1983)

206180 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.21132 - 962.001/(221.852 + t/^{\circ}C)$, temp range -71.77 to $6.858^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

202620 (Daubert & Danner 1985)

206000 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 7.08212 - 960.242/(221.67 + t/^{\circ}C)$, temp range -72 to $6^{\circ}C$ (Antoine eq., Dean 1985, 1992)

196800 (quoted lit., Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.18886 - 1.024.40/(238.0 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

205300 (interpolated-Antoine eq.-II., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.29031 - 993.586/(-48.12 + T/\text{K})$, temp range 201–280 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.20646 - 965.728/(-50.151 + T/\text{K})$, temp range 277–360 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.81489 - 2369.425/(141.433 + T/\text{K})$, temp range 358–438 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 36.9182 - 2.4965 \times 10^3/(T/\text{K}) - 10.417 \cdot \log (T/\text{K}) - 1.6287 \times 10^{-9} \cdot (T/\text{K}) + 4.6496 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 181–438 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

1.796 (exptl., Hine & Mookerjee 1975; quoted, Howard 1990)

1.796, 1.03 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2.718 (calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

−0.38 (shake flask-RC at pH 13, Wolfenden 1978)

−0.38 (Hansch & Leo 1985)

−0.38 (recommended, Sangster 1989; 1993)

−0.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.00 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

−0.523 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

2.638 (adsorption isotherm average for five soils, Rao & Davidson 1982; quoted, Howard 1990)

0.602; 2.212; 2.706 (Podzol soil; Alfisol soil; sediment, von Oepen et al. 1991)

2.63 (soil, calculated-MCI, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 35.1$ h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; selected, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated:

$k_{OH} = 6.54 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (Atkinson et al. 1977; quoted, Carlier et al. 1986; Atkinson 1989)

photooxidation $t_{1/2} = 5.9$ h in air was estimated for the vapor phase reaction with hydroxyl radical of 5×10^5 radicals/ cm^3 in air (Atkinson et al. 1978; Atkinson 1985; quoted, Howard 1990);

$k_{O_3} = (2.61 \pm 0.30) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Atkinson & Carter 1984; quoted, Atkinson 1985)

$k_{OH} = 6.5 \times 10^{-11} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with 5×10^5 OH radicals/ cm^3 at room temp. having a loss rate of 2.8 d^{-1} (Atkinson 1985)

$k_{OH}(\text{calc}) = 63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1987).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 2\text{--}79$ h, based on river die-away test data (Digeronimo et al. 1979; Dojlido 1979; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 8\text{--}316$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 5.9$ h was estimated for the vapor phase reaction with hydroxyl radical of 5×10^5 radicals/cm³ in air (Atkinson et al. 1978; Atkinson 1985; quoted, Howard 1990);

photooxidation $t_{1/2} = 0.892\text{--}9.20$ h, based on measured rate constant for the gas-phase reaction with OH radical (Atkinson 1985; quoted, Howard et al. 1991) and ozone (Tuazon et al. 1978; selected, Howard et al. 1991).

Surface water: $t_{1/2} = 2\text{--}79$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 4\text{--}158$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 86\text{--}336$ h, based on soil die-away test data (Tate & Alexander 1976; Greene et al. 1981; selected, Howard et al. 1991).

Biota:

TABLE 16.1.2.1.1

Reported vapor pressures of dimethylamine at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

$$\log P = A - B/(T/K) - C \log (T/K) + D \cdot (T/K) - E \cdot (T/K)^2 + F \cdot (T/K)^3 \quad (5)$$

Ashton et al. 1939				Stull 1947	
static method				summary of literature data	
T/K	P/Pa			t/°C	P/Pa
201.387	648	bp/K	280.04	-87.7	133.3
213.802	1959	mp/K	180.97	-72.2	666.6
222.078	3780	$\Delta H_v/(\text{kJ mol}^{-1}) = 26.48$ (bp)		-64.6	1333
232.137	7775	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 5.94$ (mp)		-56.0	2666
242.078	14743			-46.7	5333
249.640	22949	eq. 5	P/mmHg	-40.7	7999
256.449	33269	A	32.26370	-32.6	13332
262.977	46404	B	2460.10	-20.4	26664
270.182	65491	C	8.6390	-7.1	53329
275.934	84860	D	7.6055×10^{-3}	7.4	101325
279.980	100974	E	3.51389×10^{-5}		
277.680	91519	F	5.3241×10^{-8}	mp/°C	-96.0
280.018	101141				

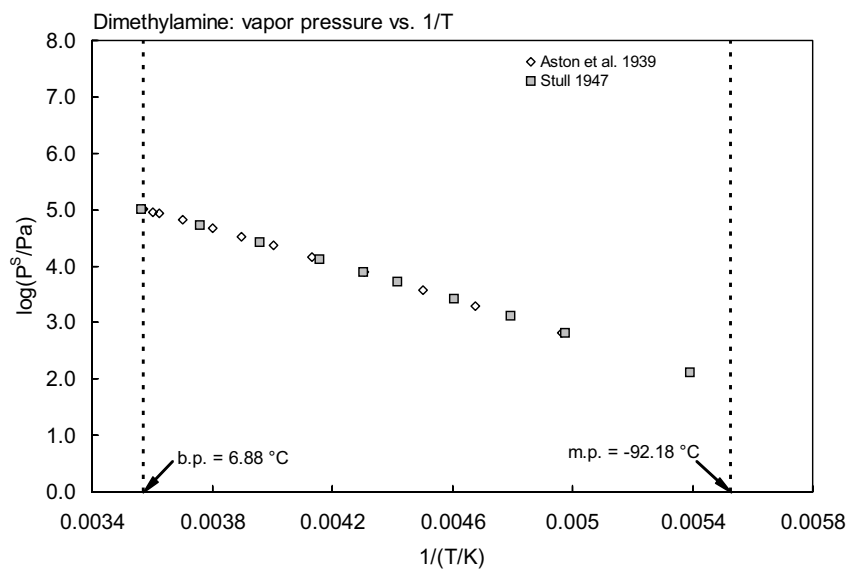


FIGURE 16.1.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethylamine.

16.1.2.2 Trimethylamine



Common Name: Trimethylamine

Synonym: dimethylamino methane, TMA

Chemical Name: trimethylamine

CAS Registry No: 75-50-3

Molecular Formula: C_3H_9N , $CH_3N(CH_3)_2$

Molecular Weight: 59.110

Melting Point ($^{\circ}C$):

-117.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

2.87 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6356 (Weast 1982–83)

Molar Volume (cm^3/mol):

93 ($20^{\circ}C$, calculated-density)

93.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

9.801, 9.987 (Perrin 1972; quoted, Howard 1990)

9.80 (pK_a , protonated cation + 1, Dean 1985)

9.79 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

22.85, 24.13 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$) or as indicated:

410000 (Dean 1985)

890000 ($30^{\circ}C$, Howard 1990)

291000 (selected, Yaws et al. 1990)

miscible (Stephenson 1993b)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this chapter):

221715* (isoteniscope, measured range 0 – $40^{\circ}C$, Swift & Hochanadel 1945)

$\log (P/mmHg) = 24.91300 - 2018.37/(T/K) - 6.0303 \cdot \log (T/K)$; temp range 0 – $40^{\circ}C$ (isoteniscope method, Swift & Hochanadel 1945)

265200* (extrapolated-regression of tabulated data, temp range -97.1 to $+2.9^{\circ}C$, Stull 1947)

226540 (calculated by formula, Dreisbach 1961)

$\log (P/mmHg) = 6.97038 - 968.7/(234.0 + t/^{\circ}C)$, temp range -58 to $32^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

$\log (P/mmHg) = [-0.2185 \times 6361.7/(T/K)] + 7.952370$; temp range -97.1 to $2.9^{\circ}C$ (Antoine eq., Weast 1972–73)

192500 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

219300, 221800 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.98554 - 1957.276/(237.664 + t/^{\circ}C)$, temp range -80.3 to $3.45^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 5.87712 - 894.366/(228.276 + t/^{\circ}C)$, temp range 0 – $40^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

214200 (Daubert & Danner 1985)

219000 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 6.85755 - 955.94/(237.52 + t/^{\circ}C)$, temp range -80 to $3^{\circ}C$ (Antoine eq., Dean 1985, 1992)

219900 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.01402 - 968.978/(-34.253 + T/\text{K})$, temp range 192–277 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 58.6807 - 2.686 \times 10^3/(T/\text{K}) - 20.36 \cdot \log (T/\text{K}) + 1.3131 \times 10^{-2} \cdot (T/\text{K}) - 6.563 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 156–433 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

6.672 (exptl., Hine & Mookerjee 1975)

12.71, 2.16 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

15.64 (calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.27 (shake flask-TN, Sandell 1962; quoted, Leo et al. 1971)

0.27; 0.20 (calculated-f const., calculated- π const., Rekker 1977)

0.16 (shake flask, Hansch & Leo 1985)

0.16 (recommended, Sangster 1989)

0.16 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

< 0.0 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.462 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

0.602 (soil, estimated-solubility, Lyman et al. 1982; quoted, Howard 1990)

0.778; 2.365; 2.831 (Podzol soil; Alfisol soil; sediments von Oepen et al. 1991)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 11$ h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 6.09 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (Atkinson et al. 1977; Atkinson 1989)

photooxidation $t_{1/2} = 62$ d in water, based on rate constant $k = 1.3 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with photochemically produced hydroxyl radicals of $1 \times 10^{-17} \text{ mol} \cdot \text{L}^{-1}$ in water (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990)

$k_{OH} = 6.10 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with $1 \times 10^6 \text{ OH radicals/cm}^3$ with a loss rate of 5.0 d^{-1} and rate constant $k_{O_3} = 9.70 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with $7 \times 10^{11} \text{ O}_3 \text{ molecules/cm}^3$ with a loss rate of 0.6 d^{-1} both at room temp. (Atkinson & Carter 1984)

calculated $k_{OH} = 64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 4.0$ h, based on rate constant $k = 6.09 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radical of $8 \times 10^5 \text{ radicals/cm}^3$ in air at 25.5°C and $t_{1/2} = 1.4$ d, based on rate constant $k = 9.73 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with ozone of $6 \times 10^{11} \text{ molecules/cm}^3$ in air at 24.4°C (Atkinson 1985; GEMS 1986; quoted, Howard 1990).

Surface water: $t_{1/2} = 62$ d, based on rate constant $k = 1.3 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with photochemically produced hydroxyl radicals of $1 \times 10^{-17} \text{ mol L}^{-1}$ in water (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990).

TABLE 16.1.2.2.1

Reported vapor pressures of trimethylamine at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & \end{aligned}$$

Aston et al. 1944		Swift & Hochanadel 1945		Stull 1947	
static method		isoteniscope		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-80.315	805	0	91059	-97.1	133.3
-74.081	1367	15	158520	-81.7	666.6
-62.339	3354	20	188651	-73.8	1333
-51.938	6777	25	221715	-65.0	2666
-46.842	9305	30	259444	-55.2	5333
-41.774	12548	35	302107	-48.8	7999
-35.617	17684	40	349437	-40.3	13332
-28.507	25624			-27.0	26664
-24.155	31772	bp/K	276.03	-12.5	53329
-23.067	33494			2.90	101325
-20.164	38401	eq. 4	P/mmHg		
-15.974	46505	A	24.91300	mp/°C	-117.1
-11.422	56802	B	2018.37		
-8.985	63039	C	6.0303		
-7.399	67346				
-3.113	80208	$\Delta H_v/(\text{kJ mol}^{-1}) = 23.93$			
0.780	93495	at bp			
2.928	101526				
3.454	103611				

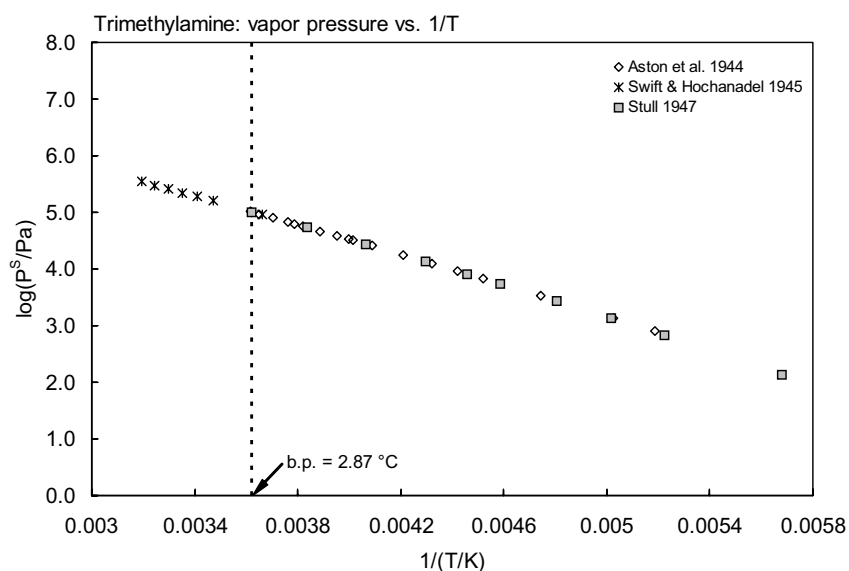
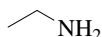


FIGURE 16.1.2.2.1 Logarithm of vapor pressure versus reciprocal temperature for trimethylamine.

16.1.2.3 Ethylamine



Common Name: Ethylamine

Synonym: aminoethane, ethanamine, monoethylamine

Chemical Name: aminoethane, ethylamine

CAS Registry No: 75-04-7

Molecular Formula: C_2H_7N , $CH_3CH_2NH_2$

Molecular Weight: 45.084

Melting Point ($^{\circ}C$):

−80.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

16.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6829 (Dreisbach 1961; Weast 1982–83)

0.6769 ($25^{\circ}C$, Dreisbach 1961)

Molar Volume (cm^3/mol):

65.4 ($5^{\circ}C$, Stephenson & Malanowski 1987)

66.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

10.79 (Perrin 1972)

10.81 ($20^{\circ}C$, Weast 1982–83)

10.63 (protonated cation + 1, Dean 1985)

10.70 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.08, 27.57 ($25^{\circ}C$, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985; Howard 1990; Stephenson 1993b)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):

156200* (extrapolated-regression of tabulated data, temp range -82.3 to $16.6^{\circ}C$, Stull 1947)

141620 (calculated by formula, Dreisbach 1961)

$\log (P/mmHg) = 7.3862 - 1137.30/(235.85 + t/^{\circ}C)$; temp range -43 to $47^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

93325* ($20^{\circ}C$, temp range 1.95 to $20^{\circ}C$, Bittrich et al. 1962)

$\log (P/mmHg) = [-0.2185 \times 6845.1/(T/K)] + 7.973674$; temp range -82.3 to $176^{\circ}C$, (Antoine eq., Weast 1972–73)

121570, 172220 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

139100 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.12561 - 559.427/(162.579 + t/^{\circ}C)$; temp range 1.95 – $14.65^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

139700 (Daubert & Danner 1985)

141000 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 7.05413 - 987.31/(220.0 + t/^{\circ}C)$; temp range -20 to $90^{\circ}C$ (Antoine eq., Dean 1985, 1992)

137500, 141200 (calculated-Antoine eq.-II, III, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.57462 - 1167.57/(-34.18 + T/K)$; temp range 213 – $297 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.43082 - 1140.62/(-32.433 + T/K)$; temp range 290 – $449 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.21526 - 1009.66/(-49.804 + T/\text{K})$; temp range 291–367 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.48782 - 1176.995/(-26.674 + T/\text{K})$; temp range 377–456 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

140900 (calculated-Cox eq., Chao et al. 1990)

$\log (P/\text{mmHg}) = 33.2962 - 2.4307 \times 10^3/(T/\text{K}) - 9.0779 \cdot \log (T/\text{K}) - 1.3848 \times 10^{-9} \cdot (T/\text{K}) + 3.8183 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 192–456 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

1.012 (partial pressure, Butler & Ramchandani 1935)

0.683 (exptl., Hine & Mookerjee 1975)

0.859, 0.730 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.421 (calculated-molecular structure, Russell et al. 1992)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

−0.30 (shake flask-titration with ion correction, Korenman et al. 1973)

−0.16, −0.14; −0.19 (calculated-fragment const.; calculated- π const., Rekker 1977)

−0.13 (Hansch & Leo 1985)

−0.13 (recommended, Sangster 1989)

−0.14 (calculated-CLOGP, Jäkel & Klein 1991)

−0.13 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

< 0.0 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 2.0$ d was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} > 9.9$ d for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH} = 2.77 \times 10^{-11} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$ at 299 K (Atkinson et al. 1977; quoted, Carlier et al. 1986)

photooxidation $t_{1/2} = 321$ d in water, based on a rate constant $k = 2.5 \times 10^9 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$ for the aqueous-phase reaction with photochemically produced OH radical of $1 \times 10^{-17} \text{ mol} \cdot \text{L}^{-1}$ (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990)

$k_{O_3} = (2.76 \pm 0.34) \times 10^{-20} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$ at 296 ± 2 K under atmospheric conditions (Atkinson & Carter 1984)

$k_{OH} = 27.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299.6 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 8.6$ h, based on rate constant $k = 6.54 \times 10^{-11} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$ for the vapor-phase reaction with an average hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ at 25.5°C (Atkinson 1985; quoted, Howard 1990).

Surface water: $t_{1/2} = 321$ d, based on a rate constant $k = 2.5 \times 10^9 \text{ L}\cdot\text{mol}^{-1}\cdot\text{s}^{-1}$ for the aqueous-phase reaction with photochemically produced hydroxyl radical of $1 \times 10^{-17} \text{ mol}\cdot\text{L}^{-1}$ (Mill et al. 1980; Güesten et al. 1981; quoted, Howard 1990).

TABLE 16.1.2.3.1
Reported vapor pressures of ethylamine at various temperatures

Stull 1947		Bittrich et al. 1962	
summary of literature data			
t/°C	P/Pa	t/°C	P/Pa
-82.3	133.3	1.95	53329
-66.4	666.6	4.55	59995
-58.3	1333	6.85	66661
-48.6	2666	9.15	73327
-39.8	5333	11.05	79993
-33.4	7999	12.85	86659
-25.1	13332	14.65	93325
-12.3	26664		
2.0	53329		
16.6	101325		
mp/°C	-80.6		

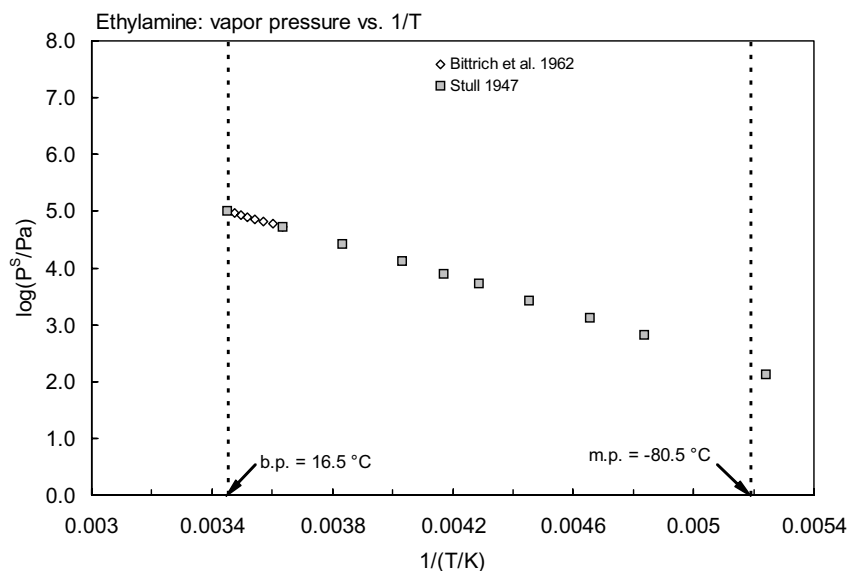
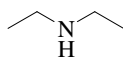


FIGURE 16.1.2.3.1 Logarithm of vapor pressure versus reciprocal temperature for ethylamine.

16.1.2.4 Diethylamine



Common Name: Diethylamine

Synonym: aminoethylethane, *N*-ethylethanamine

Chemical Name: aminoethylethane, diethylamine

CAS Registry No: 109-89-7

Molecular Formula: $C_4H_{11}N$, $CH_3CH_2NHCH_2CH_3$

Molecular Weight: 73.137

Melting Point ($^{\circ}C$):

−49.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

55.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6993, 0.6926 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach. 1961)

0.7056 (Weast 1982–83)

0.7070, 0.7016 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

103.4 ($20^{\circ}C$, calculated-density)

109.0 (exptl. at normal bp, Lee et al. 1972)

111.9 (calculated-Le Bas method at normal boiling point.)

Dissociation Constant, pK_a :

10.98 (Perrin 1965; quoted, Howard 1990)

10.80 ($35^{\circ}C$, Perrin 1972)

10.80 (protonated cation + 1, Dean 1985)

11.07 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.38, 29.50 ($25^{\circ}C$, bp, Dreisbach 1961)

31.32, 29.07 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

815000 ($14^{\circ}C$, quoted, Verschueren 1983)

miscible (Dean 1985; Riddick et al. 1986; Yaws et al. 1990)

miscible (Stephenson 1993b)

Vapor Pressure (Pa at $25^{\circ}C$ and or as indicated reported temperature dependence equations. Additional data at other temperatures designated* are compiled at the end of this section):

26664* ($21^{\circ}C$, summary of literature data, temp range -33.0 to $55.5^{\circ}C$, Stull 1947)

31130 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.14099 - 1209.9/(229.0 + t/^{\circ}C)$; temp range -15 to $90^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

39997* ($31.45^{\circ}C$, temp range 31.45 – $60.58^{\circ}C$, Bittrich & Kauer 1962)

31471* ($25.17^{\circ}C$, temp range 19.73 – $40.22^{\circ}C$, Kilian & Bittrich 1965)

$\log(P/mmHg) = [-0.2185 \times 7307.5/(T/K)] + 7.701718$; temp range -33.0 to $210^{\circ}C$ (Antoine eq., Weast 1972–73)

26660, 38660 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

30110, 31310 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 4.97981 - 580.448/(143.68 + t/^{\circ}C)$; temp range 31.45 – $60.58^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 5.84728 - 994.478/(203.53 + t/^{\circ}C)$; temp range 19.758 – $40.22^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

31130 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 4.92649 - 583.297/(144.145 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

31490 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.96802 - 1058.538/(-61.331 + T/\text{K})$; temp range 302–328 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.92678 - 1028.405/(-66.2061 + T/\text{K})$; temp range 325–437 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 5.8016 - 583.3/(144.1 + t/^{\circ}\text{C})$; temp range 31–61 $^{\circ}\text{C}$ (Antoine eq., Dean 1992)

$\log (P/\text{mmHg}) = 32.626 - 2.4918 \times 10^3/(T/\text{K}) - 9.3285 \cdot \log (T/\text{K}) + 3.990 \times 10^{-3} \cdot (T/\text{K}) + 1.1732 \times 10^{-12} \cdot (T/\text{K})^2$; temp range 223–497 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$):

2.596 (exptl., Hine & Mookerjee 1975)

2.537, 2.37 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

6.67 (calculated-vapor liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.43 (shake flask, Collander 1951)

0.57 (shake flask-titration, Sandell 1962)

0.60, 0.61; 0.70 (calculated-fragment const.; calculated- π const., Rekker 1977)

0.58 (Hansch & Leo 1985)

0.58 (20 $^{\circ}\text{C}$, shake flask-GC, Takayama et al. 1985)

0.81 (HPLC- k' correlation, Eadsforth 1986)

0.58 (recommended, Sangster 1989)

0.58 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.210 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.699 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 31.6$ h for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: photooxidation $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 0.21$ d in air, based on an estimated second-order rate constant $k = 77.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5×10^5 radicals/ cm^3 in air (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radicals in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 0.21$ d, based on an estimated rate constant $k \sim 77.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5×10^5 radicals/ cm^3 in air (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.4.1

Reported vapor pressures of diethylamine at various temperatures

Stull 1947		Bittrich & Kauer 1962		Kilian & Bittrich 1965	
summary of literature data					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-33.0	1333	31.45	39997	19.73	24718
-22.6	2666	34.75	46663	25.17	31471
-11.3	5333	38.05	53329	30.31	39343
-4.0	7999	41.1	59995	34.99	47596
6.0	13332	43.85	66661	40.22	58582
21.0	26664	46.5	73327		
38.0	53329	48.85	79993		
55.5	101325	51.10	86659		
		53.20	93325		
mp/°C	-38.9	55.53	101325		
		57.05	106658		
		59.00	113324		
		60.58	119990		

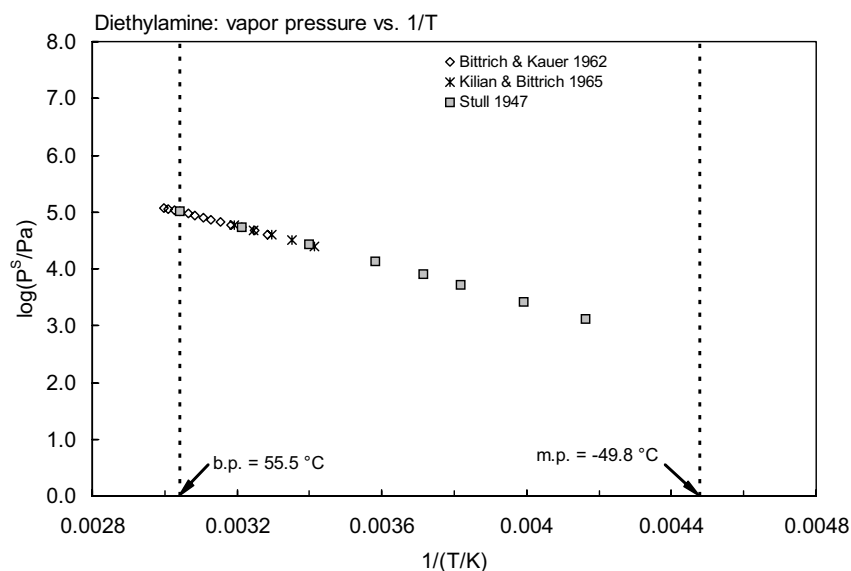
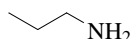


FIGURE 16.1.2.4.1 Logarithm of vapor pressure versus reciprocal temperature for diethylamine.

16.1.2.5 *n*-Propylamine

Common Name: Propylamine

Synonym: 1-aminopropane, 1-propanamine, *n*-propylamine

Chemical Name: aminopropane, *n*-propylamine

CAS Registry No: 107-10-8

Molecular Formula: C₃H₉N, CH₃CH₂CH₂NH₂

Molecular Weight: 59.110

Melting Point (°C):

−84.75 (Lide 2003)

Boiling Point (°C):

47.22 (Lide 2003)

Density (g/cm³ at 20°C):

0.7173 (Dreisbach 1961; Weast 1982–83; Dean 1985; Riddick et al. 1986)

0.7123 (25°C, Dreisbach 1961)

Molar Volume (cm³/mol):

82.4 (liquid molar volume, Kamlet et al. 1986, 1987)

88.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:

10.74, 10.789 (20°C, Perrin 1972)

10.71 (pK_a, 20°C, Weast 1982–83)

10.57 (pK_{BH}⁺, Dean 1985; Riddick et al. 1986)

10.68 (pK_a, Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.13, 29.73 (25°C, bp, Dreisbach 1961)

31.26, 29.54 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.974 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Dean 1985; Stephenson 1993b)

miscible (Riddick et al. 1986; Howard 1990; Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

41800* (interpolated-regression of tabulated data, temp range −64.4 to 48.5°C, Stull 1947)

41050 (calculated by formula, Dreisbach 1961)

log (P/mmHg) = 7.2672 − 1218.1/(229.9 + t/°C); temp range −20 to 81°C (Antoine eq. for liquid state, Dreisbach 1961)

42100* (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

log (P/mmHg) = 6.92646 − 1044.028/(t/°C + 210.833); temp range 23–77.6°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)

log [(P/atm) = [1 − 320.379 ± (T/K)] × 10⁴{0.922208 − 10.51259 × 10^{−4}·(T/K) + 11.25530 × 10^{−7}·(T/K)²}, temp range: 34–77.6°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)

log (P/mmHg) = [−0.2185 × 7408.0/(T/K)] + 7.867998; temp range −64.4 to 214.5°C (Antoine eq., Weast 1972–73)

32660 (20°C, 31°C, Verschueren 1983)

38550; 42110 (22.97°C, quoted exptl., calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.05146 − 1044.082/(210.84 + t/°C); temp range 22.97–77.6°C (Antoine eq. from reported exptl. data of Osborn & Douslin 1968, Boublik et al. 1984)

42120 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.92651 - 1044.05/(210.84 + t/^{\circ}\text{C})$; temp range: 23–77°C (Antoine eq., Dean 1985, 1992)
 41050 (Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.05136 - 1044.028/(210.833 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 42120 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.04693 - 1041.725/(-62.596 + T/\text{K})$; temp range 295–351 K (Antoine eq., Stephenson & Malanowski 1987)
 42125 (calculated-Cox eq., Chao et al. 1990)
 $\log (P/\text{mmHg}) = 24.6420 - 2.3152 \times 10^3/(T/\text{K}) - 5.8711 \cdot \log (T/\text{K}) - 4.6258 \times 10^{-11} \cdot (T/\text{K}) + 1.582 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 190–497 (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1.274 (partial pressure, Butler & Ramchandani 1935)
 0.784; 0.732 (exptl.; calculated-group contribution, Hine & Mookerjee 1975)
 1.330 (calculated-bond contribution, Hine & Mookerjee 1975)
 0.637 (calculated-molecular structure, Russell et al. 1992)
 2.01 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.28 (shake flask-GC, Korenman et al. 1973)
 0.37, 0.39; 0.31 (calculated-f const.; calculated- π const., Rekker 1977)
 0.48 (shake flask-GC, pH 13, Yakayama et al. 1985)
 0.48 (recommended, Sangster 1989)
 0.48 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

–0.886 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

< 1.699 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 2.44$ d was estimated for a model river 1 m deep flowing at 1 m/s with a wind speed of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 12$ h in air, based on estimated rate constant $k = 3.21 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ for the vapor-phase reaction with hydroxyl radical of $5 \times 10^5/\text{cm}^3$ at 25°C in the atmosphere (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 12$ h, based on estimated second-order rate constant of $3.21 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ for the vapor-phase reaction with hydroxyl radical of $5 \times 10^5/\text{cm}^3$ at 25°C in the atmosphere (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.5.1
Reported vapor pressures of *n*-propylamine at various temperatures

Stull 1947		Osborn & Douslin 1968	
summary of literature data		ebulliometric method	
t/°C	P/Pa	t/°C	P/Pa
-64.4	133.3	22.973	38547
-46.3	666.6	27.750	47359
-37.2	1333	32.564	57803
-27.1	2666	37.414	70109
-16.0	5333	42.304	84525
-9.0	7999	47.229	101325
0.50	13332	52.193	120798
15.0	26664	57.195	143268
31.5	53329	62.235	169052
48.5	101325	67.314	198530
		72.430	232087
mp/°C	-83.0	77.587	270110

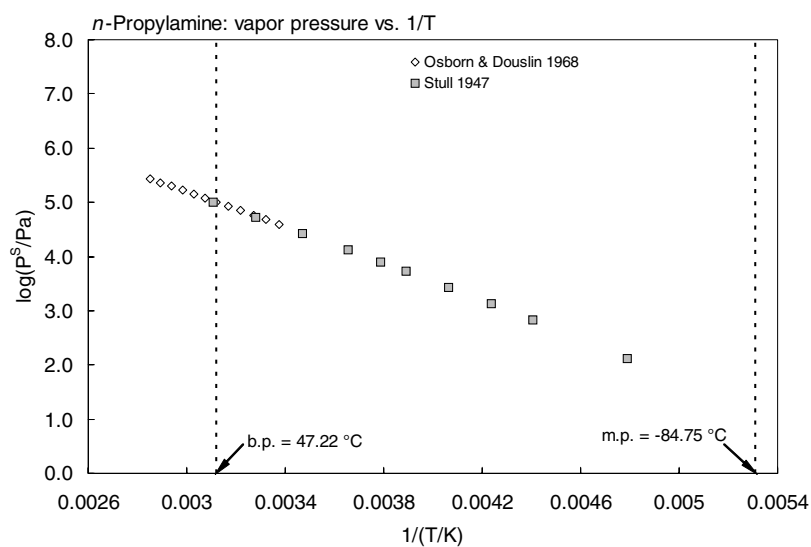
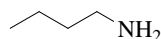


FIGURE 16.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-propylamine.

16.1.2.6 *n*-Butylamine

Common Name: Butylamine

Synonym: 1-aminobutane, *n*-butylamine, 1-butanamine

Chemical Name: 1-aminobutane, *n*-butylamine

CAS Registry No: 109-73-9

Molecular Formula: C₄H₁₁N, CH₃CH₂CH₂CH₂NH₂

Molecular Weight: 73.137

Melting Point (°C):

−49.1 (Dreisbach 1961; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):

77.0 (Lide 2003)

Density (g/cm³ at 20°C):

0.7414 (Dreisbach 1961; Weast 1982–83)

0.7392 (Riddick et al. 1986)

Molar Volume (cm³/mol):

98.8 (20°C, calculated-density)

110.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:

10.77 (Perrin 1965; pK_a, 20°C, Weast 1982–83; Howard 1990)

10.65 (Perrin 1972)

10.64 (pK_a, protonated + 1, Dean 1985; Sangster 1989)

10.77 (pK_{BH+}, Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.54, 32.11 (25°C, bp, Dreisbach 1961)

35.74, 31.80 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Dean 1985; Howard 1990; Yaws et al. 1990)

miscible (Riddick et al. 1986)

miscible (Stephenson 1993b)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

13850 (Hoy 1970; Abraham 1984)

12230 (calculated by formula, Dreisbach 1961)

log (P/mmHg) = 7.213 − 1308.4/(224.2 + t/°C); temp range 4–114°C (Antoine eq. for liquid state, Dreisbach 1955)

9600 (20°C, Verschueren 1983)

12230 (quoted lit., Riddick et al. 1986; quoted, Howard 1990)

log (P/kPa) = 6.07009 − 1157.810/(207.80 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

12520 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.2635 − 1258.745/(−54.49 + T/K); temp range 313–350 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 25.0711 − 2.5701 × 10³/(T/K) − 5.8985 · log (T/K) + 7.9399 × 10^{−10} · (T/K) + 1.192 × 10^{−6} · (T/K)²; temp range 124–532 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

1.526 (partial pressure, Butler & Ramchandani 1935)

1.528 (exptl., Hine & Mookerjee 1975)

- 1.676, 1.68 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.880 (calculated-molecular structure, Russell et al. 1992)
 1.785 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW} :

- 0.68 (shake flask, Collander 1951)
 0.88 (shake flask-titration, Sandell 1962)
 0.81 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1987)
 0.74 (shake flask-titration, Korenman et al. 1973)
 0.90, 0.92; 0.81 (calculated- f const.; calculated- π const., Rekker 1977)
 0.80 (inter-lab. shake flask average, Eadsforth & Moser 1983)
 0.97 (shake flask-GC, Takayama et al. 1985)
 0.86 (recommended, Sangster 1989)
 0.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

- 3.61 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 0.505 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, log K_{OC} :

- 1.903 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)
 1.176, 2.021, 2.029 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
 1.880 (soil, quoted exptl., Meylan et al. 1992)
 1.780 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 1.95$ d was predicted for evaporation from a model river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: estimated vapor phase photooxidation $t_{1/2} = 0.479$ d in air, based on a result of reaction with photochemically produced hydroxyl radical at a concentration of 5×10^5 radicals/cm³ (USEPA 1986; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

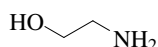
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated vapor phase $t_{1/2} = 0.479$ d, based on a result of reaction with photochemically produced hydroxyl radical at a concentration of 5×10^5 radicals/cm³ (USEPA 1986; quoted, Howard 1990).

16.1.2.7 Ethanolamine



Common Name: Ethanolamine

Synonym: β -aminoethyl alcohol, ethylolamine, 2-hydroxyethylamine, β -hydroxyethylamine, monoethanolamine, MEA

Chemical Name: ethanolamine, 2-aminoethanol

CAS Registry No: 141-43-5

Molecular Formula: $\text{C}_2\text{H}_7\text{NO}$, $\text{HOCH}_2\text{CH}_2\text{NH}_2$

Molecular Weight: 61.098

Melting Point ($^{\circ}\text{C}$):

10.5 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

171 (Lide 2003)

Density (g/cm^3 at 20°C):

1.0180 (Weast 1982–83)

1.0147 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

60.4 (Stephenson & Malanowski 1987)

73.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK :

9.48, 9.4994 (Perrin 1972; quoted, Howard 1990)

9.50 (pK_{BH^+} , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_{v} (kJ/mol):

92.09, 49.831 (25°C , bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.50 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} $\text{J}/\text{mol K}$:

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

miscible (Dean 1985)

miscible (Riddick et al. 1986; quoted, Howard 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

893* (65.4°C , Ramsay-Young method, measured range 65.4 – 170.9°C , Matthews et al. 1950)

$\log (P/\text{mmHg}) = 44.008 - 4089/(T/\text{K}) - 11.446 \pm \log (T/\text{K})$; temp range 65.4 – 170.9°C (Kirchhoff eq., ebulliometry, Matthews et al. 1950)

8707* (106.1°C , ebulliometry, measured range 106.1 – 170.37°C , McDonald et al. 1959)

$\log (P/\text{mmHg}) = 7.7380 - 1772.11/(186.25 + t/^{\circ}\text{C})$; temp range 106 – 170°C , or pressure range 65.31 – 760 mmHg (ebulliometry, McDonald et al. 1959)

53.32 (20°C , Verschueren 1983)

41.64, 46.67 (extrapolated values-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.54175 - 1554.149/(171.175 + t/^{\circ}\text{C})$; temp range 65.5 – 170.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.86239 - 1725.168/(185.556 + t/^{\circ}\text{C})$; temp range 106.1 – 170.37°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

42.51 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.4568 - 1577.67/(172.37 + t/^{\circ}\text{C})$; temp range 65 – 171°C (Antoine eq., Dean 1985, 1992)

48.0 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.86290 - 1732.11/(186.215 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

47.34 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 6.8629 - 1732.11/(-86.6 + T/\text{K})$; temp range 310 – 444 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

34.66 (from Dow Chemical's Handbook, Howard 1990)

$\log(P/\text{mmHg}) = 72.9125 - 5.8595 \times 10^3/(T/K) - 21.914 \cdot \log(T/K) - 7.1511 \times 10^{-10} \cdot (T/K) + 5.9841 \times 10^{-6} \cdot (T/K)^2$;
temp range 284–638 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.0041 (calculated-bond method, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

−1.31 (shake flask, Collander 1951)

−1.29; −1.35 (calculated- f const., calculated- π const., Rekker 1977)

−1.31 (recommended, Sangster 1993)

−1.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

< 0.0 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

0.699 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation $t_{1/2} = 11$ h in air, based on an estimated rate constant $k \sim 3.5 \times 10^{-11} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ in air (Atkinson 1987; quoted, Howard 1990).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: half-life of 11 h, based on an estimated rate constant of $3.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ in air (Atkinson 1987; quoted, Howard 1990).

TABLE 16.1.2.7.1

Reported vapor pressures of ethanolamine at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

Matthews et al. 1950				McDonald et al. 1959	
Ramsay-Young method				ebulliometric method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
65.4	893	137.9	32264	106.1	8707
65.5	947	144.6	42236	108.43	10058
69.5	1160	150.0	54195	112.29	11427
70.0	1253	161.4	73860	114.55	12702
75.4	1760	170.9	100125	116.79	14049
81.1	2320			125.73	20454
86.4	3280	bp/K	444.1	159.79	71862
90.0	3813			169.20	97584
96.4	5440	$\Delta H_v/(\text{kJ mol}^{-1}) = 46.07$ at bp		170.37	101325
101.7	7146	Kirchhoff, Rankine, Dupre			
105.5	8559	eq. 4	P/mmHg	mp/°C	10.31
112.1	11306	A	44.008	eq. 2	P/mmHg
117.3	14012	B	4809	A	7.7380
125.0	19452	C	11.446	B	173211
132.0	25771			C	186.215

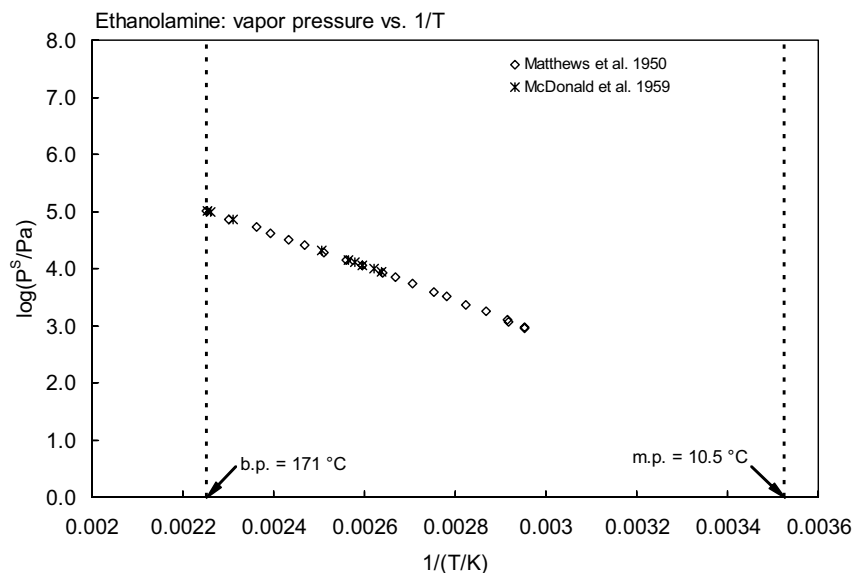
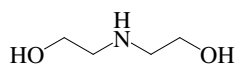


FIGURE 16.1.2.7.1 Logarithm of vapor pressure versus reciprocal temperature for ethanolamine.

16.1.2.8 Diethanolamine



Common Name: Diethanolamine

Synonym: 2,2'-amino-diethanol, 3-aza-1,5-pentanediol, diethylolamine, bis(hydroxyethyl)amine, 2,2'-dihydroxydiethylamine, β,β' -dihydroxydiethylamine, 2,2'-iminobisethanol, 2,2'-iminodiethanol

Chemical Name: diethanolamine

CAS Registry No: 111-42-2

Molecular Formula: $C_4H_{11}NO_2$, $HOCH_2CH_2NHCH_2CH_2OH$

Molecular Weight: 105.136

Melting Point ($^{\circ}C$):

28.0 (Weast 1982–83; Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

268.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0966 (Weast 1982–83)

1.0936 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

96.5 ($30^{\circ}C$, Stephenson & Malanowski 1987)

126.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK :

8.88, 8.97 (Perrin 1972)

8.88 (pK_{BH^+} , Dean 1985; Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.3, 65.229 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.104 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.934 (mp at $28^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

954000 (Verschuere 1983)

964000 (Dean 1985)

954000 ($20^{\circ}C$, Riddick et al. 1986)

miscible (from Dow Chemical's Handbook, Howard 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

< 1.333 ($20^{\circ}C$, Verschuere 1983)

0.040 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 8.1388 - 2327.9/(174.4 + t/^{\circ}C)$; temp range 194 – $241^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.030 (quoted lit., Riddick et al. 1986)

$\log(P/kPa) = 7.26458 - 2328.56/(174.399 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 7.26044 - 2326.23/(-98.907 + T/K)$; temp range: 423 – $542 K$ (liquid, Antoine eq., Stephenson & Malanowski 1987)

0.0373 (quoted from Dow Chemical's Handbook, Howard 1990)

$\log(P/mmHg) = 122.0877 - 8.8422 \times 10^3/(T/K) - 40.422 \cdot \log(T/K) + 1.4062 \times 10^{-2} \cdot (T/K) + 1.1986 \times 10^{-12} \cdot (T/K)^2$; temp range 301 – $542 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.42×10^{-9} (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.43 (shake flask, Collander 1951)
- 1.51 (calculated-fragment const., Rekker & De Kort 1979)
- 1.43 (recommended, Sangster 1993)
- 1.43 (recommended, Hansch et al 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- < 0.0 (estimated- K_{OW} , Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.602 (soil, estimated- K_{OW} , Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation $t_{1/2} = 0.72\text{--}7.2$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1990; Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 14.4\text{--}168$ h, based on measured half-life in surface water grab sample experiment (Boethling & Alexander 1979; quoted, Howard et al. 1991) and aqueous aerobic screening test data (Gerike & Fischer 1979; Bridie et al. 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 57.6\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.72\text{--}7.2$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1990; Howard et al. 1991);

atmospheric transformation lifetime by reaction with water was estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 14.4\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

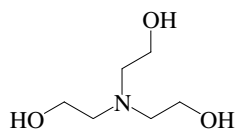
Groundwater: $t_{1/2} = 28.8\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 14.4\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.2.9 Triethanolamine



Common Name: Triethanolamine

Synonym: 2,2',2''-nitrilotriethanol, 2,2',2''-nitrilotrisethanol, triethylolamine, trihydroxytriethylamine, trolamine, tris(hydroxyethyl)-amine, TEA

Chemical Name: triethanolamine

CAS Registry No: 102-71-6

Molecular Formula: $C_6H_{15}NO_3$, $(HOCH_2CH_2)_3N$

Molecular Weight: 149.188

Melting Point ($^{\circ}C$):

20.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

335.4 (Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1242 (Weast 1982–83; Dean 1985)

1.1196 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

133.3 (Stephenson & Malanowski 1987)

182.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK :

7.92 (Perrin 1972; quoted, Howard 1990)

7.76 (pK_{BH^+} , Dean 1985; Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

67.475 (bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.20 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985; Howard 1990)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

< 1.33 ($20^{\circ}C$, Verschueren 1983)

0.0131 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 9.19319 - 4543.817/(297.839 + t/^{\circ}C)$, temp range: 252.7 – $305.6^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.0100 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 10.0675 - 4542.78/(297.76 + t/^{\circ}C)$, temp range: 252 – $305^{\circ}C$ (Antoine eq., Dean 1985, 1992)

< 1.30 ($20^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 7.67989 - 2962.73/(186.75 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 9.53861 - 4951.87/(49.99 + T/K)$, temp range: 523 – $579\ K$, (Antoine eq., Stephenson & Malanowski 1987)

4.79×10^{-4} (quoted from Dow Chemical's Handbook, Howard 1990)

$\log(P/mmHg) = 135.3206 - 1.0312 \times 10^4/(T/K) - 44.637 \cdot \log(T/K) + 1.4368 \times 10^{-2} \cdot (T/K) - 1.7552 \times 10^{-13} \cdot (T/K)^2$; temp range 294 – $787\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.42×10^{-14} (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.32, -1.75 (calculated, Verschueren 1983)
- 1.59 (Howard 1990)
- 1.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- < 0.0 (estimated- K_{OW} , Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.477 (soil, estimated- K_{OW} , Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: photooxidation $t_{1/2} = 4.0$ h in air, based on an estimated rate constant $k \sim 10.4 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ in air at 25°C (Atkinson 1987; quoted, Howard 1990).

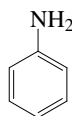
Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 4.0$ h, based on an estimated rate constant $k \sim 10.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ radicals/cm}^3$ in air at 25°C (Atkinson 1987; quoted, Howard 1990).

16.1.3 AROMATIC AMINES**16.1.3.1 Aniline**

Common Name: Aniline

Synonym: phenylamine, aminobenzene, benzeneamine, benzenamine

Chemical Name: aniline

CAS Registry No: 62-53-3

Molecular Formula: $C_6H_5NH_2$

Molecular Weight: 93.127

Melting Point ($^{\circ}C$):

-6.02 (Lide 2003)

Boiling Point ($^{\circ}C$):

184.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.02173, 1.01750 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.02173 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

91.2 ($20^{\circ}C$, calculated-density)

110.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.596 (Perrin 1972; Howard 1989)

4.600 (McLeese et al. 1979; Riddick et al. 1986; Sangster 1989)

4.630 (Weast 1982–83)

4.58, 3.96 (quoted, HPLC, Miyake et al. 1987)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

54.28, 43.17 ($25^{\circ}C$, bp, Dreisbach 1955)

55.843, 44.53 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

36650 (Hill & Macy 1924)

36070 (Seidell 1941)

38670 (shake flask-residue volume method, Booth & Everson 1948)

36220 (shake flask-interferometry, Donahue & Bartell 1952)

34100 (Stephen & Stephen 1963)

36600 (Kenaga 1980)

34000 (Verschueren 1983)

56900 (calculated-activity coeff. γ by UNIFAC, Fu & Luthy 1985, 1986)

33800 (selected, Riddick et al. 1986)

34200 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3 ($43.7^{\circ}C$, static method, measured range 43.7 – $183.9^{\circ}C$, Kahlbaum 1898)

85.71* (extrapolated-regression of tabulated data, temp range 34.8 – $184.4^{\circ}C$ Stull 1947)

$\log(P/mmHg) = 7.57170 - 1941.7/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

10351* ($112.92^{\circ}C$, ebulliometry, measured range 112.92 – $183.93^{\circ}C$, Dreisbach & Shrader 1949)

89.52 (calculated by formula, Dreisbach 1955; quoted, Riddick et al. 1986)

$\log (P/\text{mmHg}) = 7.24179 - 1674.3/(200.0 + t/^{\circ}\text{C})$; temp range 90–250°C (Antoine eq. for liquid state, Dreisbach 1955)

6806* (102.59°C, ebulliometry, measured range 102.59–185.15°C, McDonald et al. 1959)

$\log (P/\text{mmHg}) = 7.25375 - 1684.35/(201.175 + t/^{\circ}\text{C})$, temp range 103–185°C (Antoine eq., ebulliometry, McDonald et al. 1959)

133.3* (31.55°C, calculated-thermodynamic properties, temp range 31.55–184.40°C, Hatton et al. 1962)

$\log (P/\text{mmHg}) = [-0.2185 \times 11307.6/(T/\text{K})] + 8.221995$; temp range 34.8–422.4°C (Antoine eq., Weast 1972–73)

88.30 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log (P/\text{mmHg}) = 7.3201 - 1731.515/(205.049 + t/^{\circ}\text{C})$; temp range 102.6–185.2°C (Antoine eq. from reported exptl. data of McDonald et al. 1959, Boublik et al. 1973)

$\log (P/\text{mmHg}) = [-0.2185 \times 11307.6/(T/\text{K})] + 8.221995$; temp range 34.8–422.4°C (Antoine eq., Weast 1972–73)

82.71 (calculated-Cox eq., Chao et al. 1983)

$\log (P/\text{atm}) = [1 - 457.025/(T/\text{K})] \times 10^4 \{0.911551 - 6.64936 \times 10^{-4} \cdot (T/\text{K}) + 5.25455 \times 10^{-7} \cdot (T/\text{K})^2\}$; temp range: 267.3–695.0 K (Cox eq., Chao et al. 1983)

80 ± 6 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)

40.0 (20°C, Verschueren 1983)

88.0, 48.24 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.43196 - 1722.154/(205.002 + t/^{\circ}\text{C})$; temp range 102.6–185.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.68977 - 1234.569/(151.207 + t/^{\circ}\text{C})$; temp range 112.9–183.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

65.18 (Daubert & Danner 1985)

89.30 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.32010 - 1731.515/(206.049 + t/^{\circ}\text{C})$; temp range 102–185°C (Antoine eq., Dean 1985, 1992)

$\log (P/\text{kPa}) = 5.69066 - 1941.7/(230.0 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

89.60 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.40627 - 1702.817/(-70.155 + T/\text{K})$; temp range 304–458 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 8.1019 - 2728/(T/\text{K})$; temp range 273–338 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.41147 - 1708.239/(-69.454 + T/\text{K})$; temp range 373–458 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.44338 - 1682.348/(-78.065 + T/\text{K})$; temp range: 455–523 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

86.70 (calculated-Cox eq., Chao et al. 1990)

$\log (P/\text{mmHg}) = 124.3764 - 7.1676 \times 10^3/(T/\text{K}) - 42.763 \cdot \log (T/\text{K}) + 1.7336 \times 10^{-2} \cdot (T/\text{K}) + 5.7138 \times 10^{-15} \cdot (T/\text{K})^2$; temp range 267–699 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

13778 (Hakuta et al. 1977)

12.16 (measured, Yoshida et al. 1983)

0.193 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.90 (shake flask-UV, Fujita et al. 1964)

0.90 (shake flask, Iwasa et al. 1965)

0.90 (shake flask-UV, Hansch et al. 1968)

0.90 (Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1983, Hansch & Leo 1985)

0.89 (shake flask-UV at pH 5.6, Umeyama et al. 1971)

0.90 (HPLC- k' correlation, Carlson et al. 1975)

0.85 (shake flask, Lu & Metcalf 1975)

0.90 (HPLC-RT correlation, Mirrlees et al. 1976)

0.93 ± 0.05 (shake flask at pH 7, Unger et al. 1978)

0.90, 0.98, 0.85 (shake flask, Hansch & Leo 1979)

0.91 (HPLC- k' correlation, Könnemann et al. 1979)

0.90 (shake flask-UV, Briggs 1981)

- 1.03 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 0.90 (HPLC- k' correlation, Hammers et al. 1982)
 0.90 (inter-laboratory studies. shake flask average, Eadsforth & Moser 1983)
 1.09 (inter-laboratory studies, HPLC-RT correlation, average, Eadsforth & Moser 1983; Brooke et al. 1990)
 1.34, 1.27, 1.08 (HPLC-RT correlation, Harnish et al. 1983)
 1.08 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
 0.79, 0.96 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
 0.89 (shake flask-UV at pH 7.4, El Tayar et al. 1984)
 0.99 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
 0.81, 1.08 (HPLC- k' correlation, Eadsforth 1986)
 0.91 (RP-HPLC-RT correlation, Eadsforth 1986)
 0.98 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
 0.93 (HPLC method average, Ge et al. 1987)
 0.78 (HPLC- k' correlation, Miyake et al. 1987)
 1.18 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 0.940 ± 0.006 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
 0.90 (recommended, Sangster 1989, 1993)
 0.942 ± 0.010 ; 0.940 ± 0.006 (shake flask/stir-flask method by BRE; RITOX, inter-laboratory studies, Brooke et al. 1990)
 0.90 (shake flask-GC, Alcorn et al. 1993)
 1.21, 0.89, 0.87, 1.09 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
 0.92 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
 0.88 (microemulsion electrokinetic chromatography-retention factor correlation, Jia et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 0.78 (fish, Lu & Metcalf 1975)
 0.30 (calculated-S, Kenaga 1980)
 < 1.0 (fish, Freitag et al. 1982)
 < 1.0, 0.602, 3.01 (golden orfe, algae, activated sludge, Freitag et al. 1982)
 0.602 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
 0.845 (alga *Chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)
 < 1.0, < 1.0, 2.70 (golden ide, algae, activated sludge, Freitag et al. 1985)
 2.77 (*Daphnia magna*, based on elimination phase, Dauble et al. 1986)
 1.87 (*Daphnia magna*, based on ^{14}C and exposure water, Dauble et al. 1986)
 0.70 (fish, correlated- K_{OW} , Isnard & Lambert 1988)
 0.78 (quoted, Isnard & Lambert 1988, 1989)
 0.41 (zebrafish, Kalsch et al. 1991)
 0.41 (zebrafish, Zok et al. 1991)
 0.41; 1.04, -0.87, 0.03 (quoted exptl.; calculated values- K_{OW} , Bintein et al. 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.11; 2.11 (H-montmorillonite at pH 8.35; pH 6.80, Bailey et al. 1968)
 1.86 (soil average, Moreale & Van Bladel 1976)
 1.41 (average of seven agricultural soils, Briggs 1981)
 3.59 (colloidal organic carbon/ground water, Means et al. 1982)
 2.11; 2.61 (soil; more acidic soil, Pillai et al. 1982)
 2.49; 2.11 (nonsterile Hagerstown soil; sterile Hagerstown soil, Pillai et al. 1982)
 2.96; 2.61 (nonsterile Palouse soil; sterile Palouse soil, Pillai et al. 1982)
 1.17 (soil, quoted as $\log K_{OM}$, Sabljic 1987)
 2.12, 2.05, 2.06 (calculated values: Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
 0.596 (calculated- K_{OW} , Kollig 1993)

- 1.08, 1.25, 0.98 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
 1.41 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.07; 1.65 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 2.70, 1.64, 2.08, 2.04, 2.29 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 2.384, 1.503, 1.279, 1.437, 2.136 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
 1.0–1.54 (5 soils, pH 2.8–7.2, batch equilibrium-sorption isotherm, Li et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 12$ d from a measured Henry's law constant of 1.2×10^{-4} atm m³ mol⁻¹ (Yoshida et al. 1983; quoted, Howard 1989) for a model river of 1-m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);
 volatilization $t_{1/2}(\text{calc}) = 55$ d (Toräng et al. 2002).

Photolysis: first-order rate constants for photosensitized reactions in water with various humic substances as sensitizers: $k = 0.17$ h⁻¹ with aquatic humus from Aucilla River, $k = 0.12$ h⁻¹ with Aldrich humic acid, $k = 0.091$ h⁻¹ with Fluka humic acid and $k = 0.11$ h⁻¹ with Contech fulvic acid in sunlight, corresponding to half-lives of 4 to 8 h (Zepp et al. 1981); photolysis $t_{1/2} = > 50$ yr at 15°C and a pH 5–9 (Toräng et al. 2002).

Oxidation: rate constant k ; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO₃ radical and k_{O_3} with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k = 1 \times 10^4$ M⁻¹ s⁻¹ for oxidation by RO₂ radical at 30°C in aquatic systems with $t_{1/2} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2$ M⁻¹ s⁻¹ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{OH}} = 1.20 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹, $k_{\text{OH}}(\text{av.}) = 1.17 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹ at 296 K (flash photolysis-RF, Rinke & Zetzsch 1984; Witte et al. 1986)

$k_{\text{OH}}^* = 1.10 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹ at 298 K, measured range: 239–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{\text{OH}}(\text{calc}) = 1.54 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson et al. 1985)

$k_{\text{OH}}(\text{obs}) \approx 6.0 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹; $k_{\text{OH}}(\text{calc.}) = 1.16 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 1.36 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹, $k_{\text{OH}}(\text{obs.}) = 1.17 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^*(\text{exptl}) = 1.18 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K, measured range: 265–455 K; and $k_{\text{O}_3} = 1.12 \times 10^{-18}$ cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{\text{OH}}^* = 1.11 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 1.385 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: completely degraded by a soil inoculum in 4 d (Alexander & Lustigman 1966; quoted, Verschuere 1983; Howard 1989);

completely degraded in 20 d by bacteria in river mud (Calamari et al. 1980; quoted, Howard 1989);

$k = 0.23$ d⁻¹ and corresponding to a $t_{1/2} = 3$ d in samples of White Lake water at 29°C (Subba-Rao et al. 1982);

average rate of biodegradation $k = 19.0$ mg COD g⁻¹ h⁻¹ for 94.5% removal (Scow 1982);

biodegradation $t_{1/2} = 4.5$ d in unpolluted and $t_{1/2} < 0.5$ d in polluted pond water as model environments (Lyons et al. 1984);

0.46 mM aniline solution degraded by strain Ani1 within 14 d in water (Schnell et al. 1989);

average exptl. $k = 0.044$ h⁻¹ compared to the group-contribution method predicted rate constants of 0.050 h⁻¹ (nonlinear) and 0.018 h⁻¹ (Tabak & Govind 1993);

first-order $k = 1.0$ d⁻¹ for batch expt. with Elbe water at 20°C (Börnack et al. 2001);

field first-order degradation $k \sim 1.8$ d⁻¹ for 2 different dates with water temperatures of 21.9 and 14.7°C, respectively, in Rhine river and rate constant obtained in laboratory shake flask batch tests with Rhine water averaged 1.5 d⁻¹ at 15°C and 2.0 d⁻¹ at 20°C (Toräng et al. 2002).

Biotransformation: mean bacteria transformation rate constant for all three sites of $(1.1 \pm 0.8) \times 10^{-11}$ L·organism⁻¹·h⁻¹ (Paris & Wolfe 1987; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.052 \pm 0.0067$ h⁻¹; $k_2 = 7.200 \pm 1.3000$ h⁻¹ (Kalsch et al. 1991)

$k_1 = 11.10 \pm 3.2000$ h⁻¹ (zebrafish, Zok et al. 1991)

Half-Lives in the Environment:

Air: atmospheric lifetimes of 2.3 h in clean troposphere and 1.2 h in moderately polluted atmosphere, based on gas-phase reaction with hydroxyl radical at room temp.; atmospheric lifetimes of 15.0 d in clean troposphere and 5.0 d in moderately polluted atmosphere, based on gas-phase reaction with O₃ at room temp. (Atkinson et al. 1987)

$t_{1/2} \sim 3.3$ h, based on reaction with photochemically produced hydroxyl radical (Howard 1989);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2} = 2.3$ d in Rhine river in case of a first order reduction process (Zoeteman et al. 1980; quoted, Howard 1989);

estimated $t_{1/2} = 0.3$ –3.0 d in river waters (Zoeteman et al. 1980);

$t_{1/2} = 4$ to 8 h in May sunlight with both commercial humic acids and aquatic humus as photosensitizers near-surface water and $t_{1/2} \sim 1$ wk in distilled water (Zepp et al. 1981);

$t_{1/2} = 6$ d in eutropic pond and $t_{1/2} = 21$ d in an oligotrophic lake (Subba-Rao et al. 1982; quoted, Howard 1989);

biodegradation $t_{1/2} = 4.5$ d in unpolluted and $t_{1/2} < 0.5$ d in polluted pond water as model environments (Lyons et al. 1984);

$t_{1/2} = 4$ –33 d at 15°C (Ingerslev & Nyholm 2000);

$t_{1/2} \sim 9$ h in the Rhine river at 15 and 22°C (Toräng et al. 2002).

Ground water: estimated $t_{1/2} \sim 30$ –300 d (Zoeteman et al. 1980).

Sediment:

Soil:

Biota:

TABLE 16.1.3.1.1

Reported vapor pressures of aniline at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959		Hatton et al. 1962	
summary of literature data		ebulliometry		ebulliometry		calc-thermodynamic properties	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
34.8	133.3	112.92	10351	102.59	6806	31.55	133.3
57.9	666.6	125.16	17039	117.22	12295	41.82	666.6
69.4	1333	153.2	42103	137.5	25439	52.59	1333
82.0	2666	168.21	67701	160.08	51913	68.62	2666
96.7	5333	183.93	101325	182.4	97103	82.11	5333
106.0	7999			184.24	101912	97.02	7999
119.9	13332	bp/°C	183.93	185.15	104589	119.41	13332
140.1	26664					138.90	26664
161.9	53329			mp/°C	–6.02	161.05	53329
184.4	101325					184.40	101325
mp/°C	–6.2			eq. 2	P/mmHg		
				A	7.25375		
				B	1684.35		
				C	201.175		

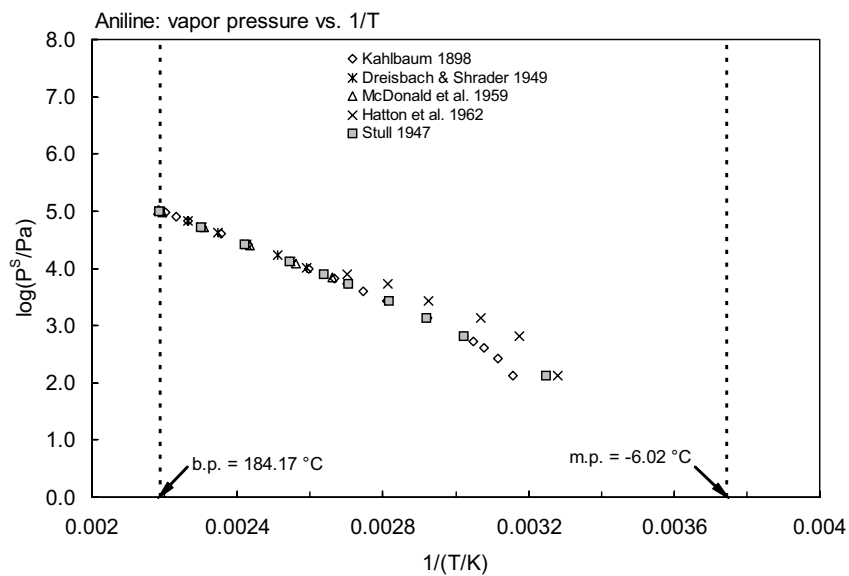
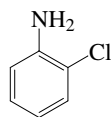


FIGURE 16.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for aniline.

16.1.3.2 2-Chloroaniline



Common Name: 2-Chloroaniline

Synonym: 1-amino-2-chlorobenzene, *o*-aminochlorobenzene, *o*-chloroaniline, 2-chlorophenylamine

Chemical Name: 1-amino-2-chlorobenzene, *o*-chloroaniline, 2-chloroaniline

CAS Registry No: 95-51-2

Molecular Formula: $C_6H_4NH_2Cl$

Molecular Weight: 127.572

Melting Point ($^{\circ}C$):

- −1.94 (β -2-chloroaniline, Dreisbach 1955; Weast 1872–83, Riddick et al. 1986)
- −14.0 (α -2-chloroaniline, Weast 1982–83; Verschueren 1983; Howard 1989)
- −1.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

- 208.8 (Kahlbaum 1898; Stull 1947; Dreisbach 1955; Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

- 1.21266, 1.20787 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)
- 1.21251, 1.20775 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

- 105.2 ($20^{\circ}C$, Stephenson & Malanowski 1987)
- 131.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

- 2.661 (Perrin 1972; quoted, Howard 1989)
- 2.650 (Weast 1982–83)
- 2.640 (protonated cation + 1, Dean 1985)
- 2.640 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

- 57.5 ± 5 ($25^{\circ}C$, Piacente et al. 1985)
- 56.756, 44.35 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

- 11.88 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

- 8760 (Dreisbach 1955)
- 3765 ($20^{\circ}C$, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)
- 3763 (calculated- K_{ow} , Müller & Klein 1992)
- 4740 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 40.31* (extrapolated-regression of tabulated data, measured range 64.4 – $208.8^{\circ}C$, Kahlbaum 1898)
- 37.77* (extrapolated-regression of tabulated data, temp range 46.3 – $208.8^{\circ}C$, Stull 1947)
- $\log (P/mmHg) = 7.63311 - 2085.5/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)
- 7605* ($124.48^{\circ}C$, ebulliometry, measured range 124.48 – $208.84^{\circ}C$, Dreisbach & Shrader 1949)
- 33.77 (calculated by formula, Dreisbach 1955; selected, Riddick et al. 1986)
- $\log (P/mmHg) = 7.19240 - 1762.74/(200.0 + t/^{\circ}C)$; temp range 110 – $330^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)
- $\log (P/mmHg) = [-0.2185 \times 12441.0/(T/K)] + 8.56946$; temp range 46.3 – $208.8^{\circ}C$ (Antoine eq., Weast 1972–73)
- 33.88 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.56265 - 1998.6/(220.0 + t/^{\circ}\text{C})$, temp range 20–108°C (Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 7.19240 - 1762.74/(200.0 + t/^{\circ}\text{C})$, temp range: 108–300°C (Antoine eq., Dean 1985, 1992)
 35.30* (torsion-weighing effusion, Piacente et al. 1985)
 $\log (P/\text{kPa}) = (8.63 \pm 0.16) - (3006 \pm 56)/(T/\text{K})$; temp range: 287–336 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)
 $\log (P/\text{kPa}) = 6.75801 - 2085.50/(230.0 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 18.97 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.84227 - 1432.2/(-108.81 + T/\text{K})$; temp range 397–482 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 90.6491 - 6.041 \times 10^3/(T/\text{K}) - 31.118 \cdot \log (T/\text{K}) + 1.1564 \times 10^{-2} \cdot (T/\text{K}) + 4.8388 \times 10^{-13} \cdot (T/\text{K})^2$;
 temp range 271–722 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.760 (calculated-P/C, Howard 1989)
 0.425 (calculated-P/C, Meylan & Howard 1991)
 0.143 (estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.81 (shake flask, Fujita et al. 1964)
 1.90 (Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
 1.92 (exptl., Leo et al. 1971; McCall 1975; Rekker 1977)
 1.92 (HPLC- k' correlation, Carlson et al. 1975)
 1.63 (calculated- π const., Norrington et al. 1975)
 1.61, 1.73 (calculated- π const., calculated- f const., Rekker 1977)
 1.90, 1.92 (shake flask, Hansch & Leo 1979)
 1.74 (HPLC- k' correlation, Könemann et al. 1979)
 1.74 (calculated- f const., Rekker & De Kort 1979)
 1.91 \pm 0.01 (HPLC- k' , Hammers et al. 1982)
 1.99 (HPLC- k' correlated, Hammers et al. 1982)
 1.926 \pm 0.021 (slow-stirring-GC, De Bruijn et al. 1989)
 1.88 (recommended, Sangster 1993)
 1.93 \pm 0.14, 1.55 \pm 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
 1.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

< 2.0 (Kawasaki 1980)
 1.30 (estimated, Canton et al. 1985)
 1.18 (zebrafish, Zok et al. 1991)
 0.301–0.57 (carp, Tsuda et al. 1993)
 1.18; 1.56, 0.73, 0.94 (quoted; calculated values- K_{OW} , Bintein et al. 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 5.6$ d was estimated for a model river of 1-m deep (Lyman et al. 1982; quoted, Howard 1989);
 estimated $t_{1/2} = 64$ d from a representative environmental pond (stagnant) (USEPA 1987; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant of $5.1 \times 10^{-12} \text{ cm}^3/\text{molecule} \cdot \text{s}$ for the reaction with hydroxyl radical in a typical ambient atmosphere at 25°C with $t_{1/2} \sim 2$ d (GEMS 1987; quoted, Howard 1989).

Hydrolysis:

Biodegradation: average biodegradation rate of 25 mg COD $\text{g}^{-1} \text{ h}^{-1}$ for 95.6% removal (Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 7.10 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

$k_2 = 0.19 \text{ h}^{-1}$ (carp, Tsuda et al. 1993)

Half-Lives in the Environment:

Air: estimated atmospheric $t_{1/2} = 2 \text{ d}$, based on the reaction with sunlight-produced hydroxyl radical (GEMS 1987; quoted, Howard 1989).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: $t_{1/2} = 3.6 \text{ h}$ in carp with excretion rate constant $k = 0.19 \text{ h}^{-1}$ (Tsuda et al. 1993).

TABLE 16.1.3.2.1

Reported vapor pressures of 2-chloroaniline at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Kahlbaum 1898		Stull 1947		Piacente et al. 1985		Piacente et al. 1985	
static method		summary of literature data		torsion-weighing effusion		torsion-weighing effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
64.4	400	46.3	133.3	run 62	average		average
72.3	666.6	72.3	666.6	14	18	23	36
84.8	1333	84.8	1333	20	32	24	41
92.9	2000	99.2	2666	27	45	28	50
99.2	2666	115.6	5333	32	72	30	66
104.2	3333	125.7	7999	34	96	31	62
108.4	4000	139.5	13332	34.5	86	32	83
112.0	4666	160.0	26664	38	117	34	87
115.2	6333	183.7	53329	43	200	35	90
118.1	6000	208.8	101325	34	203	38	112
120.7	6666			48.5	251	41	167
131.4	9999	mp/°C	-	52.5	347	43	190
139.5	13332			54	362	45	200
160.0	26664			63	505	47	218
173.6	39997	Dreisbach & Shrader 1949				49	269
183.7	53329	ebulliometry				51	275
192.0	66661	t/°C	P/Pa			51	309
199.4	79993					55	343
208.8	101325					56	354
		124.48	7605			57	398
		131.54	10114				
		145.3	16500			overall vapor pressure eq.	
		154.55	42066			eq. 1	P/kPa
		192.71	67661			A	8.63 ± 0.16
		208.84	101325			B	3006 ± 56
						ΔH _v /(kJ mol ⁻¹) = 57.5 ± 5	
						at 25°C	

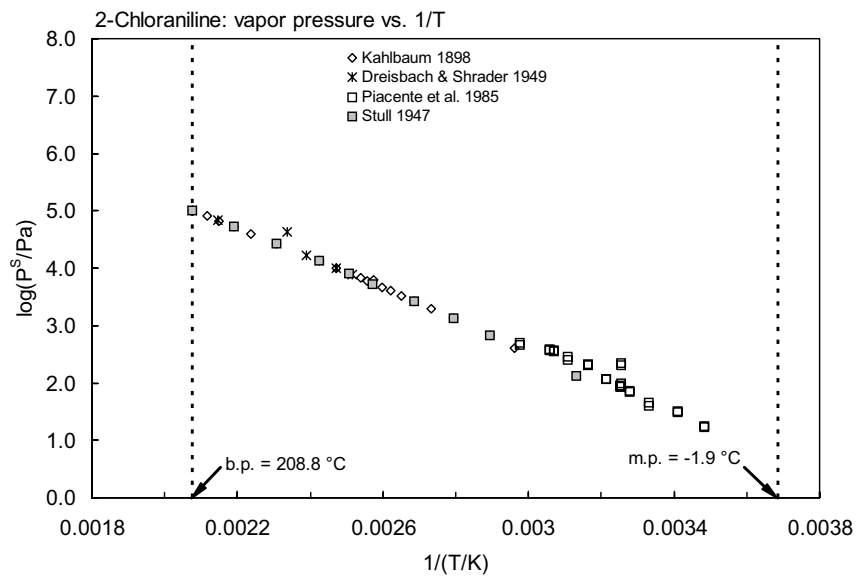
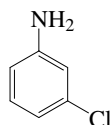


FIGURE 16.1.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2-chloroaniline.

16.1.3.3 3-Chloroaniline



Common Name: 3-Chloroaniline

Synonym: 1-amino-3-chlorobenzene, *m*-chloroaniline, 3-chlorophenylamine

Chemical Name: 1-amino-3-chlorobenzene, *m*-chloroaniline, 3-chloroaniline

CAS Registry No: 108-42-9

Molecular Formula: $C_6H_4NH_2Cl$

Molecular Weight: 127.572

Melting Point ($^{\circ}C$):

−10.28 (Lide 2003)

Boiling Point ($^{\circ}C$):

230.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.21606 ($20^{\circ}C$, Weast 1982–83)

1.2150 ($22^{\circ}C$, Dean 1985; Budavari 1989)

Molar Volume (cm^3/mol):

105.0 ($22^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

131.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.52 (Perrin 1972)

3.50 (McLeese et al. 1979)

3.46 (Weast 1982–83)

3.52 (protonated cation + 1, Dean 1985)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

61.04, 46.016 ($25^{\circ}C$, bp, Dreisbach 1955)

60.9 ± 5 ($25^{\circ}C$, Piacente et al. 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.25 (Dreisbach 1955)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5442 ($20^{\circ}C$, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)

5447 (calculated- K_{ow} , Müller & Klein 1992)

4740 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

13.14* (extrapolated-regression of tabulated data, measured range 81.7 – $228.5^{\circ}C$, Kahlbaum 1898)

11.94* (extrapolated-regression of tabulated data, temp range 63.5 – $228.5^{\circ}C$, Stull 1947)

11.17 (calculated by formula, Dreisbach 1955)

$\log (P/mmHg) = 7.23603 - 1857.75/(196.64 + t/^{\circ}C)$; temp range 125 – $350^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log (P/mmHg) = [-0.2185 \times 133854.6/(T/K)] + 8.761546$; temp range 63.5 – $228.5^{\circ}C$ (Antoine eq., Weast 1972–73)

11.06 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 7.59939 - 2073.75/(215.0 + t/^{\circ}C)$, temp range 15 – $125^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 7.23603 - 1857.75/(196.64 + t/^{\circ}C)$, temp range 125 – $310^{\circ}C$ (Antoine eq., Dean 1985, 1992)

15.60* (torsion-weighing effusion, Piacente et al. 1985)

$\log (P/\text{kPa}) = (8.86 \pm 0.10) - (3180 \pm 40)/(T/\text{K})$; temp range ~290–345 K (Antoine eq., combined torsion-weighing effusion, Piacente et al. 1985)

9.530 (extrapolated from Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.36093 - 1857.75/(-76.51 + T/\text{K})$; temp range 398–573 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 65.6033 - 5.3779 \times 10^3/(T/\text{K}) - 20.518 \cdot \log (T/\text{K}) + 6.7861 \times 10^{-3} \cdot (T/\text{K}) + 2.1167 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 263–751 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.223 (calculated-P/C)

0.102 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.88 (shake flask-UV, Fujita et al. 1964)

1.88 (Ichikawa et al. 1969)

1.88 (Leo et al. 1971; Hansch & Leo 1979)

1.90 (exptl., Leo et al. 1971; Rekker 1977)

1.98 (calculated- π const., Norrington et al. 1975)

1.73, 1.75; 1.61 (calculated-f const., calculated- π const., Rekker 1977)

1.90, 1.88 (shake flask, Hansch & Leo 1979)

1.57 (HPLC- k' correlation, Könemann et al. 1979)

1.89 ± 0.01 (HPLC- k' correlation, Hammers et al. 1982)

2.00 (HPLC- k' correlation, Hammers et al. 1982)

1.910 ± 0.013 (slow-stirring-GC, De Bruijn et al. 1989)

1.88 (recommended, Sangster 1993)

1.91 ± 0.14 , 1.52 ± 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)

1.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.06 (zebrafish, Zok et al. 1991)

-0.097 to 0.342 (average for carp, Tsuda et al. 1993)

1.06; 1.55, 0.70, 0.92 (quoted; calculated values, Bintein et al. 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct aqueous photolysis rate constant $k = 0.393 \pm 0.006 \text{ min}^{-1}$ with a calculated $t_{1/2} = 1.76 \text{ min}$ (Stegeman et al. 1993).

Oxidation:

Hydrolysis: direct photohydrolysis rate constant $k = 0.393 \pm 0.006 \text{ min}^{-1}$ with a calculated $t_{1/2} = 1.76 \text{ min}$ (Stegeman et al. 1993).

Biodegradation: average biodegradation rate of $6.2 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 97.2% removal (Scow 1982).

Biotransformation: mean bacteria transformation rate constant for all three sites of $(2.2 \pm 1.7) \times 10^{-12} \text{ L} \cdot \text{organism}^{-1} \cdot \text{h}^{-1}$ (Paris & Wolfe 1987; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 19.1 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

$k_2 = 0.21 \text{ h}^{-1}$ (carp, Tsuda et al. 1993)

Half-Lives in the Environment:

Biota: $t_{1/2} = 3.3 \text{ h}$ in carp with excretion rate $k = 0.21 \text{ h}^{-1}$ (Tsuda et al. 1993).

TABLE 16.1.3.3.1

Reported vapor pressures of 3-chloroaniline at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Kahlbaum 1898		Stull 1947		Piacente et al. 1985			
static method		summary of literature data		torsion-weighing effusion			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				run 63	average	run 64	average
81.7	400	63.5	133.3	19	8	31	19
89.8	666.6	89.8	666.6	29	17	39	41
102	1333	102	1333	36.5	33	42	50
110.4	2000	116.7	2666	43	49	44	52
116.8	2666	133.6	5333	50	89	45	56
122.0	3333	144.1	7999	57.5	145	46	66
126.2	4000	158	13332	65	250	47	70
129.8	4666	179.5	26664	73	376	49	89
133.2	6333	203.5	53329			50	85
136.2	6000	228.5	101325			51	95
138.8	6666					52	105
149.9	9999	mp/°C	–10.4			53	102
158.0	13332					55	126
179.5	26664					57	146
193.2	53329					59	151
203.5	66661					60.5	170
211.9	79993					62	190
228.5	101325					63	204
						65	240
						69	296
				overall vapor pressure eq.			
				eq. 1			
				P/kPa			
				A			
				8.86 ± 0.10			
				B			
				3180 ± 40			
				ΔH _v /(kJ mol ^{–1}) = 60.9 ± 5			
				at 25°C			

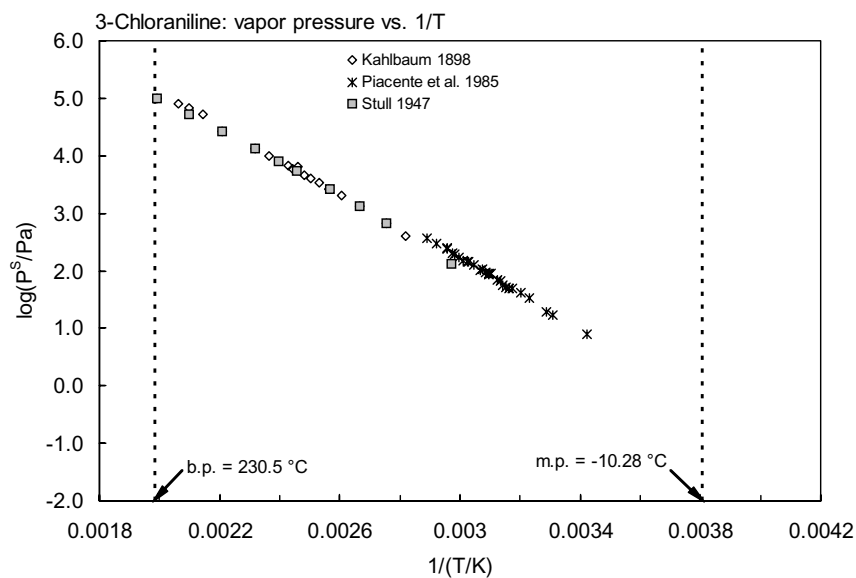
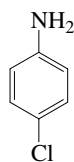


FIGURE 16.1.3.3.1 Logarithm of vapor pressure versus reciprocal temperature for 3-chloroaniline.

16.1.3.4 4-Chloroaniline



Common Name: 4-Chloroaniline

Synonym: 1-amino-4-chlorobenzene, *p*-chloroaniline, 4-chlorophenylamine

Chemical Name: 1-amino-4-chlorobenzene, *p*-chloroaniline, 4-chloroaniline

CAS Registry No: 106-47-8

Molecular Formula: $\text{NH}_2\text{C}_6\text{H}_4\text{Cl}$

Molecular Weight: 127.572

Melting Point ($^{\circ}\text{C}$):

70.5 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

232.0 (Weast 1982–83; Verschueren 1983; Howard 1989)

Density (g/cm^3 at 20°C):

1.429 (19°C , Weast 1982–83)

Molar Volume (cm^3/mol):

131.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.98 (Perrin 1972; Freitag et al. 1984; quoted, Howard 1989)

4.20 (McLeese et al. 1979)

4.15 (Weast 1982–83)

3.99 (protonated + 1, Dean 1985)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

79 ± 5 (25°C , Piacente et al. 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.69 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

57.74 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.358 (mp at 70.5°C)

Water Solubility (g/m^3 or mg/L at 25°C):

3000 (Philpot et al. 1940)

3900 (Kilzer et al. 1979)

2620 (Schmidt-Bleek et al. 1982; Rott et al. 1982)

2487 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.707* (20°C , Knudsen effusion, measured range 10 – 30°C , Swan & Mack 1925)

15.19* (extrapolated-regression of tabulated data, temp range 59.3 – 230.5°C , Stull 1947)

$\log (P/\text{mmHg}) = [-0.2185 \times 12832.8/(T/\text{K})] + 8.461034$; temp range 59.3 – 230.5°C (Antoine eq., Weast 1972–73)

3.173 (effusion method, DePablo 1976)

3.33 (extrapolated, Verschueren 1977)

2.00, 6.67 (20°C , 30°C , quoted, Verschueren 1983)

0.224 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 3.55438 - 521.556/(47.392 + t/^{\circ}\text{C})$; temp range 90 – 150°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.636* (torsion-weighing effusion, Piacente et al. 1985)

$\log (P/\text{kPa}) = (11.20 \pm 0.20) - (4170 \pm 60)/(T/K)$; temp range ~298–360 K (Antoine eq., combined torsion-weighting effusion, Piacente et al. 1985)

3.66 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 13.448 - 4736/(T/K)$, temp range 283–303 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.3489 - 2729/(T/K)$, temp range 363–505 K (Antoine eq.-II, Stephenson & Malanowski 1987)

3.33, 32.0 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = -15.3259 - 2.8592 \times 10^3/(T/K) + 11.527 \cdot \log (T/K) - 1.8071 \times 10^{-2} \cdot (T/K) + 7.2359 \times 10^{-6} \cdot (T/K)^2$; temp range 343–754 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1.0840 (calculated-P/C, Howard 1989)

0.0395 (calculated-P/C, Meylan & Howard 1991)

0.1430 (estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.84 (Ichikawa et al. 1969)

1.83 (quoted exptl., Leo et al. 1969, 1971; Hansch & Leo 1985)

1.83 (HPLC- k' correlation; Carlson et al. 1975)

1.83 (shake flask, Hansch & Leo 1979)

1.57 (HPLC- k' correlation, Könemann et al. 1979)

1.83, 20.2 (HPLC- k' correlation, Hammers et al. 1982)

1.64 (inter-laboratory studies, HPLC-RT correlation average, Eadsforth & Moser 1983)

1.88 ± 0.02 (HPLC-RV correlation-ALPM; Garst & Wilson 1984)

2.78 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)

1.83 (shake flask, Log P Database, Hansch & Leo 1987)

1.83 (RP-HPLC- k' correlation, Minick et al. 1988)

1.88 ± 0.014 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)

1.83 (shake flask, Leahy et al. 1989)

1.80, 1.82 (shake flask, HPLC-RT correlation, Wang et al. 1989)

2.01 (centrifugal partition chromatography CPC-RV correlation, El Tayar et al. 1991)

1.83 (recommended, Sangster 1993)

1.83 (pH 7.4, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

< 1.30 (golden orfe for 3-d exposure, Körte et al. 1978)

3.08 (green algae for 24-h exposure of dry wt. basis, Körte et al. 1978)

2.42 (green algae for 24-h exposure of wet wt. basis, Körte et al. 1978)

< 1.0, 2.41, 3.11 (golden orfe, algae, activated sludge, Freitag et al. 1982)

2.42 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)

2.06 (alga *Chlorella fusca*, calculated- K_{ow} , Geyer et al. 1984)

1.11, 2.42, 2.45 (golden ide, algae, activated sludge, Freitag et al. 1985)

0.91 (zebrafish, Zok et al. 1991)

−0.097–0.23 (carp, Tsuda et al. 1993)

0.91; 1.52, 0.63, 0.88 (quoted; calculated values, Bintein et al. 1993)

2.58 (algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, $\log K_{oc}$:

2.36–2.67 (five Belgium soils, Van Bladel & Moreale 1977)

1.98–3.18 (five German soils, Rott et al. 1982)

3.74 (colloidal org. matter in ground water, Means 1983)

1.86 (calculated-MCI χ , Sabljic 1987)

2.08 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)

1.96, 1.86 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)

- 1.61 (calculated- K_{OW} , Kollig 1993)
 1.96 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.28; 1.86 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.086, 2.21, 2.48, 2.374, 2.973 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 2.801, 2.326, 2.145, 2.420 (second generation Eurosoils ES-1, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 6.4$ h from using Henry's law constant for a model river of 1-m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} = 3$ d in an experimental pond with spiked 4-chloroaniline (Schauerte et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant k ; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (8.3 \pm 0.42) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner & Zetzsch 1983)

$k_{OH}(\text{obs.}) = 83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH}(\text{calc.}) = 34.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. in air (Atkinson 1985; Atkinson et al. 1985)

$k_{OH}(\text{calc.}) = 54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH}(\text{obs.}) = 83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{OH} = (83 \text{ to } \sim 44) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295–296 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 42.9 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

$k_2 = 0.16 \text{ h}^{-1}$ (carp, Tsuda et al. 1993)

$k_1 = 17.74 \text{ h}$, $k_2 = 0.0465 \text{ h}$ (algae *Chlorella fusca*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 4.6$ h, based on estimated reaction rate with photochemically produced hydroxyl radical of 5×10^5 radicals/cm³ in atmosphere (Wahner & Zetzsch 1983; quoted, Howard 1989).

Surface water: estimated $t_{1/2} = 0.3$ – 3.0 d in river waters in case of a first order reduction process (Zoeteman et al. 1980);

72.1 mg/L total organic carbon (TOC) degraded to 92% TOC after 5 h illumination with a 250 watt tungsten lamp by photo-Fenton reaction in distilled water (Ruppert et al. 1993).

Groundwater: estimated $t_{1/2} = 30$ – 300 d in Rhine River (Zoeteman et al. 1980).

Sediment:

Soil:

Biota: $t_{1/2} = 4.3$ h in carp with excretion rate $k = 0.16 \text{ h}^{-1}$ (Tsuda et al. 1993).

TABLE 16.1.3.4.1

Reported vapor pressures of 4-chloroaniline at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Swan & Mack 1925		Stull 1947		Piacente et al. 1985			
Knudsen effusion		summary of literature data		torsion-weighing effusion			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				Run 58	average	Run 66	average
10	0.513	59.3	133.3	26	3.0	52	56
20	1.707	87.9	666.6	31	6.0	56.5	75
30	6.493	102.1	1333	34	8.0	61	128
		117.8	2666	39	13	63	136
		135.0	5333	40	17	65	152
		145.8	7999	43	20	68	238
eq. 4	P/mmHg	159.9	13332	48	31	71	275
A	415.007	182.3	26664	49.5	35	72	316
B	22322	206.6	53329	53	48		
C	138.475	230.5	101325	59	87		
				60.5	100	overall vapor pressure eq.	
ΔH _v /(kJ mol ⁻¹) = 90.37		mp/°C	70.5	63.5	127	eq. 1	P/kPa
at 20°C				67	170	A	11.20 ± 0.20
				69.5	224	B	4170 ± 60
				82.5	549		
				88.5	832	ΔH _v /(kJ mol ⁻¹) = 70.9 ± 5	
						at 25°C	

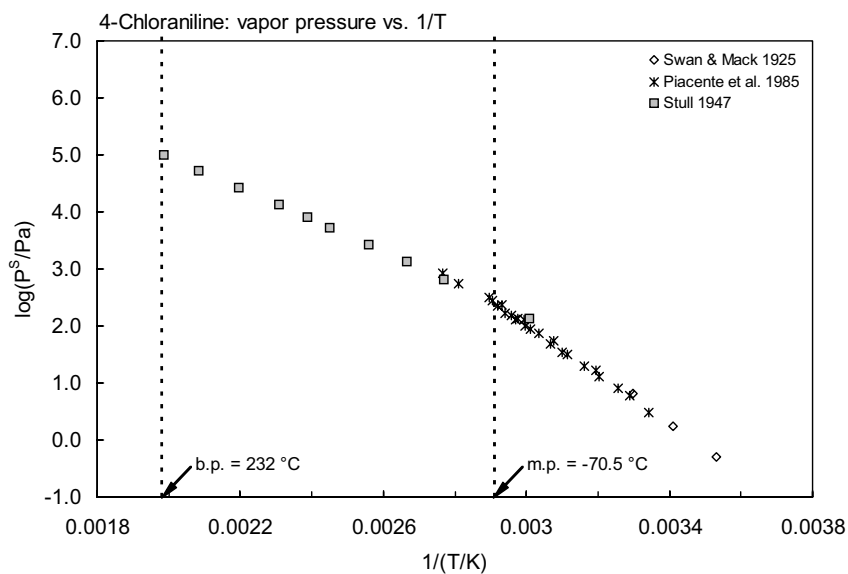
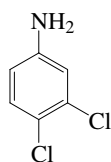


FIGURE 16.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for 4-chloroaniline.

16.1.3.5 3,4-Dichloroaniline



Common Name: 3,4-Dichloroaniline

Synonym:

Chemical Name: 3,4-dichloroaniline

CAS Registry No: 95-76-1

Molecular Formula: $C_6H_5Cl_2N$, $C_6H_3NH_2Cl_2$

Molecular Weight: 162.017

Melting Point ($^{\circ}C$):

72.0 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

272.0 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

111.7 (calculated-density, Jaworska & Schultz 1993)

152.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.968, 3.0 (Perrin 1972)

2.00 (estimated, Wolff & Crossland 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.346 (mp at $72^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

92.03 ($20^{\circ}C$, Wolff & Crossland 1985)

93.2; 740 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.30 ($20^{\circ}C$, Wolff & Crossland 1985)

2.27 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 7.6189 - 3060.03/(T/K)$; temp range 420–545 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = -15.2685 - 3.3857 \times 10^3/(T/K) + 11.926 \cdot \log (T/K) - 1.9227 \times 10^{-2} \cdot (T/K) + 7.4179 \times 10^{-6} \cdot (T/K)^2$;
temp range 345–800 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.289 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.69 (unpublished result, Leo et al. 1971, Hansch & Leo 1979)

2.12 (HPLC- k' correlation, Könemann et al. 1979)

2.78 ($20^{\circ}C$, shake flask-UV, Briggs 1981)

2.69, 2.67 (HPLC- k' correlation, Hammers et al. 1982)

2.62 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)

2.30 (inter-laboratory studies, HPLC-RT correlation average, Eadsforth & Moser 1983)

2.14, 2.63 (HPLC- k' correlation, Eadsforth 1986)

2.69 (shake flask, Log P Database, Hansch & Leo 1987)

2.68 (recommended, Sangster 1993)

2.69 (recommended, Hansch et al. 1995)

2.69 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.48 (zebrafish, Zok et al. 1991)

1.48; 2.02, 1.88, 1.75 (fish: quoted; calculated values- K_{OW} , Bintein et al. 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

2.29 (20°C, sorption isotherm-GC, converted from K_{OM} multiplied by 1.724, Briggs 1981)

1.40 (calculated- K_{OW} , wet sediment, Wolff & Crossland 1985)

2.29 (Sabljic 1987)

2.05 (soil, quoted, Sabljic 1987)

2.29, 2.08 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

2.29 (calculated-MCI $^1\chi$, Sabljic et al. 1995)

2.26, 2.39 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: first order rate constant $k(\text{calc}) = 5.0 \times 10^{-3} \text{ d}^{-1}$ (Wolff & Crossland 1985).

Photolysis: phototransformation rate constant $k = 0.12$ to 0.20 d^{-1} (Wolff & Crossland 1985).

Oxidation:

Hydrolysis: not expected to occur (Wolff & Crossland 1985).

Biodegradation:

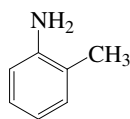
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 78.5 \text{ h}^{-1}$ (zebrafish, Zok et al. 1991)

Half-Lives in the Environment:

Surface water: overall rate of loss predicted from outdoor ponds was calculated based on direct phototransformation, and indirect phototransformation $k = 0.13$ to 0.22 d^{-1} corresponding to $t_{1/2} = 3.2$ to 5.3 d ; the observed rate of loss varied from 0.11 to 0.17 d^{-1} corresponding to $t_{1/2} = 4.1 - 6.3 \text{ d}$ (Wolff & Crossland 1985).

16.1.3.6 *o*-Toluidine (2-Methylbenzeneamine)

Common Name: *o*-Toluidine

Synonym: 2-aminotoluene, *o*-aminotoluene, 2-methylaniline, 2-methylbenzeneamine

Chemical Name: 2-aminotoluene, *o*-methylaniline, *o*-toluidine

CAS Registry No: 95-53-4

Molecular Formula: C_7H_9N , $C_6H_4(CH_3)NH_2$

Molecular Weight: 107.153

Melting Point ($^{\circ}C$):

−14.41 (Lide 2003)

Boiling Point ($^{\circ}C$):

200.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9984, 0.99430 (10, $25^{\circ}C$, Dreisbach 1955, Riddick et al. 1986)

0.9984 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

107.3 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

132.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.40, 4.447, 4.46 (Perrin 1972)

4.44 (Weast 1982–83)

4.45 (protonated cation + 1, Dean 1985)

4.43 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.739, 44.597 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.535 (Dreisbach 1955)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

16330 ($20^{\circ}C$, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)

15000 (quoted, Verschueren 1983)

16300 (calculated- K_{ow} , Müller & Klein 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($48.2^{\circ}C$, static method, measured range 48.2 – $199.7^{\circ}C$, Kahlbaum 1898)

42.72* (extrapolated-regression of tabulated data, temp range 44 – $199.7^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.60681 - 2033.6/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

7605* ($118.46^{\circ}C$, ebulliometry, measured range 118.46 – $200.30^{\circ}C$, Dreisbach & Shrader 1949)

42.26 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.28896 - 1768.7/(201.0 + t/^{\circ}C)$; temp range 103 – $320^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [-0.2185 \times 12663.4/(T/K)] + 8.440371$; temp range 41 – $203.3^{\circ}C$ (Antoine eq., Weast 1972–73)

42.93 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/mmHg) = [1 - 473.369/(T/K)] \times 10^{[0.907135 - 6.44774 \times 10^{-4} \cdot (T/K) + 4.94693 \times 10^{-7} \cdot (T/K)^2]}$; temp range: 300.0 – $710.0 K$ (Cox eq., Chao et al. 1983)

13.33, 40.0 ($20^{\circ}C$, $30^{\circ}C$, quoted, Verschueren 1983)

33.96 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.20039 - 1623.158/(186.641 + t/^{\circ}\text{C})$; temp range 118.5–200.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

43.0 (selected lit., Riddick et al. 1986)

$\log (P/\text{mmHg}) = 6.73171 - 2033.6/(230.0 + t/^{\circ}\text{C})$; temp range: not specified (Antoine eq., Riddick et al. 1986)

34.18 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.08203 - 1627.72/(187.13 + t/^{\circ}\text{C})$; temp range 118–200°C (Antoine eq., Dean 1985, 1992)

36.46 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.26948 - 1672.87/(-81.47 + T/\text{K})$; temp range 391–474 K, (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 96.5685 - 6.2643 \times 10^3/(T/\text{K}) - 32.265 \cdot \log (T/\text{K}) + 1.2361 \times 10^{-2} \cdot (T/\text{K}) + 6.2915 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 249–694 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.095 (calculated-P/C)

0.201 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.29 (shake flask-UV, Leo et al. 1971)

1.43 (HPLC- k' correlation, Carlson et al. 1975)

1.63 (RP-HPLC-RT correlation, Veith et al. 1979a)

1.42 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)

1.34 (HPLC-RT correlation, average, Ge et al. 1987)

1.32 (shake flask, Log P Database, Hansch & Leo 1987)

1.32 (recommended, Sangster 1989)

1.44, 1.57 (shake flask, HP:C-RT correlation, Wang et al. 1989)

1.43 (recommended, Sangster 1993)

1.32 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.24 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radicals at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

rate constant $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 62.4 - 3480 \text{ h}$ in water, based on estimated rate constants for reactions of representative aromatic amines with OH and RO_2 radicals (Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.394 - 3.94 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: decomposition by a soil microflora in $> 64 \text{ d}$ (Alexander & Lustigman 1966; quoted, Verschuereen 1983);

aqueous aerobic $t_{1/2} = 24 - 168 \text{ h}$, based on aqueous aerobic screening test data (Baird et al. 1977; Sasaki 1978; quoted, Howard et al. 1991);

average biodegradation $k = 15.1 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 97.7% removal (Scow 1982);

aqueous anaerobic $t_{1/2} = 96 - 672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.394 - 3.94$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2} = 1.0$ d for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

photooxidation $t_{1/2} = 62.4 - 3480$ h, based on estimated rate constants for reactions of representative aromatic amines with OH and RO₂ radicals (Mill & Mabey 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 48 - 336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24 - 168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.3.6.1

Reported vapor pressures of *o*-toluidine at various temperatures

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949	
static method-manometer*		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
48.2	133.3	44.0	133.3	118.46	7605
55.3	266.6	69.3	666.6	122.22	8851
61.4	400.0	81.4	1333	125.99	10106
65.7	533.3	95.1	2666	139.0	16500
69.3	666.6	110.0	5333	168.06	42066
81.4	1333.2	119.8	7999	184.80	67661
94.9	2666.4	133.0	13332	200.30	101325
103.6	3999.7	153.0	26664		
110.0	5332.9	170.2	53329		
115.1	6666.1	199.7	101325		
125.4	9999.2				
133.0	13332	mp/°C	-16.3		
154.0	26664				
166.2	39997				
176.2	53329				
183.9	66661				
190.5	79993				
196.2	93326				
199.7	101325				

*complete list see [ref.](#)

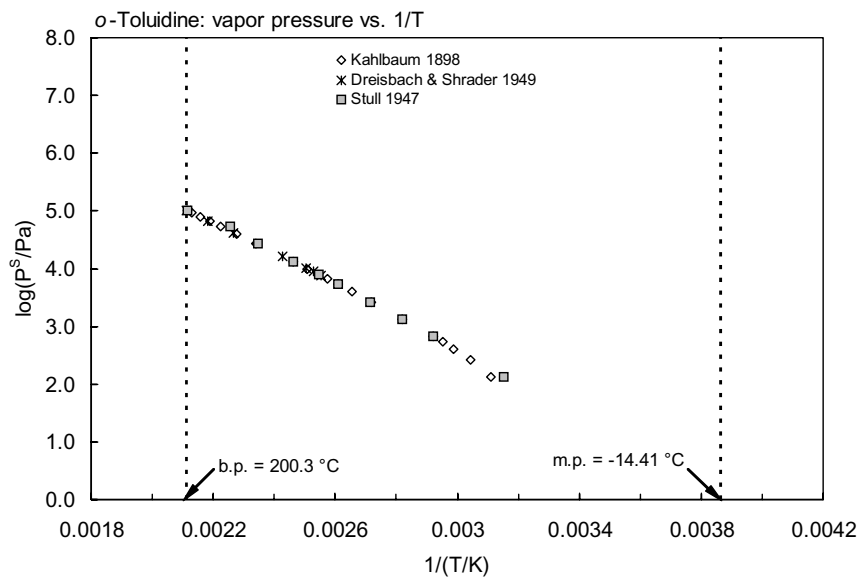
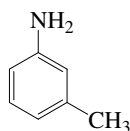


FIGURE 16.1.3.6.1 Logarithm of vapor pressure versus reciprocal temperature for *o*-toluidine.

16.1.3.7 *m*-Toluidine (3-Methylbenzeneamine)

Common Name: *m*-Toluidine

Synonym: 3-aminotoluene, 3-methylbenzeneamine, 3-methylaniline

Chemical Name: 3-aminotoluene, *m*-amino-methylbenzene, *m*-methylaniline, *m*-toluidine

CAS Registry No: 108-44-1

Molecular Formula: $C_6H_4(CH_3)NH_2$

Molecular Weight: 107.153

Melting Point (°C):

−31.3 (Lide 2003)

Boiling Point (°C):

203.3 (Stull 1947; Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):

0.9889 (Dreisbach 1955; Weast 1982–83)

Molar Volume (cm³/mol):

108.4 (20°C, Stephenson & Malanowski 1987)

132.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.66, 4.712, 4.72 (Perrin 1972)

4.73 (Weast 1982–83)

4.71 (protonated cation + 1, Dean 1985)

4.70 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

57.283, 44.848 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.08 (Dreisbach 1955)

3.891 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

15031 (20°C, shake flask-GC, Chiou 1981; Chiou & Schmedding 1981; Chiou et al. 1982)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (49.8°C, static method, measured range 49.8–203.3°C, Kahlbaum 1898)

49.54* (extrapolated-regression of tabulated data, temp range 41–203.3°C, Stull 1947)

$\log(P/\text{mmHg}) = 7.616512 - 2052.0/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

7605* (121.77°C, ebulliometry, measured range 121.77–203.34°C, Dreisbach & Shrader 1949)

36.64 (calculated by formula, Dreisbach 1955)

$\log(P/\text{mmHg}) = 7.27435 - 1772.06/(200.0 + t/^\circ\text{C})$; temp range 105–320°C (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/\text{mmHg}) = [-0.2185 \times 12104.1/(T/K)] + 8.440371$; temp range 41–203°C (Antoine eq., Weast 1972–73)

33.49 (calculated-Cox eq., Chao et al. 1983)

$\log(P/\text{atm}) = [1 - 476.329/(T/K)] \times 10^4 \{0.923479 - 6.91988 \times 10^{-4} \cdot (T/K) + 5.41104 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 280.0–705.0 K (Cox eq., Chao et al. 1983)

27.91 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.21454 - 1620.608/(203.346 + t/^\circ\text{C})$; temp range 121.9–203.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

25.66 (extrapolated-Antoine eq., Dean 1985, 1992)

- $\log (P/\text{mmHg}) = 7.09367 - 1631.43/(183.91 + t/^{\circ}\text{C})$; temp range 122–203°C (Antoine eq., Dean 1985, 1992)
 36.0 (quoted lit., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 17.6292 - 3200.9/(T/\text{K}) - 3.323 \cdot \log (T/\text{K})$, temp range not specified (vapor pressure eq., Riddick et al. 1986)
 26.86 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.27299 - 1669.26/(-85.339 + T/\text{K})$; temp range 394–447 K (Antoine eq., Stephenson & Malanowski 1987)
 25.50 (calculated-Cox eq., Chao et al. 1990)
 $\log (P/\text{mmHg}) = 7.0317 - 3.2034 \times 10^3/(T/\text{K}) + 2.3006 \cdot \log (T/\text{K}) - 9.7791 \times 10^{-3} \cdot (T/\text{K}) + 4.6824 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 243–709 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.257 (calculated-P/C)
 0.169 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.40 (shake flask-UV, Fujita et al. 1964)
 1.43 (HPLC- k' correlation, Carlson et al. 1975)
 1.42 (20°C, shake flask-UV, Briggs 1981)
 1.43 (shake flask, Log P Database, Hansch & Leo 1987)
 1.40 (recommended, Sangster 1989)
 1.49, 1.37 (shake flask, HPLC-RT correlation, Wang et al. 1989)
 1.40 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.41 (soil, quoted obs. as $\log K_{\text{OM}}$, Sabljic 1987)
 1.65 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982).

Biodegradation: decomposition by a soil microflora in 8 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average biodegradation rate of $30.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 97.7% removal (Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

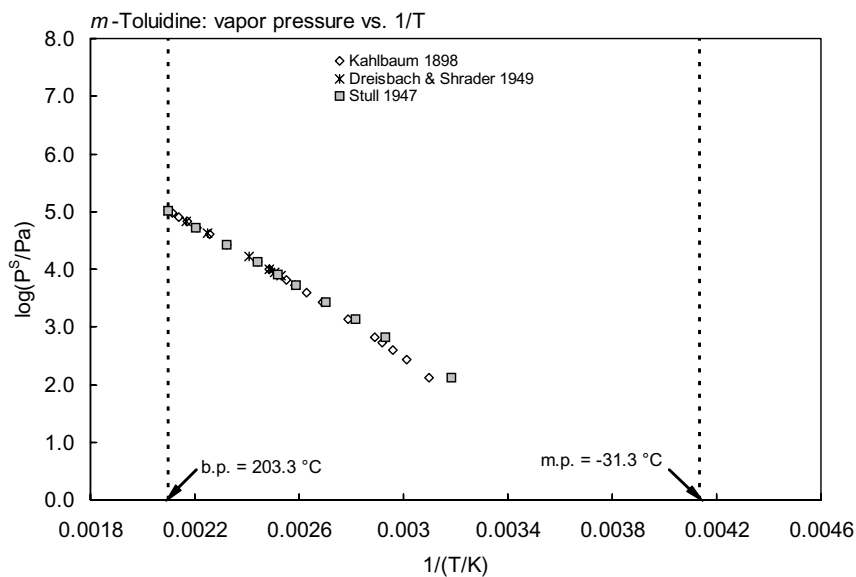
Half-Lives in the Environment:

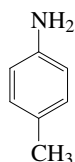
Surface water: estimated $t_{1/2} = 1.0 \text{ d}$ for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.3.7.1

Reported vapor pressures of *m*-toluidine at various temperatures

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949	
static method-manometer*		summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
49.8	133.3	41.0	133.3	121.77	7605
58.9	266.6	68.0	666.6	125.57	8851
64.8	400.0	82.0	1333	129.03	10114
69.3	533.3	96.7	2666	142.27	16500
72.8	666.6	113.5	5333	171.18	42066
85.3	1333.2	123.8	7999	187.87	67661
98.5	2666.4	136.7	13332	203.34	101325
107.1	3999.7	157.6	26664		
113.6	5332.9	180.6	53329		
118.7	6666.1	203.3	101325		
129.0	9999.2				
136.6	13332	mp/°C	−31.5		
157.6	26664				
169.8	39997				
179.8	53329				
187.5	66661				
194.0	79993				
199.8	93326				
203.3	101325				

*complete list see [ref.](#)FIGURE 16.1.3.7.1 Logarithm of vapor pressure versus reciprocal temperature for *m*-toluidine.

16.1.3.8 *p*-Toluidine (4-Methylbenzeneamine)

Common Name: *p*-Toluidine

Synonym: 4-aminotoluene, 4-methylaniline, 4-methylbenzenamine

Chemical Name: 4-aminotoluene, *p*-amino-methylbenzene, *p*-methylaniline, *p*-toluidine

CAS Registry No: 106-49-0

Molecular Formula: $C_6H_4(CH_3)NH_2$

Molecular Weight: 107.153

Melting Point ($^{\circ}C$):

43.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

200.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9619 ($20^{\circ}C$, Weast 1982–83)

1.043 (Verschueren 1983)

Molar Volume (cm^3/mol):

132.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

5.02, 5.08, 5.084 (Perrin 1972)

5.08 (Weast 1982–83; Sangster 1989)

5.08 (protonated cation + 1, Dean 1985)

5.17 (shake flask-HPLC/UV, Johnson & Westall 1990)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.195, 44.271 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.32 (Tsonopoulos & Prausnitz 1971)

18.91 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

54.81 (Tsonopoulos & Prausnitz 1971)

57.61 (observed, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.657 (mp at $43.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ as indicated):

65400 (20 – $25^{\circ}C$, shake flask-gravimetric, Dehn 1917)

8965 (Seidell 1941, 1952)

7400 ($21^{\circ}C$, Verschueren 1983)

6643, 5370 ($20^{\circ}C$, shake flask-UV, calculated, Hashimoto et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($46.9^{\circ}C$, static method, measured range 46.9 – $200.4^{\circ}C$, Kahlbaum 1898)

$\log(P/mmHg) = -2597/(T/K) + 8.366$ (isoteniscope method, temp range not specified, Kobe et al. 1941)

46.27* (extrapolated-regression of tabulated data, temp range 42 – $200.4^{\circ}C$, Stull 1947)

44.70 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.25173 - 1755.0/(201.0 + t/^{\circ}C)$; temp range 103 – $330^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/atm) = [-0.2185 \times 12428.6/(T/K)] + 8.748585$; temp range 42 – $200.4^{\circ}C$ (Antoine eq., Weast 1972–73)

38.13 (calculated-Cox eq., Chao et al. 1983)

- $\log (P/\text{mmHg}) = [1 - 473.445/(T/K)] \times 10^{\{0.915691 - 6.57014 \times 10^{-4} \cdot (T/K) + 5.11261 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 290.0–700.0 K (Cox eq., Chao et al. 1983)
 40.17 (calculated-Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 7.26022 - 1758.55/(201.0 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Dean 1985, 1992)
 45.0 (quoted lit., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 18.2818 - 3269.3/(T/K) - 3.877 \cdot \log (T/K)$; temp range not specified (vapor pressure eq., Riddick et al. 1986)
 27.03 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.17451 - 1585.0/(-93.44 + T/K)$; temp range 393–474 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = -13.9927 - 2.5795 \times 10^3/(T/K) - 10.823 \cdot \log (T/K) - 1.7705 \times 10^{-2} \cdot (T/K) + 7.6741 \times 10^{-6} \cdot (T/K)^2$; temp range 317–693 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.656 (calculated-P/C)
 0.0768 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 1.39 (shake flask-UV, Fujita et al. 1964)
 1.41 (HPLC- k' correlation, Carlson et al. 1975)
 1.56 (shake flask-UV, Ezumi & Kubota 1980)
 1.40 (20°C , shake flask-UV, Briggs 1981)
 1.44 ± 0.03 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
 1.42 (HPLC- k' correlation, Haky & Young 1984)
 1.39 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)
 1.41 (HPLC-RT correlation, average, Ge et al. 1987)
 1.39 (shake flask, Leahy et al. 1989)
 1.39 (recommended, Sangster 1989, 1993)
 1.38, 1.39 (shake flask, HPLC-RT correlation, Wang et al. 1989)
 1.40 (shake flask-HPLC/UV, Johnson & Westall 1990)
 1.40 (shake flask-UV, Roberts et al. 1991)
 1.40 (32°C , shake flask-UV, pH 7, Takahashi et al. 1993)
 1.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.51, 2.70, 2.71 (Morocco soil, Oakville soil, Milford soil, Graveel et al. 1986)
 1.66 (soil, quoted obs. as $\log K_{OM}$, Sabljic 1987)
 2.74, 2.22, 2.20 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
 1.24 (calculated- K_{OW} , Kollig 1993)
 1.90 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.21; 1.86 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.28, 2.01, 2.30, 2.084 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 2.138, 2.133, 2.212, 2.041 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask-batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization:
 Photolysis:
 Hydrolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982).

Biodegradation: decomposition by a microflora in 4 d (Alexander & Lustigman 1966; quoted, Verschueren 1983); average biodegradation rate of $20 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 97.7% removal (Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 1.0 \text{ d}$ for methylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.3.8.1
Reported vapor pressures of *p*-toluidine at various temperatures

Kahlbaum 1898		Stull 1947	
static method-manometer*		summary of literature data	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
46.9	133.3	42.0	133.3
55.9	266.6	68.2	666.6
62.0	400.0	81.8	1333
66.4	533.3	95.8	2666
70.1	666.6	111.5	5333
82.2	1333.2	121.5	7999
95.6	2666.4	133.7	13332
104.3	3999.7	154.0	26664
110.7	5332.9	176.9	53329
115.8	6666.1	200.4	101325
126.1	9999.2		
133.7	13332	mp/ $^\circ\text{C}$	44.5
154.7	26664		
166.9	39997		
176.9	53329		
184.6	66661		
191.1	79993		
196.9	93326		
200.4	101325		

*complete list see [ref.](#)

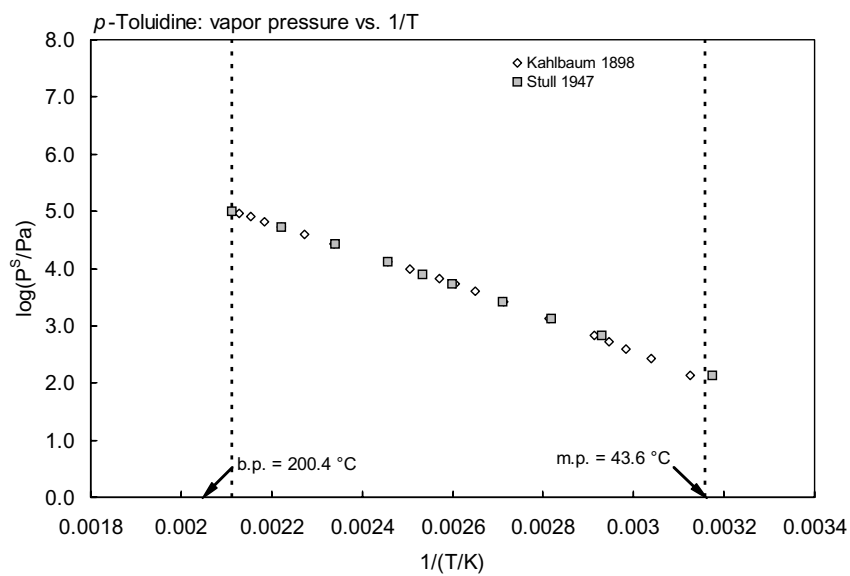
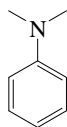


FIGURE 16.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-toluidine.

16.1.3.9 N,N'-Dimethylaniline



Common Name: N,N'-Dimethylaniline

Synonym: N,N'-dimethylbenzenamine

Chemical Name: N,N'-dimethylaniline

CAS Registry No: 121-69-7

Molecular Formula: $C_8H_{11}N$, $C_6H_5N(CH_3)_2$

Molecular Weight: 121.180

Melting Point ($^{\circ}C$):

2.42 (Lide 2003)

Boiling Point ($^{\circ}C$):

194.0 (Weast 1982–83)

194.15 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9557 (Weast 1982–83)

Molar Volume (cm^3/mol):

154.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK:

5.15 (pK_{BH}^{+} , Riddick et al. 1986)

5.10 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.42 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

41.46 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1105 (shake flask-GC, Chiou et al. 1982)

1540, 1680 (20, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $90^{\circ}C$, Stephenson 1993c)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

106.3 (extrapolated-regression of tabulated data, temp range 20.0 – $193.1^{\circ}C$, Stull 1947)

133.3 ($29.5^{\circ}C$, Stull 1947)

83.90 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/atm) = [-0.2185 \times 11320.4/(T/K)] + 8.197379$; temp range: 29.5 – $193^{\circ}C$, (Antoine eq., Weast 1972–73)

68.95 (calculated-Cox eq., Chao et al. 1983)

$\log(P/mmHg) = [1 - 466.445/(T/K)] \times 10^{\{0.909397 - 7.07673 \times 10^{-4} \pm (T/K) + 5.69581 \times 10^{-7} \pm (T/K)^2\}}$; temp range 275.0 – $685.0 K$ (Cox eq., Chao et al. 1983)

84.5 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.5031 - 1865.084/(211.171 + t/^{\circ}C)$; temp range 71.02 – $196.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

83.91 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.91048 - 946.35/(246.68 + t/^{\circ}C)$; temp range -87 to $7^{\circ}C$ (Antoine eq., Dean 1985, 1992)

670.0 (quoted from Stull 1947, Riddick et al. 1986)

107.0 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.07329 - 2301.63/(-12.001 + T/K)$; temp range 302 – $467 K$ (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.55663 - 1864.075/(-55.854 + T/K)$; temp range 363 – $418 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 2-.177 - 3.1095 \times 10^3/(T/K) - 4.0127 \cdot \log (T/K) + 5.8538 \times 10^{-10} \cdot (T/K) + 3.5387 \times 10^{-7} \cdot (T/K)^2;$$

temp range 276–687 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

11.73 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.31 (shake flask-UV, Fujita et al. 1964)
 2.62 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)
 1.66 (shake flask-UV, Leo et al. 1971)
 2.29 (shake flask-UV, Yaguzhinskii et al. 1973)
 2.30 (shake flask at pH 7, Unger et al. 1978)
 2.43 (HPLC-RT correlation, Miyake et al. 1986)
 2.28 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
 2.32 (CPC correlation, El Tayar et al. 1991)
 2.31 (recommended, Sangster 1993)
 2.31 (recommended, Hansch et al. 1995)
 2.05 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.99; 2.53; 2.06 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
 2.26, 1.89 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 2.26 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k ; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{OH}}^*(\text{exptl}) = (1.48 \pm 0.11) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, measured range 278–464 K; $k_{\text{O}_3} = (9.1 \pm 1.0) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1987)

$k_{\text{OH}} = 1.5 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes of 1.9 h in clean troposphere and 1.0 h in moderately polluted atmosphere; $k_{\text{O}_3} = 9.1 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes of 1.8 d in clean troposphere and 14 h in moderately polluted atmosphere at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 4.66 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs}) = 1.48 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}(\text{calc}) = 1.78 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: aerobic $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aqueous screening test data and anaerobic $t_{1/2} = 2880\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetimes of 1.9 h in clean troposphere and 1.0 h in moderately polluted atmosphere, based on the gas-phase reaction with hydroxyl radical in air at room temp.; atmospheric lifetimes of 1.8 d in clean

troposphere and 14 h in moderately polluted atmosphere, based on the gas-phase reaction with O_3 in air at room temp. (Atkinson et al. 1987);

$t_{1/2} = 2.7\text{--}21$ h, based on photooxidation half-life in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: estimated $t_{1/2} = 2.3$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2} = 19.3\text{--}1925$ h, based on reaction with singlet oxygen in aqueous solution (Howard et al. 1991)

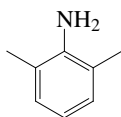
Groundwater: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota:

16.1.3.10 2,6-Xylidine (2,6-Dimethylbenzeneamine)



Common Name: 2,6-Xylidine

Synonym: 2,6-dimethylaniline, 2,6-dimethylbenzeneamine

Chemical Name: 2,6-dimethylaniline

CAS Registry No: 87-62-7

Molecular Formula: $C_8H_{11}N$, 2,6- $(CH_3)_2C_6H_3NH_2$

Molecular Weight: 121.180

Melting Point ($^{\circ}C$):

11.20 (Weast 1982–83; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

214.0 (at 739 mm Hg, Weast 1982–83; Verschueren 1983)

215 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9842 (Weast 1982–83; Riddick et al. 1986)

Molar Volume (cm^3/mol):

123.1 ($20^{\circ}C$, calculated-density)

154.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK :

3.95 (pK_{BH}^{+} , Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

slightly soluble (Dean 1985; Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

43.03 (extrapolated-regression of tabulated data, temp range 44 – $217.9^{\circ}C$, Stull 1947)

$\log(P/atm) = [1 - 490.795/(T/K)] \times 10^{0.926009 - 6.89676 \times 10^{-4} \cdot (T/K) + 5.31053 \times 10^{-7} \cdot (T/K)^2}$; temp range: 285.0 – $720.0\ K$ (Cox eq., Chao et al. 1983)

17.33 (Howard et al. 1986)

670.0 (quoted from Stull 1947, Riddick et al. 1986)

35.99 (calculated-solvatochromic parameters, Banerjee et al. 1990)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

17.28 (calculated- P/C from selected value)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.96 (calculated, Verschueren 1983)

1.91 (calculated-CLOGP, Jäckel & Klein 1991)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982); $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);photooxidation $t_{1/2} = 0.33\text{--}3.3 \text{ h}$ in air, based on estimated reaction rate constant with OH radical (Atkinson 1987; selected, Howard et al. 1991) and photooxidation $t_{1/2} = 62.4\text{--}3480 \text{ h}$ in water, based on reaction rate constants of amine class with $\text{RO}_2\cdot$ and OH radicals in water (Güesten et al. 1981; Mill & Mabey 1985; selected, Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 672\text{--}4320 \text{ h}$, based on a biological screening study (Baird et al. 1977; selected Howard et al. 1991) and a soil degradation study (Bollag et al. 1978; selected, Howard et al. 1991); aqueous anaerobic biodegradation $t_{1/2} = 2688\text{--}17280 \text{ h}$, based on estimated aqueous biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

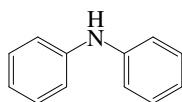
Air: $t_{1/2} = 0.33\text{--}3.3 \text{ h}$, based on estimated photooxidation half-lives in air from estimated reaction rate constant with OH radical in air (Atkinson 1987; selected, Howard et al. 1991).Surface water: estimated $t_{1/2} = 2.0 \text{ d}$ for dimethylaniline in Rhine River in case of a first order reduction process (Zoeteman et al. 1980) $t_{1/2} = 62.4\text{--}3480 \text{ h}$, based on photooxidation half-life in water (Howard et al. 1991).Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 72\text{--}7584 \text{ h}$, based on soil persistence and soil biodegradation studies (Bollag et al. 1978; Medvedev & Davidov 1981; selected, Howard et al. 1991).

Biota:

16.1.3.11 Diphenylamine



Common Name: Diphenylamine

Synonym: N-diphenylamine, N-phenyl aniline, DPA

Chemical Name: N-diphenylamine, diphenylamine

CAS Registry No: 122-39-4

Molecular Formula: $C_{12}H_{11}N$, $C_6H_5NHC_6H_5$

Molecular Weight: 169.222

Melting Point ($^{\circ}C$):

53.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

302.0 (Stull 1947; Weast 1982–83; Verschueren 1983; Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.160 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

145.9 ($20^{\circ}C$ calculated-density)

200.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

0.89 (Perrin 1972)

0.90 (protonated cation + 1, Dean 1985)

0.78 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.53 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

53.56 (Tsonopoulos & Prausnitz 1971)

54.81; 56.5 (exptl., calculated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.529 (mp at $53.2^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ as indicated):

150 (20 – $25^{\circ}C$, shake flask-gravimetric method, Dehn 1917)

308 (Briggs 1981)

48 ($20^{\circ}C$, shake flask and membrane filter-fluorophotometric, Hashimoto et al. 1982)

52, 54 ($20^{\circ}C$, shake flask and glass fiber filters-fluorophotometric, Hashimoto et al. 1982)

300 (Verschueren 1983)

53 ($20^{\circ}C$, Yalkowsky et al. 1987)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.5682* (extrapolated-regression of tabulated data, temp range 108.3 – $302^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 14920.3/(T/K)] + 8.564067$; temp range 108.3 – $302^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/atm) = [1 - 575.114/(T/K)] \times 10^4 \{0.936992 - 6.17195 \times 10^{-4} \cdot (T/K) + 4.32696 \times 10^{-7} \cdot (T/K)^2\}$; temp range 335.0 – $670.0\ K$ (Cox eq., Chao et al. 1983)

0.0612 (calculated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 12.704 - 5043.9/(T/K)$; temp range 298 – $323\ K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.15045 - 2778.28/(-35.102 + T/K)$; temp range 381 – $575\ K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.5746 - 2430.7/(-41.15 + T/K)$; temp range 573 – $673\ K$ (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 9.7736 - 3.9008 \times 10^3/(T/K) + 0.91207 \cdot \log(T/K) - 5.898 \times 10^{-3} \cdot (T/K) + 2.3012 \times 10^{-6} \cdot (T/K)^2$; temp range 326 – $817\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 0.285 (calculated-P/C, Meylan & Howard 1991)
- 0.106 (estimated-bond contribution, Meylan & Howard 1991)
- 0.035 (calculated-P/C from selected values)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.23 (shake flask-UV, pH 7.4, Rogers & Cammarata 1969)
- 3.34 (unpublished result, Leo et al. 1971)
- 3.34, 3.50, 3.72 (unpublished results, Rekker 1977)
- 2.37 (RP-HPLC-RT correlation, Veith et al. 1979a)
- 3.45 (Hansch & Leo 1979)
- 3.42 (shake flask-UV, Briggs 1981)
- 3.37 (inter-laboratory shake flask average, Eadsforth & Moser 1983)
- 3.72 ± 0.03 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
- 2.69 (HPLC-RT correlation, average, Ge et al. 1987)
- 3.42 (shake flask, Log P Database, Hansch & Leo 1987)
- 3.50 (recommended, Sangster 1989, 1993)
- 3.70, 3.68 (shake flask, HPLC-RT correlation, Wang et al. 1989)
- 3.50 (recommended, Hansch et al. 1995)
- 2.99, 3.13, 3.04, 3.18 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
- 3.35 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 7.64 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.48 (fathead minnow, Veith et al. 1979b)
- 1.48, 2.10 (quoted, calculated- K_{OW} , Mackay 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.78 (sorption isotherm-GC, converted from K_{OM} organic matter-water in various soils, Briggs 1981)
- 2.78, 3.28 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 3.30 (calculated- K_{OW} , Kollig 1993)
- 2.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 2.80, 2.93 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 31\text{--}1740 \text{ h}$ in water, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 0.247\text{--}2.47 \text{ h}$, based on estimated rate data for the reaction with hydroxyl radicals in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis: rate constant $k = 1.2 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$ for reactions with hydroxyl radical in aqueous solution, (Buxton et al. 1986; quoted, Armbrust 2000);

measured hydroxy radical rate constant $k = 4.9 \times 10^{13} \text{ M}^{-1} \cdot \text{h}^{-1}$ (Armbrust 2000)

Biodegradation: aqueous aerobic $t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation screening test data (Malaney 1960; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 672\text{--}2688$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.247\text{--}2.47$ h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 31\text{--}1740$ h in water, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991); $t_{1/2} = 31\text{--}672$ h, based on estimated unacclimated aqueous aerobic degradation half-life and photooxidation half-life in water (Howard et al. 1991).

Groundwater: $t_{1/2} = 336\text{--}1344$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.3.11.1
Reported vapor pressures of diphenylamine at various temperatures

Stull 1947

summary of literature data

$t/^{\circ}\text{C}$	P/Pa
108.3	133.3
141.7	666.6
157.0	1333
175.2	2666
194.3	5333
206.9	7999
222.9	13332
247.5	26664
274.1	53329
302.0	101325
mp/ $^{\circ}\text{C}$	52.9

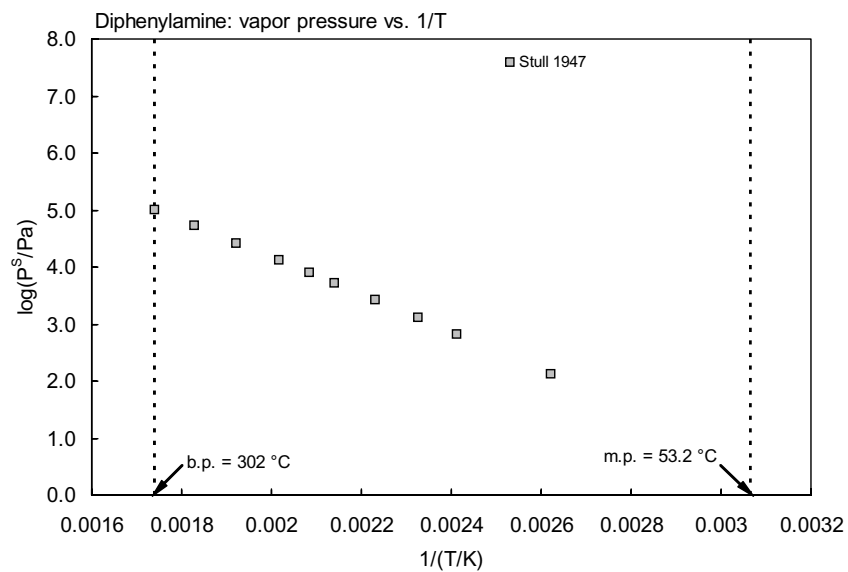
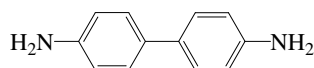


FIGURE 16.1.3.11.1 Logarithm of vapor pressure versus reciprocal temperature for diphenylamine.

16.1.3.12 Benzidine



Common Name: Benzidine

Synonym: *p,p'*-bianiline, 4,4'-diaminobiphenyl, 4,4'-biphenyldiamine, (1,1'-biphenyl)-4,4'-diamine

Chemical Name: *p*-benzidine

CAS Registry No: 92-87-5

Molecular Formula: C₁₂H₁₂N₂, NH₂C₆H₄C₆H₄NH₂

Molecular Weight: 184.236

Melting Point (°C):

128 (Weast 1982–83)

120 (Lide 2003)

Boiling Point (°C):

400 (Weast 1982–83)

401 (Lide 2003)

Density (g/cm³ at 20°C):

1.250 (Verschuereen 1983)

Molar Volume (cm³/mol):

213.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

4.66 (pK₁), 3.57 (pK₂) (30°C, Perrin 1965; quoted, Mabey et al. 1982; Howard 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.117 (mp at 120°C)

Water Solubility (g/m³ or mg/L at 25°C as indicated):

400 (12°C, Verschuereen 1977, 1983)

520 (Shriner et al. 1978)

360 (24°C at pH 5.9, shake flask-LSC, Means et al. 1980)

276 (20°C, Schmidt-Bleek et al. 1982)

359 (Gerstl & Helling 1987)

Vapor Pressure (Pa at 25°C):

0.724 (calculated-Trouton's rule, Mabey et al. 1982)

1.0 × 10⁻⁶ (20°C, Schmidt-Bleek et al. 1982)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

3.93 × 10⁻⁶ (estimated, Hine & Mookerjee 1975)

0.0394 (calculated-P/C at 12°C, Mabey et al. 1982)

4.60 × 10⁻⁷ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.34 (shake flask, Korenman 1971)

1.34 (recommended, Sangster 1993)

1.34 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.74, 2.66, 2.81, 3.4 (fish, mosquitoes, snail, algae; Lu et al. 1977)

1.60 (bluegills, USEPA 1980; quoted, Howard 1989)

1.00 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)

1.90, 2.93, 3.08 (golden ide, algae, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.66 (soil/sediment, equilibrium sorption isotherm by shake flask-LSC at pH 5.9, Means et al. 1980)
- 1.02 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
- 5.95; 5.68; 5.35; 5.91 (Russell soil; Chalmers soil; Kokomo soil; Milford soil, Graveel et al. 1986)
- 3.00 (calculated-MCI χ , Gerstl & Helling 1987)
- 3.46, 3.44 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 1.26 (calculated- K_{OW} , Kollig 1993)
- 3.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical of $1.1 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 0.312\text{--}3.12 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 48\text{--}192 \text{ h}$, based on aerobic soil die-away test data (Lu et al. 1977; quoted, Howard et al. 1991);

overall biodegradation $t_{1/2} = 76 \text{ d}$, when in sludge was applied to a sandy loam soil in a biological soil reactor and worked into the top 20 cm of soil (Kincannon & Lin 1985; quoted, Howard 1989);

aqueous aerobic $t_{1/2} = 192\text{--}768 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation of $1 \times 10^{-10} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.312\text{--}3.12 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated $t_{1/2} \sim 1 \text{ d}$ for the reaction with hydroxyl radical and ozone (Howard 1989);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

Surface water: estimated $t_{1/2} \sim 1 \text{ d}$ for the reaction with radicals and redox reactions with naturally occurring cations, etc. and perhaps with photodegradation (Howard 1989);

$t_{1/2} = 31.2\text{--}192 \text{ h}$, based on estimated photooxidation half-life in water and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 96\text{--}484 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

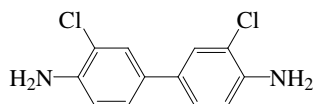
Soil: $t_{1/2} < 10 \text{ d}$ in soil (USEPA 1979; quoted, Ryan et al. 1988);

$t_{1/2} = 48\text{--}192 \text{ h}$, based on aerobic soil die-away test data (Lu et al. 1977; quoted, Howard et al. 1991);

overall biodegradation $t_{1/2} = 76 \text{ d}$, when in sludge was applied to a sandy loam soil in a biological soil reactor and worked into the top 20 cm of soil (Kincannon & Lin 1985; quoted, Howard 1989).

Biota: depuration $t_{1/2} \sim 7 \text{ d}$ from bluegills (Lu et al. 1977; quoted, Howard 1989).

16.1.3.13 3,3'-Dichlorobenzidine



Common Name: 3,3'-Dichlorobenzidine

Synonym: 3,3'-dichloro-4,4'-diamino(1,1'-biphenyl), DCB

Chemical Name: 3,3'-dichlorobenzidine

CAS Registry No: 91-94-1

Molecular Formula: $C_{12}H_{10}Cl_2N_2$, $NH_2C_6H_3(Cl)C_6H_3(Cl)NH_2$

Molecular Weight: 253.126

Melting Point ($^{\circ}C$):

132.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

254.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_b :

11.7 (Kollig 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0882 (mp at $132.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.00 ($22^{\circ}C$, as dihydrochloride, Banerjee et al. 1978)

3.99 ($22^{\circ}C$, at pH 6.9 as DCB.2HCl, quoted, Verschueren 1983)

3.11 (shake flask-UV/LSC, Banerjee et al. 1980)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00133 (estimated, Mabey et al. 1982)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0811 (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.02 (calculated as per Leo et al.1971)

3.51 ($23^{\circ}C$, shake flask, Banerjee et al. 1980)

3.35 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

3.51 (recommended, Sangster 1993)

3.51 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.70 (bluegill sunfish, Appleton & Sikka 1980)

2.97 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

2.79, 2.97, 3.49 (fish, algae, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

3.19 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

4.35, 3.87 (soil: quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

3.30 (calculated- K_{OW} , Kollig 1993)

4.35 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

direct aqueous photolysis rate constant $k = 2.1 \times 10^{-6} \text{ h}^{-1}$ in summer at 40°N latitude (Mabey et al. 1982); both aqueous and atmospheric photolysis $t_{1/2} = 0.025\text{--}0.075 \text{ h}$, based on direct photolysis in distilled water in midday summer sunlight (Banerjee et al. 1978; Sikka et al. 1978; quoted, Callahan et al. 1979; Howard et al. 1991) and approximate winter sunlight direct photolysis half-life (Banerjee et al. 1978; Sikka et al. 1978; Lyman et al. 1982; quoted, Howard et al. 1991).

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical $k < 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 31.2\text{--}1740 \text{ h}$ in water, based on estimated rate constants for reactions with OH and RO_2 radicals in water (Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.905\text{--}9.05 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320 \text{ h}$, based on lake die-away study test data (Appleton et al. 1978; quoted, Howard et al. 1991) and a soil die-away test (Boyd et al. 1984; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^{-12} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.905\text{--}9.05 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

estimated $t_{1/2} \sim 1 \text{ d}$ for the reaction with hydroxyl radical and ozone (Howard 1989);

atmospheric transformation lifetime by photolysis was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

Surface water: $t_{1/2} = 0.025\text{--}0.075 \text{ h}$, based on direct photolysis in distilled water in midday summer sunlight (Banerjee et al. 1978; Sikka et al. 1978; quoted, Howard et al. 1991) and approximate winter sunlight direct photolysis half-life (Banerjee et al. 1978; Sikka et al. 1978; Lyman et al. 1982; quoted, Howard et al. 1991).

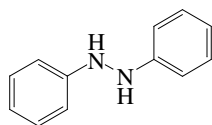
Ground water: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} = 30 \text{ min}$ by suspended microcrystalline clays may be considered the most important fate process in the aquatic environment (Callahan et al. 1979).

Soil: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.3.14 N,N'-Bianiline



Common Name: N,N'-Bianiline

Synonym: 1,2-diphenylhydrazine, hydrazobenzene

Chemical Name: 1,2-diphenylhydrazine, hydrazobenzene

CAS Registry No: 122-66-7

Molecular Formula: $C_{12}H_{12}N_2$, $C_6H_5NHNHC_6H_5$

Molecular Weight: 184.236

Melting Point ($^{\circ}C$):

131 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

293 (as azobenzene, IARC 1975)

Density (g/cm^3 at $20^{\circ}C$):

1.158 ($16^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

213.0 (calculated-Le Bas method at normal boiling point)

Dissociation constant pK_b :

13.2 (Kollig 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.0912 (mp at $131^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.252 ($20^{\circ}C$, as azobenzene, Takagishi et al. 1968)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00347 (quoted, Mabey et al. 1982)

$\log(P/mmHg) = 16.8982 - 5.0039 \times 10^3/(T/K) - 0.35846 \cdot \log(T/K) - 9.9629 \times 10^{-3} \cdot (T/K) + 4.2938 \times 10^{-6} \cdot (T/K)^2$;
temp range 404–573 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.45×10^{-4} (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.82 (shake flask-UV as for azobenzene, Fujita et al. 1964)

3.03 (calculated as per Leo et al. 1971, Callahan et al. 1979)

2.94 (shake flask, Hansch & Leo 1979; 1987)

2.94 (recommended, Sangster 1993)

2.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.46 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

2.62 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.40 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: aqueous oxidation rate constants for singlet oxygen $k < 4 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical, $k < 1 \times 10^9 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 31 - 1740 \text{ h}$, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.3 - 3.0 \text{ h}$ in air, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 672 - 4320 \text{ h}$, based on acclimated aerobic aqueous screening test data (Malaney 1960; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2880 - 17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: bacterial transformation $k = 1 \times 10^{-10} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.3 - 3.0 \text{ h}$, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

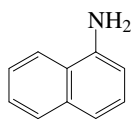
Surface water: photooxidation $t_{1/2} = 31 - 1740 \text{ h}$, based on photooxidation rate constants with OH and RO_2 radicals for the amine class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 1344 - 8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672 - 4320 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.3.15 α -Naphthylamine (1-Aminonaphthalene)

Common Name: 1-Naphthylamine

Synonym: 1-naphthalenamine, α -naphthylamine, 1-NA, 1-aminonaphthalene, naphthalidine

Chemical Name: 1-naphthalenamine

CAS Registry No: 134-32-7

Molecular Formula: $C_{10}H_7NH_2$

Molecular Weight: 143.185

Melting Point ($^{\circ}C$):

49.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

300.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1229 ($25^{\circ}C$, Weast 1982–8)

1.123 (Dean 1985)

Molar Volume (cm^3/mol):

161.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

3.92 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.23 ± 0.105 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

44.35 ± 3.35 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 0.579 (mp at $49.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1700 (Verschueren 1983)

590 parts in water (Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.803 (extrapolated-regression of tabulated data, temp range 104.3 – $300.8^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 14529.5/(T/K)] + 8.29900$; temp range 104.3 – $300.8^{\circ}C$ (Antoine eq., Weast 1972–73)

0.557 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 574.066/(T/K)] \times 10^4 \{0.822931 - 2.94554 \times 10^{-4} \cdot (T/K) + 2.19845 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 325.0 – $645.0\ K$ (Cox eq., Chao et al. 1983)

0.446 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.88407 - 2570.55/(-46.989 + T/K)$; temp range 377 – $574\ K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.197 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.23 (Leo et al. 1969)

2.25 (shake flask, Hansch & Leo 1979)

2.27 (shake flask-UV at pH 7.5, Martin-Villodre et al. 1986)

2.33 (HPLC- k' correlation, Minick et al. 1988)

2.25 (recommended, Sangster 1993)

2.25 (recommended, Hansch et al. 1995)

2.34 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

3.58, 3.43, 3.50	(Milford soil, Morocco soil, Oakville soil, Graveel et al. 1986)
2.63, 2.68, 3.15	(sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
3.51, 3.48	(soil, quoted exptl., calculated-MCI χ , Meylan et al. 1992)
3.51	(soil, calculated-MCI χ , Sabljic et al. 1995)
2.0–2.65	(5 soils, pH 2.8–7.4, batch equilibrium-sorption isotherm, Li et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

rate constant $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

atmospheric $t_{1/2} = 0.292\text{--}2.92 \text{ h}$, based on estimated rate constants for the reaction with OH radical in air and aqueous photooxidation $t_{1/2} = 62.4\text{--}3480 \text{ h}$, based on estimated rate constants for reaction of representative aromatic amines with OH and RO_2 radicals in aqueous solution (Howard et al. 1991);

photooxidation $t_{1/2} = 0.08\text{--}0.13 \text{ h}$ under sunlight and $t_{1/2} = 0.25\text{--}9.1 \text{ h}$ under UV light when adsorbed on silica; $t_{1/2} = 0.10\text{--}0.15 \text{ h}$ under sunlight and $t_{1/2} = 0.15\text{--}10.5 \text{ h}$ under UV light when adsorbed on alumina on the TLC plates under simulated atmospheric conditions (Hasegawa et al. 1993).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 672\text{--}4320 \text{ h}$ and aqueous anaerobic biodegradation $t_{1/2} = 2688\text{--}17280 \text{ h}$, based on slow biodegradation observed in aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.292\text{--}2.92 \text{ h}$, based on estimated photooxidation half-life in air (Howard et al. 1991).

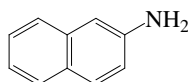
Surface water: $t_{1/2} = 0.62\text{--}3840 \text{ h}$, based on estimated rate constants for reactions of aromatic amines with OH and RO_2 radicals in aqueous solutions (Howard et al. 1991).

Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on slow biodegradation observed in an aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on slow biodegradation observed in an aerobic soil die-away test study and aerobic activated sludge screening tests (Howard et al. 1991).

Biota:

16.1.3.16 β -Naphthylamine (2-Aminonaphthalene)

Common Name: 2-Naphthylamine

Synonym: 2-naphthalenamine, β -naphthylamine, 2-NA, 2-aminonaphthalene, naphthalidine

Chemical Name: 2-naphthalenamine

CAS Registry No: 91-59-8

Molecular Formula: $C_{10}H_7NH_2$

Molecular Weight: 143.185

Melting Point ($^{\circ}C$):

113 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

306.2 (Lide 2003)

Density (g/cm^3):

1.0614 (at $98^{\circ}C$, Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

161.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

4.15 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.97 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

57.32 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.137 (mp at $113^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

6.40 ($18^{\circ}C$, Ciusa 1922; quoted, Tsonopoulos & Prausnitz 1971)

0.19 (18 – $20^{\circ}C$, Neish 1948; quoted, Tsonopoulos & Prausnitz 1971)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.634 (extrapolated-regression of tabulated data, temp range 108 – $306.1^{\circ}C$, Stull 1947)

$\log(P/atm) = [-0.2185 \times 14679.6/(T/K)] + 8.435133$; temp range 108 – $306.1^{\circ}C$ (Antoine eq., Weast 1972–73)

0.369 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 579.422/(T/K)] \times 10^{\{0.860256 - 4.44286 \times 10^{-4} \cdot (T/K) + 3.71453 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 385.0 – $645.0\ K$ (Cox eq., Chao et al. 1983)

0.035 (Howard et al. 1986)

0.035 (interpolated, solid, Antoine eq., Stephenson & Malanowski 1987)

0.362 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.4859 - 3859/(T/K)$, temp range: 283 – $323\ K$, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.88978 - 2604.31/(-46.068 + T/K)$, temp range 388 – $579\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

0.340 (calculated-solvatochromic parameters, Banerjee et al. 1990)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.28 (shake flask, Hansch & Leo 1979)

2.26 ($20^{\circ}C$, shake flask, Korenman & Polumestnaya, 1982)

2.40 (calculated-UNIFAC activity coeff., Campbell & Luthy 1985)

2.40 (shake flask-AS, pH 7.5, Martin-Villodre et al. 1986)

2.34 (recommended, Sangster 1993)

2.28 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.77 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radicals at 30°C in aquatic systems with $t_{1/2} = 0.8 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

rate constant $k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 0.30\text{--}2.90 \text{ h}$ in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

aqueous photooxidation $t_{1/2} = 62\text{--}3480 \text{ h}$, based on estimated rate constants for reaction of representative aromatic amines with OH and RO_2 radicals in aqueous solution (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.05\text{--}0.14 \text{ h}$ under sunlight and $0.20\text{--}10.0 \text{ h}$ under UV light when adsorbed on silica and $t_{1/2} = 0.16\text{--}0.19 \text{ h}$ under sunlight and $t_{1/2} = 0.22\text{--}10.8 \text{ h}$ under UV light when adsorbed on alumina TLC plates under simulated atmospheric conditions (Hasegawa et al. 1993).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic screening test data (Fochtman & Eisenberg 1979; quoted, Howard et al. 1979) and unacclimated soil grab sample data (Medvedev & Davidov 1981; quoted, Howard et al. 1991); aqueous anaerobic biodegradation $t_{1/2} = 2880\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.30\text{--}2.90 \text{ h}$, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 62.0\text{--}3840 \text{ h}$, based on estimated rate constants for reactions of aromatic amines with OH and RO_2 radicals in aqueous solutions (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991).

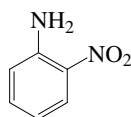
Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aerobic screening test data (Fochtman & Eisenberg 1979; quoted, Howard et al. 1991) and unacclimated aerobic soil grab sample data (Medvedev & Davidov 1981; quoted, Howard et al. 1981).

Biota:

16.1.3.17 2-Nitroaniline



Common Name: 2-Nitroaniline

Synonym: 1-amino-2-nitrobenzene, *o*-aminonitrobenzene, *o*-nitroaniline, 2-nitrophenylamine, 2-nitrobenzeneamine

Chemical Name: 1-amino-2-nitrobenzene, *o*-nitroaniline, 2-nitroaniline

CAS Registry No: 88-74-4

Molecular Formula: $C_6H_6N_2O_2$, $C_6H_4NH_2NO_2$

Molecular Weight: 138.124

Melting Point ($^{\circ}C$):

71.0 (Lide 2003)

Boiling Point ($^{\circ}C$):

284 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.442 ($15^{\circ}C$, Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

138.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

16.11 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} (J/mol K):

46.86 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.354 (mp at $71.0^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1212, 2423 ($25, 40^{\circ}C$, synthetic method-shake flask-titration, Collet & Johnson 1926)

1740 (calculated- K_{ow} , Yalkowsky & Morozowich 1980)

1260 (Verschueren 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 8.81842 - 3336.52/(T/K)$; measured range 150 – $215^{\circ}C$ (isoteniscope, Berliner & May 1925)

$\log(P/mmHg) = 9.55950 - 4037.7/(T/K)$; measured range 190 – $250^{\circ}C$ (isoteniscope, Berliner & May 1925)

0.620 (extrapolated-regression of tabulated data, temp range 104 – $284.5^{\circ}C$, Stull 1947)

0.072 (Knudsen method, calculated-Antoine eq., Hoyer & Peperle 1958)

$\log(P/mmHg) = 12.50 - 4701/(T/K)$, temp range 0 – $50^{\circ}C$ (Knudsen effusion method, Hoyer & Peperle 1958)

$\log(P/mmHg) = [-0.2185 \times 15284.0/(T/K)] + 8.868383$; temp range 104 – $284.5^{\circ}C$ (Antoine eq., Weast 1972–73)

< 13.3 ($30^{\circ}C$, Verschueren 1983)

0.650 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 8.8684 - 3336.5/(T/K)$; temp range 150 – $260^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_s/kPa) = 11.625 - 4701/(T/K)$; temp range 273 – 323 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 11.3629 - 7444.3/(240.83 + T/K)$; temp range 423 – 553 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -112.5774 - 1.5945 \times 10^3/(T/K) + 54.577 \cdot \log(T/K) - 7.6775 \times 10^{-2} \cdot (T/K) + 3.6152 \times 10^{-5} \cdot (T/K)^2$; temp range 345 – 558 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.44 (shake flask-UV, Fujita et al. 1964)

1.83 (shake flask-UV, Hansch & Anderson 1967)

1.62 (HPLC-RT correlation, Carlson et al. 1975)

1.81 (Hansch & Leo 1979)

- 1.72 (shake flask, Eadsforth & Moser 1983)
- 1.67 (calculated-HPLC- k' correlation, Deneer et al. 1987)
- 1.50 (calculated-linear extrapolation exptl. log k at various solvent compositions, Deneer et al. 1987)
- 1.93, 1.73 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
- 1.85 (recommended, Sangster 1993)
- 1.80 \pm 0.14, 1.35 \pm 0.51 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
- 1.85 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

0.91; 1.49, 0.55, 0.83 (quoted exptl.; calculated values- K_{OW} , Bintein et al. 1993)

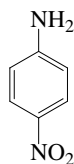
Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 1.4$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

16.1.3.18 4-Nitroaniline



Common Name: 4-Nitroaniline

Synonym: 1-amino-4-nitrobenzene, *p*-aminonitrobenzene, *p*-nitroaniline, 4-nitrobenzenamine, 4-nitrophenylamine

Chemical Name: 1-amino-4-nitrobenzene, *p*-nitroaniline, 4-nitroaniline

CAS Registry No: 100-01-6

Molecular Formula: $C_6H_6N_2O_2$, $C_6H_4NH_2NO_2$

Molecular Weight: 138.124

Melting Point ($^{\circ}C$):

147.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

332 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.424 (Weast 1982–83; Verschueren 1983)

1.4370 ($14^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

138.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.09 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

50.21 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.0628 (mp at $147.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

568, 1157 ($25, 40^{\circ}C$, synthetic method-shake flask-titration, Collet & Johnson 1926)

728 ($30^{\circ}C$, shake flask-interferometry, Gross et al. 1931)

603 (calculated- K_{ow} , Yalkowsky & Morozowich 1980)

380 ($20^{\circ}C$, shake flask-membrane filter-fluorophotometry, Hashimoto et al. 1982)

390, 400 ($20^{\circ}C$, shake flask-glass fiber filters-fluorophotometry, Hashimoto et al. 1982)

800; 22000 ($19^{\circ}C, 100^{\circ}C$, Verschueren 1983)

800 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 9.55950 - 4037.7/(T/K)$; measured range 190 – $250^{\circ}C$ (isoteniscope, Berliner & May 1925)

0.035 (extrapolated-regression of tabulated data, temp range 142.4 – $336^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 13.69 - 5707/(T/K)$, temp range 30 – $90^{\circ}C$, (Knudsen effusion method, Hoyer & Peperle 1958)

$\log(P/mmHg) = [-0.2185 \times 17220.2/(T/K)] + 9.041879$; temp range 142.4 – $336^{\circ}C$ (Antoine eq., Weast 1972–73)

0.200, 0.933 ($20^{\circ}C, 30^{\circ}C$, Verschueren 1983)

0.014 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 9.5595 - 4039.73/(T/K)$; temp range 190 – $260^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_s/kPa) = 11.1109 - 5093/(T/K)$; temp range 346 – $366\ K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.7988 - 4071.3/(T/K)$; temp range 473 – $538\ K$ (liquid, Antoine eq.-II., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 56.1642 - 5.3655 \times 10^3/(T/K) - 17.958 \cdot \log(T/K) + 9.092 \times 10^{-3} \cdot (T/K) + 7.0305 \times 10^{-10} \cdot (T/K)^2$; temp range 421 – $609\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.39 (shake flask-UV, Fujita et al. 1964; Hansch & Leo 1979)
- 0.59 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
- 1.16 (HPLC- k' correlation, Deneer et al. 1987)
- 1.10 (calculated-linear extrapolation exptl. values of $\log k$ at various solvent compositions, Deneer et al. 1987)
- 1.15 (HPLC-RT correlation, Wang et al. 1989)
- 1.51, 1.36 (25°C , 60°C , shake flask-UV, Kramer & Henze 1990)
- 1.30 (CPC-RV correlation, Tsai et al. 1991)
- 1.30 (CPC-RV correlation, El Tayar et al. 1991)
- 1.35 (recommended, Sangster 1993)
- 1.39 ± 0.14 , 0.75 ± 0.48 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
- 1.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.26; 2.66; 2.12 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
- 0.64; 1.25, -0.18 , 0.41 (quoted exptl.; calculated values- K_{OW} , Bintein et al. 1993)
- 2.16, 2.22, 2.19 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
- 1.86, 1.84 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)

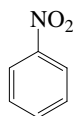
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

- Surface water: estimated $t_{1/2} = 2.3$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

16.1.4 NITROAROMATIC COMPOUNDS

16.1.4.1 Nitrobenzene



Common Name: Nitrobenzene

Synonym: nitrobenzol, oil of mirbane

Chemical Name: nitrobenzene

CAS Registry No: 98-95-3

Molecular Formula: $C_6H_5NO_2$

Molecular Weight: 123.110

Melting Point ($^{\circ}C$):

5.7 (Stull 1947; Dreisbach 1955; Weast 1982–83; Howard 1989; Lide 2003)

Boiling Point ($^{\circ}C$):

210.8 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2032, 1.1982 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.2036 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

102.0 (calculated from density, Rohrschneider 1973; Chiou 1985)

112.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

55.186, 43.421 ($25^{\circ}C$, bp, Dreisbach 1961)

55.013, 40.769 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.59 (Dreisbach 1955)

12.13 (Tsonopoulos & Prausnitz 1971)

11.63 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

43.51 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1780, 2050 (15, $30^{\circ}C$, shake flask-interferometry, Gross et al. 1931)

2060* ($30^{\circ}C$, shake flask-interferometry and titration, measured range 0 – $60^{\circ}C$, Vermillion et al. 1941)

1204 (shake flask-centrifuge, Booth & Everson 1948)

1930 (Seidell 1941)

2018 (shake flask-interferometry, Donahue & Bartell 1952)

1950 (Deno & Berkheimer 1960)

2259 ($35^{\circ}C$, shake flask-UV spectrophotometry, Hine et al. 1963)

2060 (Hansch et al. 1968)

1900 ($20^{\circ}C$, Verschueren 1977, 1983)

2093 (shake flask-LSC, Banerjee et al. 1980)

2090 (shake flask-radioactive analysis, Veith et al. 1980)

2043 (20 – $27^{\circ}C$, shake flask-GC, Chiou 1985)

1900 ($20^{\circ}C$, Riddick et al. 1986; quoted, Howard 1989)

1930* ($20^{\circ}C$, shake flask-UV spectrophotometry, measured range 10 – $40^{\circ}C$, Beneš & Dohnal 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 133.3* (53.1°C, static-manometer, measured range 53.1–208.3°C, Kahlbaum 1898)
 38.80 (saturated vapor density-gas saturation, Puck & Wise 1946)
 42.06* (extrapolated-regression of tabulated data, temp range 44.4–210.6°C, Stull 1947)
 10063* (134.1°C, ebulliometry, measured range 134.1–210.629°C, Brown 1952)
 37.86 (calculated by formula, Dreisbach 1955; quoted, Hine & Mookerjee 1975)
 $\log(P/\text{mmHg}) = 7.08283 - 1722.2/(199.0 + t/^\circ\text{C})$; temp range 108–300°C (Antoine eq. for liquid state, Dreisbach 1955)
 32.3* (23.14°C, gas saturation, measured range 6.09–23.14°C, Lynch & Wilke 1960)
 $\log(P/\text{mmHg}) = 7.545 - 2064/(t/^\circ\text{C} + 230)$; temp range 6.09–23.14°C (gas saturation, Lynch & Wilke 1960)
 80.0 (35°C, gas saturation-gravitational or UV spectrophotometry, Hine et al. 1963)
 $\log(P/\text{mmHg}) = [-0.2185 \times 12168.2/(T/\text{K})] + 8.416268$; temp range 44.4–210.6°C (Antoine eq., Weast 1972–73)
 34.60 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 7.11562 - 1746.585/(201.783 + t/^\circ\text{C})$, temp range 134–210.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
 20.00 (20°C, Verschueren 1977, 1983)
 28.37 (calculated-bp, Mackay et al. 1982)
 34.36 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.23424 - 1741.779/(201.257 + t/^\circ\text{C})$; temp range 134–210.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 4.06596 - 323.457/(-58.276 + t/^\circ\text{C})$; temp range 239–291°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 34.63 (extrapolated-Antoine eq., Dean 1985; 1992)
 $\log(P/\text{mmHg}) = 6.91048 - 946.35/(246.68 + t/^\circ\text{C})$; temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
 37.0 (quoted lit., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.670 - 2064.0/(230.0 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 37.65 (extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.22069 - 1732.222/(-72.886 + T/\text{K})$; temp range 407–484 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.6699 - 2064/(-43.15 + T/\text{K})$; temp range 279–296 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 33.33 (Howard et al. 1986)
 $\log(P/\text{mmHg}) = -54.4937 - 2.1123 \times 10^3/(T/\text{K}) + 29.321 \cdot \log(T/\text{K}) - 4.4839 \times 10^{-2} \cdot (T/\text{K}) + 2.0162 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 279–719 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

- 2.367, 4.51, 4.723 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 1.327 (calculated-P/C, Mabey et al. 1982)
 2.472 (estimated, Lyman et al. 1982)
 5.06 (calculated-molecular structure, Russell et al. 1992)
 0.868 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.85 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968; Leo et al. 1969, 1971; Hansch & Leo 1979, 1985;)
 1.74 (Neely et al. 1974)
 1.85, 1.84 (Hansch & Leo 1979)
 1.82 (HPLC-RT correlation, Veith et al. 1979a)
 1.83 (shake flask-LSC, Banerjee et al. 1980)
 1.98, 1.78 (HPLC-k' correlation, McDuffie 1981)
 1.85 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982;)
 1.88 (shake flask-UV, Unger & Chiang 1981)
 1.99 (RP-HPLC-k' correlation, Miyake & Terada 1982)
 1.83, 1.84 (calculated-activity coeff. γ from UNIFAC, octanol and water solubility considered; calculated-activity coeff. γ from UNIFAC, octanol and water solubility not considered, Arbuckle 1983)
 1.85, 1.88 (lit. values, Verschueren 1983)

- 1.83 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
- 1.84 (calculated-activity coefficient γ from UNIFAC, Campbell & Luthy 1985)
- 1.87 (Lu et al. 1986)
- 1.85 (RP-HPLC- k' correlation, Minick et al. 1988)
- 1.89 (HPLC- k' correlation, Deneer et al. 1987)
- 1.84 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
- 1.70 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
- 1.828 ± 0.001 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
- 1.85 (recommended, Sangster 1989, 1993)
- 1.836 ± 0.051; 1.828 ± 0.001 (average values, stir-flask method by BRE; by RITOX, Brooke et al. 1990)
- 1.83, 1.85, 1.88 (CPC-retention volume correlation; Gluck & Martin 1990)
- 1.94, 2.25 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
- 1.57 (shake flask-UV, Nakagawa et al. 1992)
- 1.85 (shake flask-GC, Alcron et al. 1993)
- 1.85 (recommended, Hansch et al. 1995)
- 2.25, 2.12, 2.20, 2.23 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995)
- 1.88 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
- 1.93 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

- 1.18 (fathead minnows, Veith et al. 1979b)
- 0.06 (calculated- K_{OW} , Veith et al. 1980)
- < 1.0; 1.36 (golden orfe; green algae, Freitag et al. 1982)
- 1.38; 1.42 (alga *Chlorella fusca*, wet wt. basis; calculated- K_{OW} , Geyer et al. 1984)
- 0.78 (*P. reticulata*, Canton et al. 1985; quoted, Howard 1989)
- < 1.0, 1.38, 1.60 (golden orfe, algae, activated sludge, Freitag et al. 1982)
- < 1.0, 1.30, 1.60 (golden ide, algae, activated sludge, Freitag et al. 1985)
- 1.47 ± 0.12 (guppy-fat wt. basis, Deneer et al. 1987)

Sorption Partition Coefficient, log K_{OC} :

- 1.94 (20°C, sorption isotherm-GC, converted from K_{OM} multiplied by 1.724, Briggs 1981)
- 2.30 (Lincoln fine sand, calculated exptl. value, Wilson et al. 1981)
- 2.23, 2.57 (Danish subsoils, Loekke 1985)
- 1.63, 1.84 (two Norwegian organic soils, Seip et al. 1986)
- 1.70 (soil, quoted, Sabljic 1987)
- 1.95 ± 0.84, 2.02 ± 1.18; 1.99 (Captina slit loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
- 1.43 (predicted- K_{OW} , Walton et al. 1992)
- 1.51 (calculated- K_{OW} , Kolliq 1993)
- 2.20 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 2.05, 2.16, 2.15 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
- 1.99, 1.84 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 2.20; 2.28 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.51, 2.03, 2.26, 2.09, 1.90 (soil: calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2}(\text{calc}) \approx 200$ h from water bodies (Mackay & Leinonen 1975; quoted, Callahan et al. 1979)
- $t_{1/2} = 45$ d was estimated in a model river 1 m deep with a 1.0 m/s current and a 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: aqueous photolysis $t_{1/2} = 67\text{--}200$ d, based on measured photolysis rate constant in distilled water under midday sun at 40°N latitude (Simmons & Zepp 1986; Howard 1989; Howard et al. 1991); atmospheric photolysis $t_{1/2} = 67\text{--}200$ d, based on measured photolysis rate constant in distilled water under midday sun at 40°N latitude (Simmons & Zepp 1986; quoted, Howard 1989; Howard et al. 1991); rate constant $k = 2.37 \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with $\text{HO}\cdot$ in the gas (Dilling et al. 1988).

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated *data at other temperatures see reference:

photooxidation $t_{1/2} = 125$ d to 22 yr in water, based on measured rate constant for reaction with hydroxyl radical in water (Dorfman & Adams 1973; Anbar & Neta 1967; quoted, Howard et al. 1991)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, $k \ll 1.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k = (0.09 \pm 0.02) \text{ M}^{-1} \text{ s}^{-1}$ for 5–10 mM to react with ozone in water using 50–1000 mM of *t*-BuOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}}(\text{obs.}) = 0.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Becker et al. 1984; quoted, Carlier et al. 1986)

$k_{\text{OH}} = 0.21 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Zetzsch 1982)

$k_{\text{OH}}(\text{calc}) = 0.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $0.27 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985; Atkinson et al. 1985)

$k_{\text{OH}}^* = 0.137 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K, measured range 259–362 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{\text{OH}}(\text{calc}) = 1.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (addition of OH for different positions of the electrophilic attack, Witte et al. 1986)

$k_{\text{O}_3} < 7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (relative rate method, Atkinson et al. 1987)

$k_{\text{OH}} = 1.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes $\tau = 180$ d in clean troposphere and 90 d in moderately polluted atmosphere; $k_{\text{O}_3} < 7 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes $\tau > 6$ yr in clean troposphere and $\tau > 2$ yr in moderately polluted atmosphere at room temp. (Atkinson et al. 1987)

$k_{\text{OH}}(\text{calc}) = 2.5 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.4 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = (0.16 - < 0.90) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (review, Atkinson 1989)

phototransformation decay rate constant of 0.17 min^{-1} on 0.20 g/L of TiO_2 , 8.8 min^{-1} on 0.20 g/L of ZnO and 3.1 min^{-1} on 1.0 g/L of Al_2O_3 (Minero et al. 1994)

Abiotic Transformation: Degradation in reductive environment:

$k = 0.187 \text{ min}^{-1}$ with solute concn of 50 μM in a 19 day-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)

$k = (7.39 \pm 1.28) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ in H_2S with (mercapto)juglone (an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Biodegradation:

decomposition by a soil microflora in more than 64 d (Alexander & Lustigman 1966; quoted, Verschuere 1983)

$t_{1/2}(\text{aq. anaerobic}) = 48\text{--}300$ h, based on anaerobic natural die-away test data for 2,4-dinitrotoluene (Spanggard et al. 1980; quoted, Howard et al. 1991)

$k = 14 \text{ mg COD g}^{-1} \text{ h}^{-1}$ average biodegradation rate for 98% removal (Scow 1982)

$t_{1/2}(\text{aq. aerobic}) = 322\text{--}4728$ h, based on aerobic soil column biodegradation study data (Kincannon & Lin 1985; quoted, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 13$ d, $t_{1/2}(\text{anaerobic}) = 2$ d in natural waters (Capel & Larson 1995)

Biotransformation: first-order rate constant of 0.7 d^{-1} corresponding to a half-life of 1 d in adopted activated sludge under aerobic conditions (Mills et al. 1982); rate constant for bacterial transformation of $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetimes: $\tau = 180$ d in clean troposphere and $\tau = 90$ d in moderately polluted atmosphere, based on gas-phase reaction with OH radical in atmosphere at room temp. and atmospheric lifetimes $\tau > 6$ yr in clean troposphere and $\tau > 2$ yr in moderately polluted atmosphere, based on gas-phase reaction with O_3 (estimated rate constant) in atmosphere at room temp. (Atkinson et al. 1987);

photooxidation $t_{1/2} = 0.544 - 5.44$ h, based on measured rate constant for reaction with hydroxyl radical in air (Atkinson et al. 1987; quoted, Howard 1989; Howard et al. 1991);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2} = 125$ d to 22 yr, based on measured rate constant for reaction with hydroxyl radical in water (Dorfman & Adams 1973; Anbar & Neta 1967; quoted, Howard et al. 1991);

estimated $t_{1/2} = 0.3 - 3.0$ d in rivers (Zoeteman et al. 1980);

$t_{1/2} = 322 - 4728$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 13$ d, $t_{1/2}(\text{anaerobic}) = 2$ d in natural waters (Capel & Larson 1995).

Groundwater: estimated $t_{1/2} = 1.0$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

$t_{1/2} = 48 - 9456$ h, based on estimated unacclimated aqueous anaerobic biodegradation half-life for 2,4-dinitrotoluene and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated degradation $t_{1/2} = 625$ d in activated sludge (Freitag et al. 1985; quoted, Anderson et al. 1991)

$t_{1/2} = 322 - 4728$ h, based on aerobic soil column biodegradation study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

calculated $t_{1/2} = 9.1$ d from first-order kinetic of degradation rate in sterilized soils (Anderson et al. 1991).

Biota:

TABLE 16.1.4.1.1

Reported aqueous solubilities of nitrobenzene at various temperatures

Gross et al. 1931		Vermillion et al. 1941		Beneš & Dohnal 1999	
shake flask-interferometry		interferometry		shake flask-UV	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
15	1780	0	1660	10	1770
30	2050	6	1700	20	1930
		30	2060	30	2060
		60	3120	40	2200
		titration		$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 5.4 \pm 0.2$	
		30	2060	at 25°C .	
		50	2640		

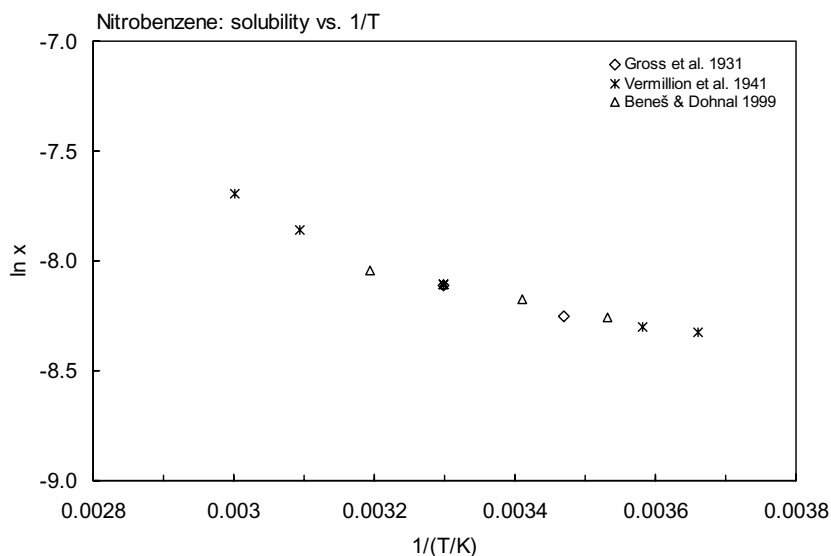


FIGURE 16.1.4.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for nitrobenzene.

TABLE 16.1.4.1.2

Reported vapor pressures of nitrobenzene at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Kahlbaum 1898*		Stull 1947		Lynch & Wilke 1960		Brown 1952	
static-manometer		summary of literature data		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
53.1	133.3	44.4	133.3	6.09	8.799	134.1	10063
59.8	266.6	71.6	666.6	12.57	14.80	139.75	13372
64.9	400.0	84.9	1333	12.67	13.33	143.17	16084
69.2	533.3	99.3	2666	14.67	16.93	149.73	18692
72.9	666.6	115.4	5333	14.72	17.73	154.61	21866
85.4	1333.2	125.8	7999	21.37	29.06	159.77	25704
99.1	2666.4	139.9	13332	21.54	29.33	164.45	29641
108.2	3999.7	161.2	26664	23.12	32.26	168.72	33649
114.9	5332.9	185.8	53329	23.14	32.26	172.96	38002
120.0	6666.1	210.6	101325			176.48	44455
131.1	9999.2			bp/°C	210.8	182.07	49014
139.9	13332	mp/°C	5.7			185.70	54019
160.5	26664			eq. 2	P/mmHg	188.90	58839
174.5	39997			A	7.545	196.63	65426
184.5	53329			B	2064	200.41	71843
192.5	66661			C	230	203.88	78997
199.5	79993					206.62	86075
205.0	93326					209.49	92023
208.3	101325					210.626	101322
						210.629	101330

*complete list see [ref.](#)

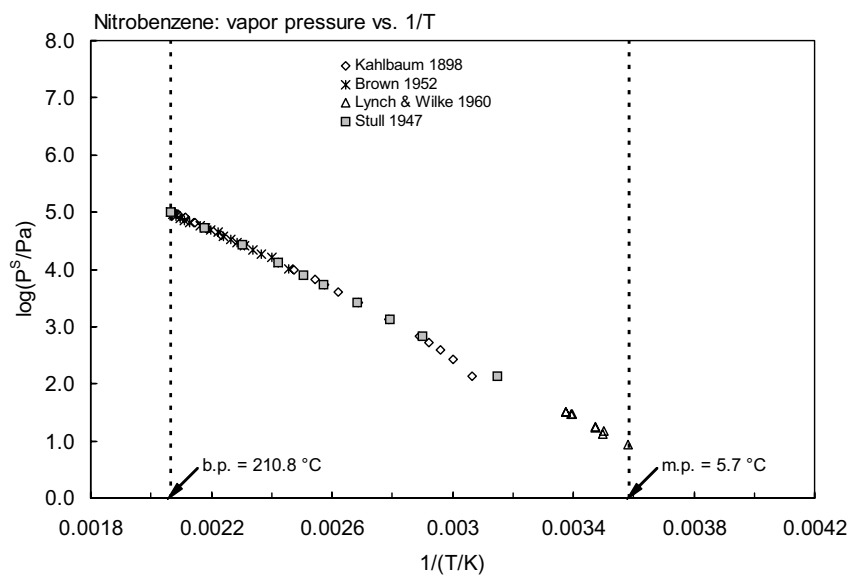
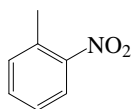


FIGURE 16.1.4.1.2 Logarithm of vapor pressure versus reciprocal temperature for nitrobenzene.

16.1.4.2 2-Nitrotoluene



Common Name: 2-Nitrotoluene

Synonym: 1-methyl-2-nitrobenzene, *o*-nitrotoluene, 2-methylnitrobenzene

Chemical Name: 2-nitrotoluene, *o*-nitrotoluene

CAS Registry No: 88-72-2

Molecular Formula: $C_7H_7NO_2$, $CH_3C_6H_4NO_2$

Molecular Weight: 137.137

Melting Point ($^{\circ}C$):

−10.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

222 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.15693, 1.15232 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

1.1629 (Weast 1982–83)

Molar Volume (cm^3/mol):

117.9 ($20^{\circ}C$, Stephenson & Malanowski 1987)

153.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$. Additional data at other temperatures designated * are compiled at the end of this section):

652 ($30^{\circ}C$, shake flask-interferometer, Gross et al. 1933)

656 (quoted, Deno & Berkheimer 1960)

< 233 (shake flask-centrifuge, Booth & Everson 1948)

324 (Hansch et al. 1968)

656, 2076 (quoted, predicted- K_{ow} , Valvani et al. 1981)

652 ($30^{\circ}C$, Verschueren 1983)

656, 771 (quoted, calculated-fragment const., Wakita et al. 1986)

641; 444 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

609* ($20^{\circ}C$, shake flask-UV spectrophotometry, measured range 10 – $40^{\circ}C$, Beneš & Dohnal 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

23.97* (extrapolated-regression of tabulated data, Kahlbaum 1898)

27.69* (extrapolated-regression of tabulated data, temp range 50 – $222.3^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.49454 - 2086.1/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

3640* ($115.842^{\circ}C$, ebulliometry, measured range 115.842 – $174.744^{\circ}C$, Dreisbach & Shrader 1949)

$\log(P/mmHg) = [-0.2185 \times 12239.7/(T/K)] + 8.286642$; temp range 50 – $222.3^{\circ}C$ (Antoine eq., Weast 1972–73)

13.33 ($20^{\circ}C$, Verschueren 1983)

1.670 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.01415 - 967.744/(99.208 + t/^{\circ}C)$; temp range 129.31 – $222.2^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.440 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 5.851 - 946/(96 + t/^{\circ}C)$, temp range 129 – $222^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_L/kPa) = 6.32043 - 1827.66/(-71.63 + T/K)$; temp range 402 – 496 K (Antoine eq., Stephenson & Malanowski 1987)

24.80* (ebulliometry, average from extrapolated-Antoine eq., Aim 1994)

$\log(P/\text{mmHg}) = 7.8266 - 2.9906 \times 10^3/(T/K) + 1.1064 \cdot \log(T/K) - 4.9168 \times 10^{-3} \cdot (T/K) + 2.2375 \times 10^{-6} \cdot (T/K)^2$;
temp range 270–720 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

5.811 (exptl., Hine & Mookerjee 1975)

4.723, 4.616 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.30 (Leo et al. 1971; Hansch & Leo 1985)

2.30 (HPLC- k' correlation, Deneer et al. 1987)

2.30 (unpublished data quoted from CLOGP Database and recommended, Sangster 1989)

2.39, 2.43, 2.58 (CPC-RV correlation, Gluck & Martin 1990)

2.46, 2.60; 2.30 (25°C , 60°C , shake flask-UV; quoted lit. value, Kramer & Henze 1990)

2.13 (shake flask-UV, Nakagawa et al. 1992)

2.30 (recommended, Sangster 1993)

2.40 ± 0.15 , 2.21 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)

2.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

< 2.0 (*carpinus carpio*, Sasaki 1978; Kawasaki 1980)

1.52, 1.20 (calculated- K_{OW} , S, Lyman et al. 1982; quoted, Howard 1989)

2.28 ± 0.06 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

2.63, 2.09 (soil, calculated- K_{OW} , S, Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 21$ h using Henry's law constant for a model river 1-m deep flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant $k = 3.0 \times 10^{-11} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ for the reaction with $8 \times 10^{-5} \text{ molecules/cm}^3$ photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989); rate constant $k = 7.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at 298 K (Atkinson 1989).

Hydrolysis:

Abiotic Transformation: Degradation in reductive environment:

$k = 0.141 \text{ min}^{-1}$ with solute concn of $50 \mu\text{M}$ in a 19 day-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)

Biodegradation: average biodegradation rate of $32.5 \text{ mg COD g}^{-1} \text{ h}^{-1}$ for 98% removal (Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 8$ h, based on a rate constant $k = 3.0 \times 10^{-11} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$ for the reaction with $8 \times 10^{-5} \text{ molecules/cm}^3$ photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989).

Surface water: estimated $t_{1/2} = 3.2$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
midday $t_{1/2}(\text{calc}) = 45$ min in Aucilla River water due to indirect photolysis using an experimentally determined reaction rate constant $k = 0.92 \text{ h}^{-1}$ (Zepp et al. 1984; quoted, Howard 1989);

estimated $t_{1/2} = 3.2$ d for a river 4 to 5 m deep, based on monitoring data (Zoeteman et al. 1980; quoted, Howard 1989).

Ground water:

Sediment:

Soil:

Biota:

TABLE 16.1.4.2.1
Reported aqueous solubilities of 2-nitrotoluene at various temperatures

Gross et al. 1931		Beneš & Dohnal 1999	
shake flask-interferometry		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	-	10	531
30	652	20	609
		30	688
		40	773
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 9.4 \pm 0.1$			
25°C			

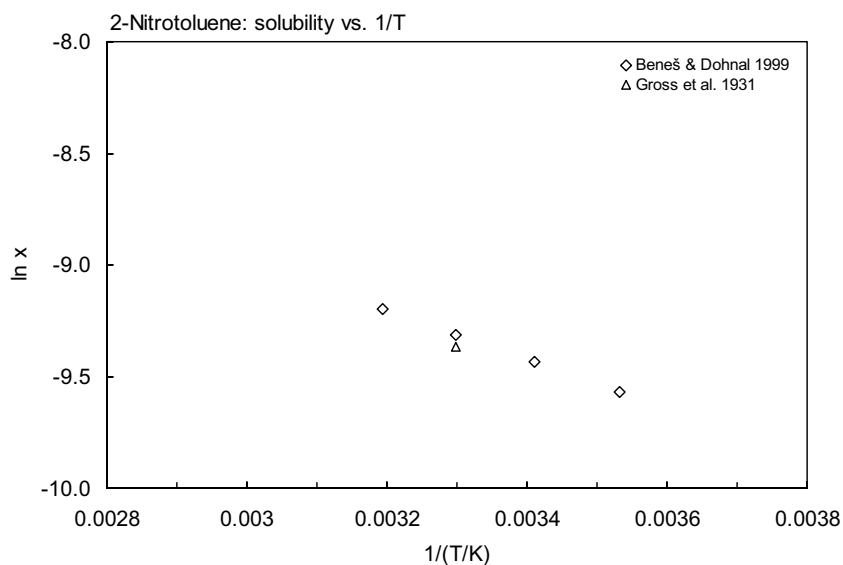


FIGURE 16.1.4.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-nitrotoluene.

TABLE 16.1.4.2.2
Reported vapor pressures of 2-nitrotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Kahlbaum 1898	Stull 1947	Dreisbach & Shrader 1949	Aim 1994				
static method	summary of literature data	ebulliometry	comparative ebulliometry				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
81.8	666.6	50.0	133.3	129.31	6287	115.842	3640
94.8	1333.2	79.1	666.6	134.51	7605	115.847	3639
109.6	2666.4	93.8	1333	138.75	8851	127.245	5773
114.8	3333.1	109.6	2666	142.43	10114	127.268	5778

TABLE 16.1.4.2.2 (Continued)

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Aim 1994	
static method		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
119.2	3999.7	126.3	5333	156.61	16500	137.028	8376
122.8	4666.3	137.6	7999	185.48	42077	137.052	8375
126.1	5333	151.5	13332	205.48	67661	144.838	11104
131.7	6666	173.7	26664	222.15	101325	151.379	13955
150.6	13332	197.7	53329			151.415	13946
172.4	26664	222.3	101325	bp/°C	222.15	157.004	16843
186.1	39997					157.028	16827
196.0	53329	mp/°C	-4.1			162.792	20322
204.2	66661					162.840	20311
211.3	79993					168.856	24597
217.5	93326					168.917	24587
220.4	101325					174.744	29405
						mp/°C	-2.90
						bp/°C	222.946
						eq. 3	P/kPa
						A	6.45342
						B	1906.532
						C	65.441
						for temp range: 115–175°C	

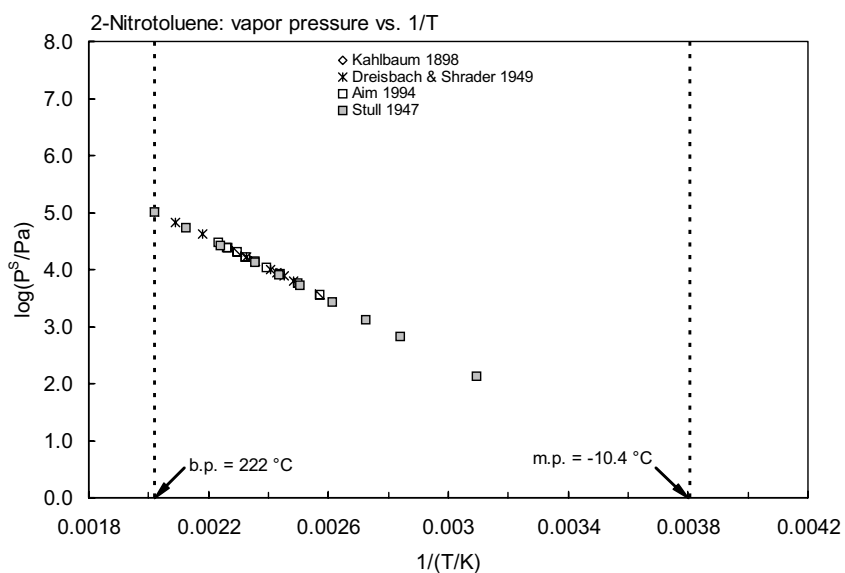
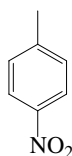


FIGURE 16.1.4.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-nitrotoluene.

16.1.4.3 4-Nitrotoluene



Common Name: 4-Nitrotoluene

Synonym: 1-methyl-4-nitrobenzene, *p*-nitrotoluene, 4-methylnitrobenzene

Chemical Name: 4-nitrotoluene, *p*-nitrotoluene

CAS Registry No: 99-99-0

Molecular Formula: $\text{CH}_3\text{C}_6\text{H}_4\text{NO}_2$

Molecular Weight: 137.137

Melting Point ($^{\circ}\text{C}$):

51.63 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

238.3 (Stull 1947; Weast 1982–83; Dean 1985; Howard 1989)

Density (g/cm^3 at 20°C):

1.16278, 1.15799 (20°C , 25°C , Dreisbach & Martin 1949)

1.392 (Dean 1985)

Molar Volume (cm^3/mol):

124.2 (75°C , Stephenson & Malanowski 1987)

153.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK :

–11.27 (Perrin 1972)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.15 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

50.21 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F : 0.548 (mp at 51.63°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

442 (30°C , shake flask-interferometer, Gross et al. 1933)

< 278 (shake flask-centrifuge, Booth & Everson 1948)

302 (Tsonopoulos & Prausnitz 1971)

442 (30°C , Verschueren 1983)

288 (20°C , shake flask-UV spectrophotometry, Hashimoto et al. 1984)

307 (calculated-group contribution method, Kühne et al. 1995)

242* (20°C , shake flask-UV spectrophotometry, measured range $10\text{--}40^{\circ}\text{C}$, Beneš & Dohnal 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

13.98* (extrapolated-regression of tabulated data, measured range $92\text{--}237^{\circ}\text{C}$, Kahlbaum 1898)

$\log (P/\text{mmHg}) = -2630/(T/\text{K}) + 8.025$ (isoteniscopes method, temp range not specified, Kobe et al. 1941)

22.81* (extrapolated-regression of tabulated data, temp range $53.7\text{--}238.2^{\circ}\text{C}$, Stull 1947)

$\log (P/\text{mmHg}) = 7.52323 - 2150.6/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

8851* (147.71°C , ebulliometry, measured range $147.71\text{--}233.25^{\circ}\text{C}$, Dreisbach & Shrader 1949)

0.622* (23.886°C , Knudsen effusion, measured range $297.036\text{--}309.518 \text{ K}$, Lenchitz & Velicky 1970)

$\log (P/\text{mmHg}) = 11.5424 - 4130.0708/(T/\text{K})$; temp range $297\text{--}310 \text{ K}$ (Knudsen effusion, Lenchitz & Velicky 1970)

$\log (P/\text{mmHg}) = [-0.2185 \times 11915.0/(T/\text{K})] + 7.965025$; temp range $53.7\text{--}238.3^{\circ}\text{C}$ (Antoine eq., Weast 1972–73)

5.50* (ebulliometry, fitted to Antoine eq., measured range $144\text{--}239^{\circ}\text{C}$, Ambrose & Gundry 1980)

9.50 (extrapolated-supercooled liq., Ambrose & Gundry 1980)

- 13.33 (20°C, Verschueren 1983; quoted, Howard 1989)
 8.347 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.11507 - 1716.897/(184.543 + t/^\circ\text{C})$; temp range 147.7–233.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 8.38 (extrapolated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.9948 - 1720.39/(184.9 + t/^\circ\text{C})$; temp range 148–233°C (Antoine eq., Dean 1985, 1992)
 0.653 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_g/\text{kPa}) = 10.6673 - 4130.07/(T/\text{K})$; temp range 296–310 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.40605 - 2889.12/(23.37 + T/\text{K})$; temp range 423–512 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 15.18* (ebulliometry, average of extrapolated-Antoine eq., Aim 1994)
 $\log(P/\text{mmHg}) = 9.9641 - 2.6549 \times 10^3/(T/\text{K}) - 0.80182 \cdot \log(T/\text{K}) + 5.3926 \times 10^{-4} \cdot (T/\text{K}) - 4.109 \times 10^{-14} \cdot (T/\text{K})^2$;
 temp range 325–736 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 5.065 (calculated, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.37 (shake flask-UV, Fujita et al. 1964)
 2.40 (unpublished result, Leo et al. 1971)
 2.34 (HPLC- k' correlation, Deneer et al. 1987)
 2.42 (recommended, Sangster 1989)
 2.10, 2.05 (25°C, 60°C, shake flask-UV, Kramer & Henze 1990)
 2.61 (shake flask-UV, Nakagawa et al. 1992)
 2.37 (recommended, Sangster 1993)
 2.37 ± 0.15 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)
 2.42 (recommended, Hansch et al. 1995)
 2.18 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

- < 2.0 (*Carprinus carpio*, Sasaki 1978; Kawasaki 1980)
 1.57, 1.30 (calculated- K_{ow} , S, Lyman et al. 1982; quoted, Howard 1989)
 2.37 ± 0.05 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.67, 2.18 (soil, calculated- K_{ow} , S, Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on Henry's law constant an estimated $t_{1/2} = 25$ h was obtained for a model river of 1- m deep with a current of 1 m/s and wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 8.0$ h in air, based on measured rate constant $k = 3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the reaction with photochemically produced $8 \times 10^5 \text{ molecules/cm}^3$ hydroxyl radical (GEMS 1986; quoted, Howard 1989).

Hydrolysis:

Abiotic Transformation: Degradation in reductive environment:

$k = 0.101 \text{ min}^{-1}$ with solute concn of 50 μM in a 19 d-old 0.2g/L magnetite suspension at pH 7 and 1.5 mM Fe(II) at 25°C (Klusen et al. 1995)

Biodegradation: average biodegradation rate of 32.5 mg COD $\text{g}^{-1} \text{ h}^{-1}$ for 98% removal (Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 8.0$ h, based on measured rate constant of 3×10^{-11} cm³ molecule⁻¹ s⁻¹ at 25°C for the reaction with photochemically produced 8×10^5 molecules/cm³ hydroxyl radical (GEMS 1986; quoted, Howard 1989).

Surface water: estimated $t_{1/2} = 2.7$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980) estimated $t_{1/2} = 2.7$ d, based on monitoring data for a river of 4 to 5-m deep (Zoeteman et al. 1980; quoted, Howard 1989).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 16.1.4.3.1
Reported aqueous solubilities of 4-nitrotoluene at various temperatures

Gross et al. 1931		Beneš & Dohnal 1999	
shake flask-interferometry		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
15	-	10	179
30	442	20	242
		30	322
		40	418
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 21.1 \pm 0.1$			
25°C			

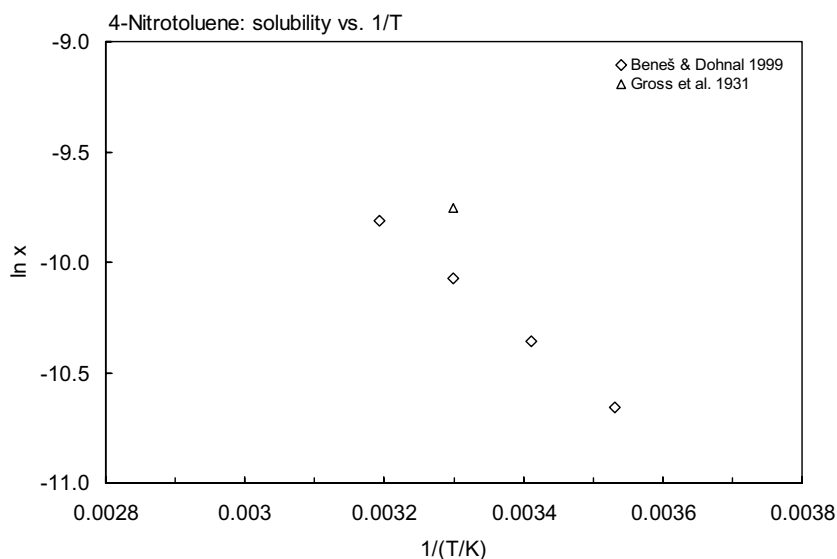


FIGURE 16.1.4.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 4-nitrotoluene.

TABLE 16.1.4.3.2

Reported vapor pressures of 4-nitrotoluene at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Kahlbaum 1898		Stull 1947		Dreisbach & Shrader 1949		Lenchitz & Velicky 1970	
static method-manometer		summary of literature data		ebulliometry		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
92.3	666.6	53.7	133.3	147.71	8851	23.886	0.6218
105.6	1333.2	85.0	666.6	151.43	10114	23.888	0.6283
120.3	2666.4	100.5	1333	165.98	16500	26.042	0.7311
125.7	3333	117.7	2666	197.75	42077	26.06	0.7330
130.4	3999.7	136.0	5333	216.17	67661	28.029	0.9426
134.4	4666	147.9	7999	233.25	101325	28.065	0.8994
137.9	5333	163.0	13332			30.205	1.0348
143.8	6666	186.7	26664	bp/°C	233.25	30.207	1.0423
164.0	13332	212.5	53329			32.012	1.3291
186.5	26664	238.3	101325			32.033	1.2987
201.2	39997					34.16	1.6681
212.2	53329	mp/°C	51.9			34.165	1.6551
220.8	66661					35.348	2.3313
228.4	79993					35.358	2.2839
234.8	93326					36.368	2.3087
237.7	101325						
						mp/°C	51.5
						enthalpy of sublimation:	
						$\Delta H_{\text{sub}} = 43.095 \text{ kJ mol}^{-1}$	
						at 25°C	
						eq. 1	P/mmHg
						A	11.5424
						B	4130.0828

2.

Ambrose & Gundry 1980		Aim 1994	
bubble-cap ebulliometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
143.498	5649	128.161	3639
148.11	7742	128.167	3639
153.159	9254	140.078	5776
158.081	10956	140.132	5787
163.205	12999	150.293	8378
168.438	15403	150.369	8400
173.494	18066	158.455	11107
180.103	22110	158.487	11118
185.757	26135	165.32	13946

(Continued)

TABLE 16.1.4.3.2 (Continued)

Ambrose & Gundry 1980		Aim 1994	
bubble-cap ebulliometer		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
192.227	31460	165.32	13967
198.564	37505	171.181	16823
205.643	44864	171.225	16845
212.568	54256	171.236	16848
218.948	63659	177.246	20306
225.722	75033	177.30	20332
233.058	89121	183.698	24639
238.685	101268		
239.269	102565	mp/°C	51.5
		bp/°C	238.343
tp/°C	51.64		
bp/°C	238.675	eq. 2	P/kPa
$\Delta H_{\text{fus}} = 16.81 \text{ kJ mol}^{-1}$		A	6.36793
$\Delta H_{\text{v}} = 46.60 \text{ kJ mol}^{-1}$, at bp		B	1931.718
		C	68.661
eq. 3	P/kPa	for temp range: 128–184°C	
A	6.27217		
B	1682.295		
C	−75.321		
for temp range: 416 to 513 K			
vapor pressure eq. for solid:			
eq. 1	P/kPa		
A	32.2514		
B	9018.0		
at triple pt	P = 67.72 Pa		
at 298.15 K	P = 5.5Pa		

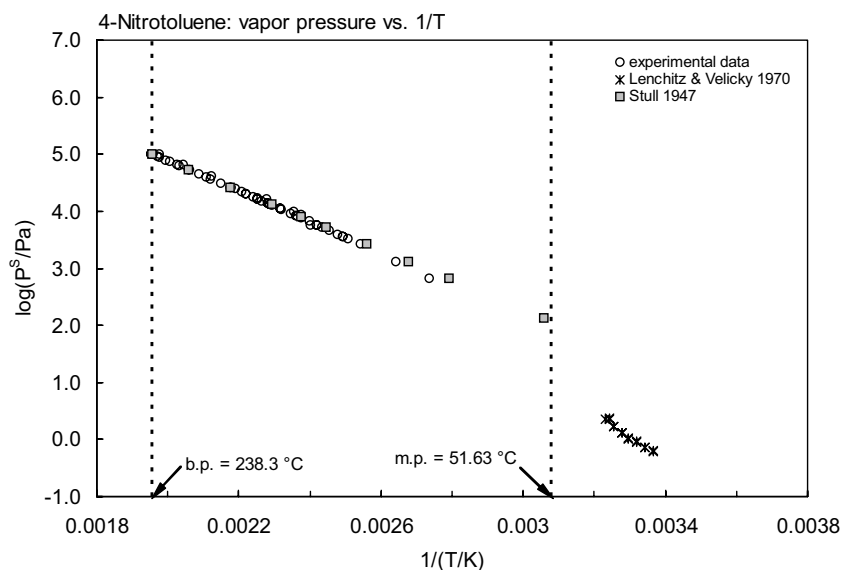
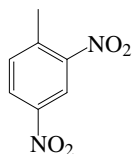


FIGURE 16.1.4.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-nitrotoluene.

16.1.4.4 2,4-Dinitrotoluene (DNT)



Common Name: 2,4-Dinitrotoluene

Synonym: dinitrotoluol, 1-methyl-2,4-dinitrobenzene, DNT

Chemical Name: 2,4-dinitrotoluene, 1-methyl-2,4-dinitrobenzene

CAS Registry No: 121-14-2

Molecular Formula: $C_7H_6N_2O_4$, $CH_3C_6H_3(NO_2)_2$

Molecular Weight: 182.134

Melting Point ($^{\circ}C$):

70.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

300 dec. (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.521 ($15^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

175.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:

–13.53 (Perrin 1972)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

58.99 (Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.358 (mp at $70.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

270 ($22^{\circ}C$, Verschueren 1977, 1983)

300 ($22^{\circ}C$, Dunlap 1981)

276; 145 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

199 ($25.2^{\circ}C$, shake flask-HPLC/UV, Phelan & Barnett 2001)

188* ($22^{\circ}C$, shake flask-HPLC/UV, measured range 12.4 – $61.8^{\circ}C$, Phelan & Barnett 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.133* ($59^{\circ}C$, Knudsen effusion, measured range 59 – $69^{\circ}C$, Lenchitz & Velicky 1970)

0.00321 (extrapolated-Antoine eq., Lenchitz & Velicky 1970)

$\log(P/mmHg) = 12.6177 - 5139.058/(T/K)$; temp range 331.913 – 342.277 K (Knudsen effusion, Lenchitz & Velicky 1970)

0.0177* ($20^{\circ}C$, gas saturation-GC/ECD, measured range 277.5 – 344.15 K, Pella 1977)

0.0290 (gas saturation-GC/ECD, interpolated-Antoine eq., measured range 277.5 – 344.15 K Pella 1977)

$\log(P/mmHg) = (13.08 \pm 0.19) - (4992 \pm 59)/(T/K)$; temp range 277.5 – 344.15 K (gas saturation, Pella 1977)

0.0147 ($20^{\circ}C$, Spangord et al. 1980)

0.6800 (quoted, Mabey et al. 1982)

$\log(P/kPa) = 5.06336 - 1216.523/(76.54 + t/^{\circ}C)$; temp range 100 – $199^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.0296, 0.0032 (extrapolated-Antoine eq.-I, eq.-II, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 12.27361 - 5009.432/(T/K)$; temp range 277 – 343 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.7426 - 5139.058/(T/K)$; temp range 331 – 342 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.1423 - 3039/(T/\text{K})$; temp range 473–572 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.04898 - 1956.095/(-108.183 + T/\text{K})$; temp range 344–572 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 5.798 - 1118/(61.8 + t/^\circ\text{C})$; temp range 200–299°C (Antoine eq., Dean 1992)

$\log (P/\text{mmHg}) = 11.5966 - 3.0079 \times 10^3/(T/\text{K}) - 1.6468 \cdot \log (T/\text{K}) + 1.5949 \times 10^{-3}(T/\text{K}) - 1.8722 \times 10^{-14} \cdot (T/\text{K})^2$; temp range 343–814 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.0160 (calculated-P/C, Smith et al. 1981)

0.4560 (calculated-P/C, Mabey et al. 1982)

0.0878 (Smith et al. 1983; quoted, Howard 1989)

32.23 (quoted from WERL Treatability database, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.98 (shake flask, Hansch & Leo 1985)

2.04 (HPLC- k' correlation, Deneer et al. 1987)

1.98 (recommended, Sangster 1993)

1.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.59 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

1.11, 1.76 (*daphnia magna*, *lumbriculus variegatus*, Liu et al. 1983)

> 3.30 (*selanastrum capricornutum*, Liu et al. 1983)

1.89, 0.602 (bluegill sunfish in viscera, bluegill sunfish in muscle, Liu et al. 1983)

2.31 \pm 0.03 (guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

1.65 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.68 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: half-life of approximately 100 d (Mills et al. 1982).

Photolysis: direct photolysis rate constant $k = 1.6 \times 10^{-2} \text{ h}^{-1}$ for summer at 40°N latitude in water (Mabey et al. 1982);

aqueous photolysis $t_{1/2} = 23\text{--}72 \text{ h}$, based on measured photolysis rates in water (Mill & Mabey 1985; Simmons & Zepp 1986; quoted, Howard et al. 1991);

atmospheric transformation lifetime $\tau \sim 1\text{--}5 \text{ d}$ (Kelly et al. 1994).

Hydrolysis:

Oxidation: aqueous oxidation rate constants $k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 144 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 284\text{--}2840 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 3\text{--}33 \text{ h}$, based on measured photooxidation rates in natural waters (Spanggord et al. 1980; Simmons & Zepp 1986; quoted, Howard et al. 1991).

Biodegradation: aqueous anaerobic $t_{1/2} = 48\text{--}240 \text{ h}$, based on anaerobic natural water die-away test data (Spanggord et al. 1980; quoted, Howard et al. 1991); aqueous aerobic $t_{1/2} = 672\text{--}4320 \text{ h}$, based on aerobic natural water die-away test data (Spanggord et al. 1981; quoted, Howard et al. 1991).

Biotransformation: rate constant of $1 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 284\text{--}2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
atmospheric transformation lifetime $\tau \sim 1\text{--}5$ d (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2} = 3\text{--}33$ h, based on measured photooxidation rates in natural waters (Spangord et al. 1980; Simmons & Zepp 1986; quoted, Howard et al. 1991);
estimated $t_{1/2} = 1.7$ d in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)
sunlight photolysis $t_{1/2} \sim 42$ h in pure water but ranged from 3 h to 10 h in three natural waters (Mabey et al. 1982).

Groundwater: $t_{1/2} = 48\text{--}8640$ h, based on estimated unacclimated aqueous anaerobic and aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 16.1.4.4.1

Reported aqueous solubilities and vapor pressures of 2,4-dinitrotoluene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Aqueous solubility		Vapor pressure			
Phelan & Barnett 2001		Lenchitz & Velicky 1970		Pella 1977	
shake flask-HPLC/UV		Knudsen effusion		gas saturation-GC	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
12.4	129	58.765	0.1731	4.0	0.00164
22.0	188	59.927	0.2073	10.0	0.0038
21.7	182	59.927	0.2138	20.0	0.0177
32.0	269	60.883	0.2328	30.0	0.0453
42.0	410	62.926	0.2568	40.0	0.171
51.0	608	62.824	0.3192	50.0	0.695
61.8	975	64.002	0.3450	60.0	1.663
41.2	397	65.115	0.3836	71.0	5.295
25.2	199	67.023	0.4380		
		68.10	0.4952	mp/°C	69.75–70.95
		69.127	0.5202		
				eq. 1	P/mmHg
				A	13.08
				B	4992
		enthalpy of sublimation: ΔH _{subl} = 98.324 kJ mol ⁻¹ (at 25°C)		enthalpy of sublimation: ΔH _{subl} = 95.81 kJ mol ⁻¹	
		eq. 1	P/mmHg		
		A	12.6177		
		B	5139.058		

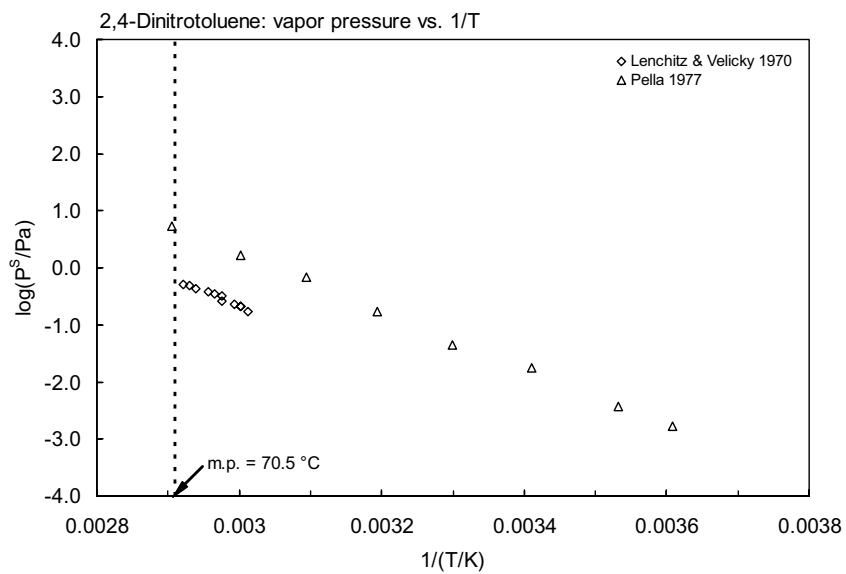
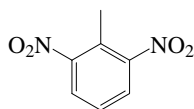


FIGURE 16.1.4.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dinitrotoluene.

16.1.4.5 2,6-Dinitrotoluene



Common Name: 2,6-Dinitrotoluene

Synonym: dinitrotoluol, 1-methyl-2,6-dinitrobenzene, 2-methyl-1,3-dinitrobenzene

Chemical Name: 2,6-dinitrotoluene, 1-methyl-2,6-dinitrobenzene

CAS Registry No: 606-20-2

Molecular Formula: $C_7H_6N_2O_4$, $CH_3C_6H_3(NO_2)_2$

Molecular Weight: 182.134

Melting Point ($^{\circ}C$):

66.0 (Weast 1982–83; Howard 1989; Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Verschuereen 1977; Callahan et al. 1979; Howard 1989; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2833 ($111^{\circ}C$, Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

141.9 ($111^{\circ}C$, Stephenson & Malanowski 1987)

175.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.396 (mp at $66.0^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated.):

180 ($20^{\circ}C$, estimated, Mabey et al. 1982)

300 (selected, Mills et al. 1982)

182; 155 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.40 ($29^{\circ}C$, Mabey et al. 1982)

0.0756* (gas saturation-GC/ECD, fitted to Antoine eq., temp range 277.5–323.15 K, Pella 1977)

$\log(P/mmHg) = (13.99 \pm 0.18) - (5139 \pm 52)/(T/K)$, temp range 277.5–323.15 K (gas saturation, Pella 1977)

0.0756 (Howard et al. 1986; quoted, Banerjee et al. 1990)

0.0767 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.9436 - 4446.22/(-21.279 + T/K)$; temp range 277–323 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.329 - 2971/(T/K)$; temp range 423–523 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.70024 - 2160.968/(-93.282 + T/K)$; temp range 330–533 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

0.0756, 1.008 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/mmHg) = 4.372 - 380/(-43.6 + t/^{\circ}C)$; temp range 150 – $260^{\circ}C$ (Antoine eq., Dean 1992)

$\log(P/mmHg) = -14.5673 - 4.2746 \times 10^3/(T/K) + 12.904 \cdot \log(T/K) - 2.380 \times 10^{-2} \cdot (T/K) + 9.4513 \times 10^{-6} \cdot (T/K)^2$; temp range 339–770 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$)

0.800 (calculated-P/C, Mabey et al. 1982)

32.23 (quoted from WERL Treatability database, Ryan et al. 1988)

0.022 (SOGC 1987; quoted, Howard 1989)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.72	(shake flask, Hansch & Leo 1985)
2.02	(HPLC- k' correlation, Deneer et al. 1987)
2.02	(shake flask-HPLC, Leggett et al. 1992)
2.07	(shake flask-UV, Nakagawa et al. 1992)
2.06	(recommended, Sangster 1993)
2.10	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

3.72	(algal biomass, Davis et al. 1981)
1.71	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
1.08	(calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)
2.44 ± 0.04	(guppy-fat basis, Deneer et al. 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

1.96	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)
2.31	(soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)
1.40	(calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 100$ d (Mills et al. 1982).

Photolysis: aqueous photolysis $t_{1/2} = 17\text{--}25$ h, based on measured photolysis rates in water (Simmons & Zepp 1986; Mill & Mabey 1985; quoted, Howard et al. 1991)

89% was photo-transformed in 24 h and none left after 72 h from seawater solution under UV light (Nipper et al. 2004).

Hydrolysis:

Oxidation: aqueous oxidation rate constants $k \ll 360 \text{ M}^{-1} \pm \text{h}^{-1}$ for singlet oxygen and $k = 144 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 2\text{--}17$ h in water, based on measured photooxidation rates in natural waters (Simmons & Zepp 1986; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 284\text{--}2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous anaerobic $t_{1/2} = 48\text{--}300$ h, based on anaerobic natural water die-away test data for 2,4-dinitrotoluene; aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on aerobic natural water die-away test data (Spanggord et al. 1981; quoted, Howard et al. 1991).

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982)

Biotransformation in marine sediments: all broken down in 28 d when incubated at 10°C , and in 7 d when incubated at 20°C in the sandy sediment; degraded by days 7 and 3 for incubation at 10 and 20°C , respectively, in fine-grained sediment (Nipper et al. 2004).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated atmospheric $t_{1/2} = 8$ h, based on the vapor phase reaction with hydroxyl radical in air (GEMS 1985; quoted, Howard 1989); photooxidation $t_{1/2} = 284\text{--}2840$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: midday $t_{1/2} \sim 12$ min in Aucilla river due to indirect photolysis using experimentally determined rate constant $k = 3.6 \text{ h}^{-1}$ (Zepp et al. 1984);

photooxidation $t_{1/2} = 2\text{--}17$ h in water, based on measured photooxidation rates in natural waters (Simmons & Zepp 1986; quoted, Howard et al. 1991)

89% was photo-transformed in 24 h and none left after 72 h from seawater solution under UV light (Nipper et al. 2004).

Ground water: $t_{1/2} = 48\text{--}8640$ h, based on estimated unacclimated aqueous anaerobic biodegradation half-life 2,4-dinitrotoluene and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: degraded by days 28 and 7 for incubation at 10 and 20°C, respectively, in sandy marine sediment; degraded by days 7 and 3 for incubation at 10 and 20°C, respectively, in fine-grain sediment (Nipper et al. 2004)

Soil: $t_{1/2} = 672 - 4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

TABLE 16.1.4.5.1
Reported vapor pressures of 2,6-dinitrotoluene at various temperatures

Pella 1977

gas saturation-GC	
t/°C	P/Pa
4.0	0.00342
10.0	0.0107
20.0	0.0383
30.0	0.147
40.0	0.483
50.0	1.718
mp/°C	57.25–57.75
eq. 1	P/mmHg
$\log P = A - B/(T/K)$	
A	13.99
B	5139
enthalpy of sublimation:	
$\Delta H_{\text{subl}} = 98.324 \text{ kJ mol}^{-1}$	

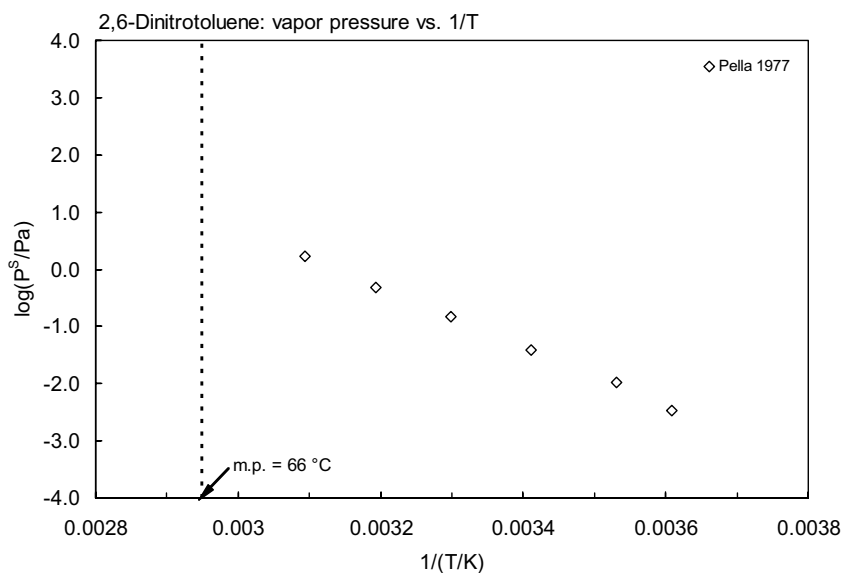
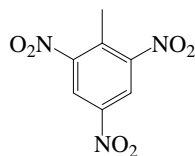


FIGURE 16.1.4.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dinitrotoluene.

16.1.4.6 2,4,6-Trinitrotoluene (TNT)



Common Name: 2,4,6-Trinitrotoluene

Synonym: TNT

Chemical Name: 2,4,6-trinitrotoluene

CAS Registry No: 118-96-7

Molecular Formula: $C_7H_5N_3O_6$, $(NO_2)_3C_6H_2CH_3$

Molecular Weight: 227.131

Melting Point ($^{\circ}C$):

80.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

240 explodes (Weast 1982–83; Dean 1992; Lide 2003)

Density (g/cm^3):

1.654 ($20^{\circ}C$, Weast 1982–83; Dean 1992)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

137.3 ($20^{\circ}C$, calculated-density)

187.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.285 (mp at $80.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

120* ($20^{\circ}C$, shake flask, measured range 0.30 – $99.5^{\circ}C$, Taylor & Rinkenbach 1923)

85.8 ($21^{\circ}C$, Hale et al. 1979)

104* ($20^{\circ}C$, temp range 10 – $30^{\circ}C$, Spanggard et al. 1983)

200 ($15^{\circ}C$, Verschueren 1983)

100 (Dean 1992)

101.5* (average value at $pH < 9.1$, shake flask-HPLC/UV, measured range 6 – $42^{\circ}C$, Ro et al. 1996)

101.6, 100.5, 110.5 (pH 3.5, pH 6.8, pH 9.1, shake flask-HPLC/UV spectrophotometry, Ro et al. 1996)

$\ln [S/(mg\ L^{-1})] = 16.12 - 3413/(T/K)$, temp range 6 – $42^{\circ}C$, ($pH < 8$, shake flask-HPLC/spec., Ro et al. 1996)

115* ($23.02^{\circ}C$, shake flask-HPLC/UV, measured range 13.6 – $61^{\circ}C$, Phelan & Barnett 2001)

99.85* 97.7* 99.9* ($20^{\circ}C$, pH 4.2, 5.7, 6.2, shake flask-HPLC/UV, measured range 2.3 – $38^{\circ}C$, Lynch et al. 2001)

$\ln [S/(mg\ L^{-1})] = 16.981 - 3607.5/(T/K)$; temp range 2.3 – $38^{\circ}C$ (composite solubility prediction correlation, shake flask-HPLC/UV measurements, Lynch et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.352* ($53^{\circ}C$, Knudsen effusion, measured range 50 – $143^{\circ}C$, Edwards 1950)

$\log (P_s/cmHg) = 14.34 - 6180/(T/K)$; range 50 – $81^{\circ}C$ (solid, Knudsen effusion, Edwards 1950)

$\log (P_L/cmHg) = 10.90 - 4960/(T/K)$; range 81 – $143^{\circ}C$ (liquid, Knudsen effusion, Edwards 1950)

0.0568* ($54.756^{\circ}C$, Knudsen effusion, measured range 55 – $76^{\circ}C$, Lenchitz & Velicky 1970)

$\log (P/mmHg) = 13.0776 - 5400.536/(T/K)$; temp range 55 – $76^{\circ}C$ (Knudsen effusion, Lenchitz & Velicky 1970)

0.00107* (gas saturation-GC/ECD, measured range 287.15 – 329.65 K, Pella 1977)

$\log (P/mmHg) = (12.31 \pm 0.34) - (5175 \pm 105)/(T/K)$, temp range 287.15 – 329.65 K (gas saturation, Pella 1977)

$\log (P/kPa) = 7.36331 - 3199.923/(248.004 + t/^{\circ}C)$; temp range 230 – $250^{\circ}C$ (liquid, Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.00078 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 13.596 - 5874.238/(T/\text{K})$; temp range 293–353 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 12.2025 - 5400.536/(T/\text{K})$; temp range 337–350 K (solid, Antoine eq.-II., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.40336 - 2191.85/(-121.43 + T/\text{K})$; temp range 353–523 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 7.67152 - 2669.4/(205.6 + t/^\circ\text{C})$; temp range 230–250°C (Antoine eq., Dean 1992)

$\log (P/\text{mmHg}) = 6.3156 - 2.6756 \times 10^3/(T/\text{K}) - 4.6215 \cdot \log (T/\text{K}) + 6.1747 \times 10^{-9} \cdot (T/\text{K}) - 2.3743 \times 10^{-12} \cdot (T/\text{K})^2$; temp range 354–518 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.60 (shake flask, Log P Database, Hansch & Leo 1987)

1.8 (shake flask-HPLC, Leggett et al. 1992)

1.73 (recommended, Sangster 1993)

2.05 (estimated-SPARC, Elovitz & Weber 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_B$:

1.09 (aquatic oligochaete *Tubifex tubifex*, Conder et al. 2004)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 14$ h in summer, $t_{1/2} = 22$ –84 h in winter in pure water and photolyzed very rapidly in natural waters (Mabey et al. 1983)

photocatalytic degradation rates of TNT in a circular photocatalytic reactor using a UV lamp as a light source and TiO_2 as a photocatalyst: 1) at different initial TNT concns: $k = 0.0989 \text{ min}^{-1}$ with $t_{1/2} = 7.07$ min at initial concn of 10 mg/L; $k = 0.0644 \text{ min}^{-1}$ with $t_{1/2} = 10.76$ min at initial concn of 20 mg/L; $k = 0.0405 \text{ min}^{-1}$ with $t_{1/2} = 17.11$ min at initial concn of 30 mg/L; $k = 0.0269 \text{ min}^{-1}$ with $t_{1/2} = 25.77$ min at initial concn of 50 mg/L; and $k = 0.0165 \text{ min}^{-1}$ with $t_{1/2} = 42.01$ min at initial concn of 100 mg/L. 2) at different pH: $k = 0.0173 \text{ min}^{-1}$ with $t_{1/2} = 27.6$ min at pH 3.0; $k = 0.0422 \text{ min}^{-1}$ with $t_{1/2} = 20.1$ min at pH 7.0 and $k = 0.0451 \text{ min}^{-1}$ with $t_{1/2} = 21.5$ min at pH 11.0 (Son et al. 2004)

Photooxidation:

Hydrolysis:

Biodegradation: 95% disappearance within 2 h under aerobic conditions, and complete loss within 10 min under anaerobic conditions in sediment-water systems (Elovitz & Weber 1999)

Biotransformation: 100 % biotransformed when incubated at both 10 and 20°C in 7 d in fine-grain sediment; in sandy sediment although some picric acid could still be measured after 28 d of incubation at 10°C, none left after 56 d of incubation at 20°C (Nipper 2004)

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air:

Surface water: photolysis $t_{1/2} = 14$ h in summer, $t_{1/2} = 22$ –84 h in water in pure water, less than 1/2 h in some natural waters (Mabey et al. 1983)

photocatalytic degradation $t_{1/2} = 7.07$ min to 42.1 min for different initial concn of TNT from 10–100 mg/L, and $t_{1/2} = 27.1$ –21.5 min at pH 3.0–7.0 in a circular reactor, using a UV lamp as a light source and TiO_2 as a photocatalyst (Son et al. 2004)

Ground water:

Sediment: rapid disappearance 95% within 2 h, of TNT in an aerobic sediment-water system; under anaerobic conditions, TNT loss was complete within 10 min (Elovitz & Weber 1999)

100 % biotransformed when incubated at both 10 and 20°C in 7 d in fine-grain sediment; in sandy sediment although some picric acid could still be measured after 28 d of incubation at 10°C, none left after 56 d of incubation at 20°C (Nipper 2004)

Soil:

Biota: steady-state concn reached within 1-h in uptake experiments, and TNT depuration after a 24-h exposure occurred completely by 3 h (aquatic oligochaete, Conder et al. 2004)

TABLE 16.1.4.6.1

Reported aqueous solubilities of 2,4,6-trinitrotoluene (TNT) at various temperatures

$$\ln S = A - B/(T/K)$$

(1)

1.

Taylor & Rinkenbach '23		Spanggord et al. 1983		Ro et al. 1996			Phelan & Barnett 2001	
shake flask				shake flask-HPLC/UV			shake flask-HPLC/UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	pH	S/g·m ⁻³	t/°C	S/g·m ⁻³
	average*							
0.30	110	10	67	6	3.7	52.5	13.9	86
5.9	113	20	104	6	6.9	51.3	23.02	115
20.0	120	30	165	12	6.9	64.0	33.3	191
33.1	203			13	3.7	72.2	42.6	266
44.2	340			13	6.9	64.4	51.8	427
45.0	370			20	4.2	86.2	61.0	641
53.0	534			20	7.3	88.5	33.2	191
57.15	614			20	9.2	96.8	13.6	90
73.25	963			20	9.4	95.7	13.6	92
94.4	1375			20	10.1	91.2		
99.5	1467			21	3.5	74.5		
				21	6.8	82.5		
				21	9.1	88.2		
				25	3.5	101.6		
				25	6.8	100.5		
				25	9	110.5		
				42	4.0	204.9		
				42	6.8	204.5		
				42	9.3	167.6		
average of 3 sets of data								
$\ln [S/(\text{mg/L})] = 16.12 - 3413/(T/K)$ <p>for pH < 8</p>								

2.

Lynch et al. 2001					
shake flask-HPLC/UV					
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
	pH 4.2		pH 5.7		pH 6.2
2.3	49.5	2.3	54.5	2.4	55.0
2.3	50.5	2.2	54.2	2.4	56.4
2.6	54.9	2.3	47.5	2.4	54.9
2.6	55.7	2.3	47.3	2.4	55.4
4.2	57.6	4.1	47.9	4.7	56.7

TABLE 16.1.4.6.1 (Continued)

Lynch et al. 2001					
shake flask-HPLC/UV					
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
4.2	57.7	4.1	48.2	4.7	57.4
4.2	45.7	4.6	58.1	5.2	56.7
4.2	48.4	4.6	59.1	5.2	56.1
20	100.7	20	96.7	20	99.6
20	99.0	20	98.7	20	100.2
20	99.2	20.1	98.9	20.1	99.5
20	101.7	20.1	100.6	20.1	96.3
20.1	96.3	20.2	98.8	20.1	99.5
20.1	95.9	20.2	99.8	20.1	99.8
20.1	96.0	20.2	97.5	20.2	94.6
20.1	97.8	20.2	100.4	20.2	97.2
36	211.7	35.7	208.5	35.9	216.5
36	213.1	35.7	213.5	35.9	213.9
36	208.5	36	215.2	36	212.2
36	211.6	36	214.3	36	215.3
37.7	219.6	37.7	229.7	37.6	229.4
37.7	219.4	37.7	230.6	37.6	231.4
37.8	218.2	37.7	226.2	38	234.4
37.8	214.8	37.7	228.3	38	235
eq. 1	S/(mg L ⁻¹)	eq. 1	S/(mg L ⁻¹)	eq. 1	S/(mg L ⁻¹)
A	22.741	A	22.399	A	23.244
B	6332	B	6230	B	6506.8

composite correlation eq. : ln [S/(mg L⁻¹) = 16981 – 3607.5/(T/K); temp range 2.3–38°C

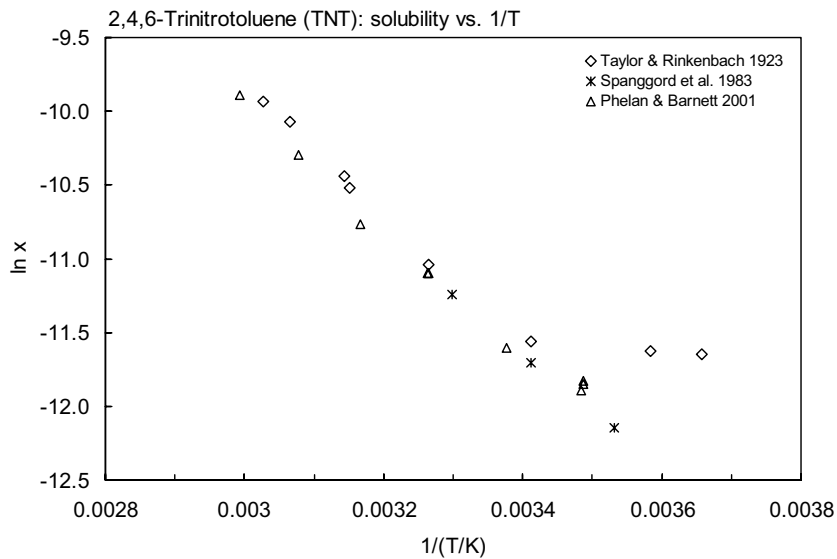


FIGURE 16.1.4.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2,4,6-trinitrotoluene.

TABLE 16.1.4.6.2

Reported vapor pressures of 2,4,6-trinitrotoluene (2,4,6-TNT) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Edwards 1950		Lenchitz & Velicky 1970		Pella 1977	
Knudsen method		Knudsen effusion		gas saturation-GC	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
53.0	0.0352	54.756	0.0568	14.0	0.000302
60.1	0.0724	59.704	0.0935	19.0	0.000412
60.8	0.0843	64.853	0.1613	25.0	0.00107
61.5	0.0915	70.02	0.3118	25.3	0.00128
61.0	0.0829	72.469	0.3665	26.5	0.00170
72.1	0.4146	72.493	0.3409	35.0	0.00676
72.1	0.4186	75.065	0.5142	40.0	0.00887
78.5	0.8586	65.91	0.1811	45.0	0.0143
78.5	0.7839	68.933	0.2342	50.0	0.0243
78.3	0.8293	73.981	0.4453	55.0	0.0446
79.8	0.8733	76.057	0.5796	56.5	0.05406
80.2	0.9546				
82.4	1.0612	mp/ $^{\circ}\text{C}$	81.1	mp/ $^{\circ}\text{C}$	80.15–81.25
86.9	1.5865				
99.5	5.2529	enthalpy of sublimation: $\Delta H_{\text{subl}} = 120.92 \text{ kJ mol}^{-1}$ (at 25 $^{\circ}\text{C}$)		eq. 2	P/mmHg
99.5	5.4262			A	12.31
110.6	11.012			B	5175
110.5	10.612				
131.5	46.396	eq. 1	P/mmHg	enthalpy of sublimation: $\Delta H_{\text{subl}} = 99.161 \text{ kJ mol}^{-1}$	
141.4	82.793	A	13.0776		
142.0	87.728	B	5400.536		
142.5	82.260				
For solid:					
eq. 1	P/cmHg				
A	14.34				
B	6180				
$\Delta H_{\text{subl}} = 118.41 \text{ kJ mol}^{-1}$					
For liquid:					
eq. 1	P/cmHg				
A	10.90				
B	4960				
$\Delta H_{\text{subl}} = 94.98.34 \text{ kJ mol}^{-1}$					

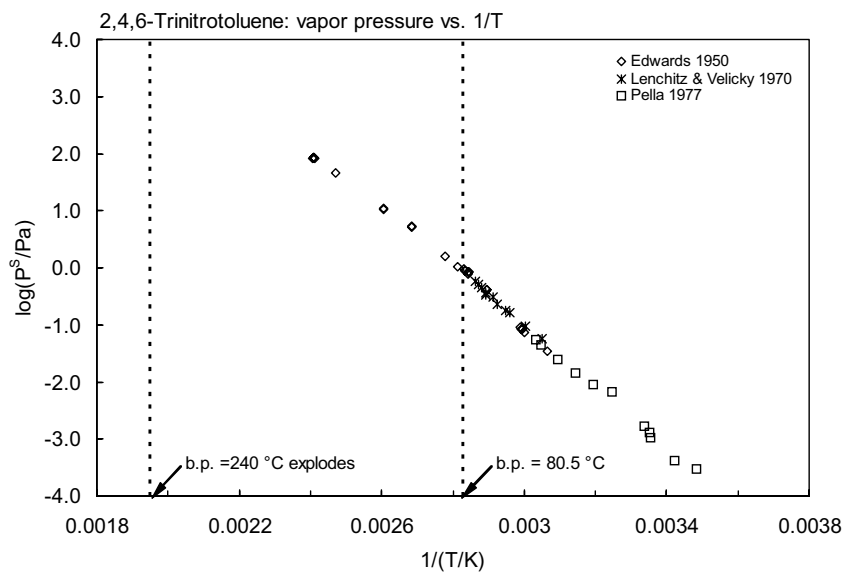
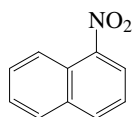


FIGURE 16.1.4.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trinitrotoluene.

16.1.4.7 1-Nitronaphthalene (α -Nitronaphthalene)

Common Name: 1-Nitronaphthalene

Synonym: α -nitronaphthalene

Chemical Name: 1-nitronaphthalene, α -nitronaphthalene

CAS Registry No: 86-57-7

Molecular Formula: $C_{10}H_7NO_2$

Molecular Weight: 173.169

Melting Point ($^{\circ}C$):

61 (Lide 2003)

Boiling Point ($^{\circ}C$):

304.0 (Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987)

Density (g/cm^3 at $20^{\circ}C$):

1.3320 (Weast 1982–83)

1.2230 (Dean 1985)

Molar Volume (cm^3/mol):

176.1 (calculated-Le Bas method at normal boiling point)

135.8 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.99 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

54.39 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F : 0.443 (mp at $61^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

50.0 (Aqueous Solubility Database, Yalkowsky et al. 1987)

9.82 (generator column-HPLC/UV, Yu & Xu 1992)

9.83 (calculated-molar concentration, Yu & Xu 1992)

50; 34.6 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.202 (effusion method-fitted to Antoine eq., Radchenko & Kitiagorodskii 1974)

0.202 (solid, extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

0.184 (liquid, extrapolated-Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.31261 - 3579.698/(T/K)$; temp range 309–326 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 13.223 - 5584/(T/K)$; temp range 325–332 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.8959 - 3468.4/(T/K)$; temp range 332–580 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

3.463 (calculated-P/C with selected values)

0.178 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.19 (Hansch & Leo 1979)

3.19 (shake flask, Hansch & Leo 1987)

- 3.19 (shake flask-UV, Debnath & Hansch 1992)
3.19 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: measured photolysis rate constant are: $15.9 \times 10^{-4} \text{ s}^{-1}$ in a 6400-L indoor all-Teflon chamber under blacklamp irradiation and $1.37 \times 10^{-4} \text{ s}^{-1}$ outdoor in a 1000-L all-Teflon chamber under natural solar irradiation (Atkinson et al. 1989);

photolysis rate $k_{\text{phot}} = 1.5 \times 10^{-4} \text{ s}^{-1}$ with a half-life of 1.7 h (Arey et al. 1990)

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (5.4 \pm 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{NO_3} \leq 7.2 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} < 6.0 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{N_2O_5} = 1.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 and at $298 \pm 2 \text{ K}$ in the atmosphere (Atkinson et al. 1989)

$k_{OH} = 5.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetime of 2.9 d; $k_{NO_3} \leq 7.2 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated lifetime of -13 d, $k_{O_3} < 6.0 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of > 28 d and $k_{N_2O_5} = 1.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with N_2O_5 a calculated lifetime of 2.4 yr at $298 \pm 2 \text{ K}$ in the atmosphere (Arey et al. 1990)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

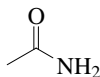
Half-Lives in the Environment:

Air: calculated lifetime of ~2 h based on measured outdoor photolysis rate and rate constants the gas-phase reactions (Atkinson et al. 1989);

photolysis $t_{1/2} = 1.7 \text{ h}$ using an average 12-h daytime NO_2 photolysis rate $k = 5.2 \times 10^{-3} \text{ s}^{-1}$ – a dominant atmospheric loss process; calculated lifetimes of 2.9 d, -13 d, > 28 d and 2.4 yr due to reactions with OH radical, NO_3 radical, O_3 and N_2O_5 (Arey et al. 1990)

16.1.5 AMIDES AND UREAS

16.1.5.1 Acetamide



Common Name: Acetamide

Synonym: ethanamide

Chemical Name: acetamide, acetic acid amine

CAS Registry No: 60-35-5

Molecular Formula: C_2H_5NO , CH_3CONH_2

Molecular Weight: 59.067

Melting Point ($^{\circ}C$):

80.16 (Lide 2003)

Boiling Point ($^{\circ}C$):

221 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):0.9986 ($78^{\circ}C$, Weast 1982–83)

1.159 (Verschueren, 1983)

Molar Volume (cm^3/mol):

59.2 (calculated-density, Stephenson & Malanowski 1987)

66.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a : 7.62Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.1 (at bp, Riddick et al. 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):78.66 ($25^{\circ}C$, Riddick et al. 1986)Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.707 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.288 (mp at $80.16^{\circ}C$)Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):975000 ($20^{\circ}C$, Verschueren 1983)408000 ($20^{\circ}C$, Riddick et al. 1986)Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):8.61 (extrapolated-regression of tabulated data, temp range 65 – $222^{\circ}C$, Stull 1947) $\log(P/mmHg) = [-0.2185 \times 14025.3/(T/K)] + 9.088352$; temp range 65.0 – $222^{\circ}C$ (Antoine eq., Weast 1972–73)

100 (Riddick et al. 1986)

 $\log(P/kPa) = 8.24516 - 3282.80/(T/K)$; temp range 65 – $150^{\circ}C$ (Antoine eq., Riddick et al. 1986) $\log(P/kPa) = 7.93409 - 2936.07/(T/K)$; temp range 65 –bp (Antoine eq., Riddick et al. 1986)

2.44 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

 $\log(P_g/kPa) = 10.9717 - 4050.1/(T/K)$; temp range 298 – $349 K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987) $\log(P_l/kPa) = 7.97079 - 1998.3/(-89.32 + T/K)$; temp range 381 – $492 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987) $\log(P/mmHg) = -413.1683 + 8.1328 \times 10^3/(T/K) + 172.9 \cdot \log(T/K) - 0.16059 \cdot (T/K) + 5.3892 \times 10^{-5} \cdot (T/K)^2$; temp range 354 – $761 K$ (vapor pressure eq., Yaws 1994)Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$): 3.53×10^{-4} (calculated-P/C with selected values)Octanol/Water Partition Coefficient, $\log K_{ow}$:

-1.09 (shake flask-radiochemical method, Cornford 1982)

- 1.26 (shake flask, Log P Database, Hansch & Leo 1987)
- 1.26 (shake flask-GC, Sotomatsu et al. 1987)
- 1.26 (recommended Sangster 1989, 1993)
- 1.23 (calculated-QSAR, Kollig 1993)
- 1.26 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.55 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 3.2\text{--}32$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Hydrolysis: overall rate constant $k_h = 5.5 \times 10^{-12} \text{ s}^{-1}$ with $t_{1/2} = 3950$ yr; acid rate constant $k_A = 8.36 \times 10^{-6} \text{ s}^{-1}$ and base rate constant $k_B = 5.5 \times 10^{-5} \text{ s}^{-1}$ at 25°C and pH 7 (Mabey & Mill 1978) acid rate constant $k = 0.03 [\text{M} \pm (\text{H}^+) \pm \text{h}]^{-1}$ at pH 5 and base rate constant $k = 0.17 [\text{M} \pm (\text{OH}^-) \pm \text{h}]^{-1}$ at pH 9 with first-order hydrolysis $t_{1/2} = 3950$ yr at pH 7 and 25°C , (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 24\text{--}168$ h, based on aerobic aqueous screening test data (Malaney & Gerhold 1962, 1969; Urano & Kato 1986; quoted, Howard et al. 1991); aqueous anaerobic biodegradation $t_{1/2} = 96\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 3.2\text{--}32$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

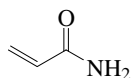
Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.5.2 Acrylamide



Common Name: Acrylamide

Synonym: 2-propenamide

Chemical Name: acrylamide

CAS Registry No: 79-06-1

Molecular Formula: C_3H_5NO , $CH_2=CHCONH_2$

Molecular Weight: 71.078

Melting Point ($^{\circ}C$):

84.5 (Lie 2003)

Boiling Point ($^{\circ}C$):

192.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.122 ($30^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

80.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.261 (mp at $84.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2050000 (quoted, Verschueren 1983)

2150000 ($30^{\circ}C$, Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.616 (average, extrapolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.395 - 3213/(T/K)$, temp range 357–413 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 10.31055 - 3994.667/(T/K)$, temp range 373–413 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 17.0034 - 4.4434 \times 10^3/(T/K) - 1.7158 \cdot \log(T/K) + 2.0063 \times 10^{-6} \cdot (T/K) - 8.0394 \times 10^{-10} \cdot (T/K)^2$; temp range 358–477 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pam^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

-0.90 (shake flask, Fujisawa & Masuhara 1980, 1981)

-1.24 (calculated-HPLC-RT correlation, Fujisawa & Masuhara 1981)

-0.67 (shake flask, Log P Database, Hansch & Leo 1987)

-0.78 (recommended, Sangster 1989)

-0.67 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

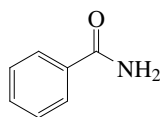
-0.969 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Surface water: measured rate constant $k = (1.0 \pm 0.1) \times 10^5 M^{-1} s^{-1}$ for direct reaction with ozone in water at pH 5.4–5.8 and $22 \pm 1^{\circ}C$, with $t_{1/2} = 0.3$ s at pH 7 (Yao & Haag 1991).

16.1.5.3 Benzamide



Common Name: Benzamide

Synonym: benzoylamide

Chemical Name: benzamide

CAS Registry No: 55-21-0

Molecular Formula: C_7H_7NO , $C_6H_5CONH_2$

Molecular Weight: 121.137

Melting Point ($^{\circ}C$):

127.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

290 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

112.2 ($130^{\circ}C$, Stephenson & Malanowski 1987)

132.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0992 (mp at $127.3^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

13500 ($20-25^{\circ}C$, shake flask-gravimetric method, Dehn 1917)

13499 (Tsonopoulos & Prausnitz 1971)

13490 (Windholz 1983)

13515 (1 g in 74 mL, Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00522 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.69847 - 5062.899/(T/K)$, temp range 325–342 K (solid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pam^3/mol at $25^{\circ}C$):

4.52×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.64 (shake flask-UV, Fujita et al. 1964)

0.65 (shake flask, Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1987)

0.66 (shake flask-UV, Yaguzhinskii et al. 1973)

0.84 (HPLC- k' correlation, Hammers et al. 1982)

0.64 (shake flask-UV, Sotomatsu et al. 1987)

0.50 (centrifugal partition chromatography CPC, Berthod et al. 1988)

0.81 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)

0.64 (recommended, Sangster 1989, 1993)

0.65 (counter-current chromatography, Vallat et al. 1990)

0.65 (CPC-RV correlation, El Tayar et al. 1991)

0.64 (shake flask-GC, Alcorn et al. 1993)

0.64 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.954; 1.301; 1.756 (sediment; Alfisol soil; Podzol soil, von Oepen et al. 1991)
- 1.46 (soil, quoted exptl., Meylan et al. 1992)
- 1.71 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 1.46 (soil, mean value, Kördel et al. 1993)
- 1.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.46; 1.71 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 1.87, 2.17, 1.12, 1.36, 1.645 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 1.46, 1.22; 2.18, 1.75, 1.88, 1.83, 1.31 (soil: quoted lit., calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)
- 1.747, 1.358, 1.236 (second generation of European reference soil set, Eurosoils ES-1, ES-3, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: aqueous photooxidation $t_{1/2} = 960 - 7.4 \times 10^4$ h, based on measured rates for reaction with OH radical in water (Anbar et al. 1966; Dorfman and Adams 1973; selected, Howard et al. 1991);
photooxidation $t_{1/2} = 3.1 - 31$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson et al. 1987; selected, Howard et al. 1991).

Hydrolysis: not expected to be significant based on estimated half-lives for hydrolysis of acetamide of 261, 3950, and 46 yr at pH 5, 7, 9, respectively, which were calculated using experimental acid and base hydrolysis rate constants for acetamide (Mabey & Mill 1978; selected, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 48 - 360$ h, and aqueous anaerobic biodegradation $t_{1/2} = 192 - 1400$ h, both based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 3.1 - 31$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson et al. 1987; selected, Howard et al. 1991).

Surface water: $t_{1/2} = 48 - 360$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

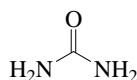
Ground water: $t_{1/2} = 96 - 720$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 48 - 360$ h, based on grab sample aerobic soil column test data (Fournier & Salle 1974; selected, Howard et al. 1991).

Biota:

16.1.5.4 Urea



Common Name: Urea

Synonym: carbamide, carbonyldiamide, Aquacare, Aqiadrate, Basodexam, Keratinamin, Nutraplus, Onychomal, Pastaron, Ureaphil, Ureophil, Ureaparl

Chemical Name: urea, carbamide, carbonyldiamide

CAS Registry No: 57-13-6

Molecular Formula: $\text{CH}_4\text{N}_2\text{O}$, H_2NCONH_2

Molecular Weight: 60.055

Melting Point ($^{\circ}\text{C}$):

133 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

decompose (Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.323 (Weast 1982–83)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

58.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol} \pm \text{K}$), F : 0.0872 (mp at 133°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

975000* (shake flask, measured range 0 – 69.5°C , Speyers 1902)

790000 (20 – 25°C , shake flask-gravimetric method, Dehn 1917)

1047000* (20°C , shake flask, measured range 0 – 70°C , Pinck & Kelly 1925)

53.97 wt %* (23.85°C , synthetic method, measured range 18.72 – 73.11°C , Shnidman & Sunier 1932)

$\log x = -609.8/(T/K) + 1.468$; temp range 20 – 70°C (synthetic method, Shnidman & Sunier 1932)

0.4388* (60°C , mole fraction solubility, synthetic method, measured range 60 – 100°C , Kakinuma 1941)

997400 (W indholz 1983)

1000000 (Dean 1985; Budavari 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

1.61×10^{-3} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 9.565 - 4579/(T/K)$; temp range 345 – 368 K (solid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pam^3/mol):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

–1.09 (Hansch & Leo 1979)

–3.00 (Kenaga & Goring 1980)

–1.21, –1.79 to –0.62 (shake flask method: mean, range of mean values, OECD 1981)

–1.54 (shake flask-radiochemical method, Cornford 1982)

–1.57 (HPLC-RT correlation, Harnish et al. 1983)

–1.56 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)

–1.66, –2.11 (shake flask, Log P Database, Hansch & Leo 1987)

–1.60 (shake flask-UV, pH 7.4, Huang 1990)

–2.11 (from Medchem software value, Chessells et al. 1992)

–2.11 (recommended, Sangster 1993)

–1.66 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 4.068 (alga *chlorella fusca*, wet wt. basis, Geyer et al. 1984)
 -0.10 (alga *chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.50, 0.62 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 0.90 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 16.1.5.4.1
Reported aqueous solubilities of urea at various temperatures

Speyers 1902		Shnidman & Sunier 1932						Kakinuma 1941	
re-calcd by Pinck & Kelly		synthetic method-heating -shake flask						synthetic method	
t/°C	S/g·m ⁻³	t/°C	wt %	x	t/°C	wt %	x	t/°C	x
		urea 1#			urea 2#				
0	674000	18.72	51.10	0.2387	21.59	52.80	0.2513	60	0.4388
11.0	875000	26.80	55.37	0.2712	23.85	53.97	0.2602	65	0.4610
19.8	975000	27.31	55.83	0.2740	30.38	57.51	0.2888	70	0.4903
31.7	1310000	35.42	59.94	0.3099	35.15	59.97	0.3102	75	0.5204
51.4	1930000	37.36	60.87	0.3183	41.11	62.95	0.3377	80	0.6617
69.5	2530000	43.94	64.19	0.3489	43.85	64.31	0.3510	85	0.5843
		46.56	65.39	0.3618	54.97	69.53	0.4065	90	0.6190
		54.77	69.33	0.4041	55.88	70.10	0.4131	95	0.6542
		67.02	70.38	0.4163	69.13	71.49	0.4294	100	0.6910
$\Delta H_{sol}/(kJ\ mol^{-1})$		61.76	72.59	0.4428	63.79	73.64	0.4561		
25°C		73.11	77.57	0.5093	70.49	76.60	0.4956	$\log x = A - B/(T/K)$	
								A	1.5314
								B	631.86
		mp/°C	132.7		mp/°C	132.6			
Pinck & Kelly 1925		mole fraction solubility expressed as:							
shake flask		$\log x = -609.8/(T/K) + 1.468$; temp range 20–70°C							
t/°C	S/g·m ⁻³								
0	670000								
10.0	840000								
20.0	1047000								
30.0	1360000								
39.7	1654000								
50.0	2050000								
50.6	2064000								
60.0	2460000								
68.5	2950000								
70.0	3146000								

urea 1# – urea made by synthetic $NH_3 + CO_2$ process—re-crystallized from water

urea 2# – urea made from calcium-cyanamid — re-crystallized from water and methanol

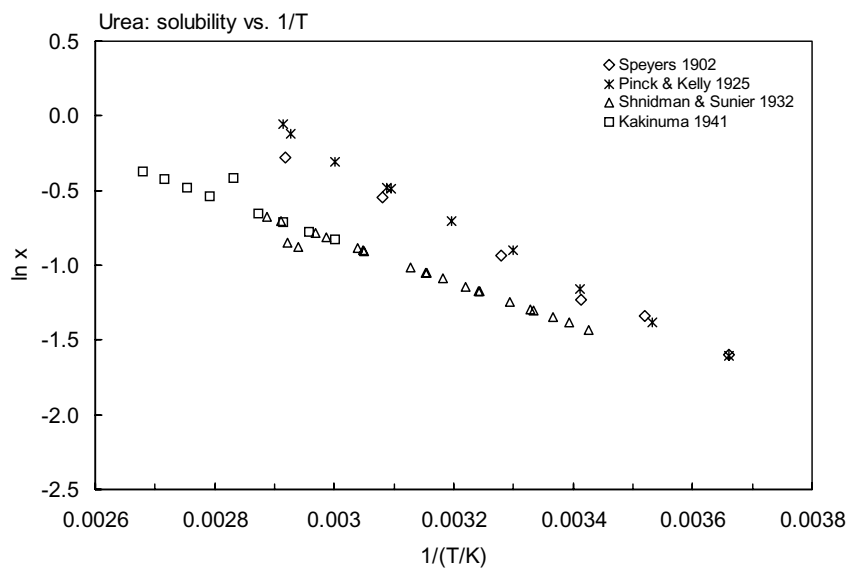


FIGURE 16.1.5.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for urea.

16.1.6 NITROSAMINES**16.1.6.1 N-Nitrosodimethylamine**

Common Name: Dimethylnitrosoamine

Synonym: *N*-nitrosodimethylamine, *N*-methyl-*N*-nitrosomethanamine, nitrous dimethylamine

Chemical Name: dimethylnitrosoamine, *N*-nitrosodimethylamine

CAS Registry No: 62-75-9

Molecular Formula: $C_2H_6N_2O$, $CH_3N(NO)CH_3$

Molecular Weight: 74.081

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

152 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.005 ($18^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

73.7 ($10^{\circ}C$, Stephenson & Malanowski 1987)

87.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

< 1.0 (Kollig 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Mirvish et al. 1976)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

1080 (Mabey et al. 1982)

730 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.10632 - 2159.476/(T/K)$, temp range 309–423 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

3.344 (calculated, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.06 (Radding et al. 1977)

−0.57 (shake flask-UV, Singer et al. 1977)

−0.68 (calculated-f const., Mabey et al. 1982)

0.46 ($30.5^{\circ}C$, shake flask-HPLC, Vera et al. 1992)

0.76 (calculated, Kollig 1993)

−0.57 (recommended, Sangster 1993)

−0.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

−0.96 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

−1.00 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

0.448 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: both aqueous and atmospheric photolysis $t_{1/2} = 0.5\text{--}1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991).

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

rate constants $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, and $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

$k_{\text{OH}} = 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{\text{O}_3} \leq 1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Tuazon et al. 1984); photooxidation $t_{1/2} = 25.4\text{--}254$ h in air, based on measured rate constant for the reaction with OH radical in air (Howard et al. 1991);

$k_{\text{OH}} = (2.53 - 3.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at 296–298 K (Atkinson 1989).

Biodegradation: aqueous aerobic $t_{1/2} = 504\text{--}4320$ h, based on aerobic soil die-away test data; and aqueous anaerobic $t_{1/2} = 2016\text{--}17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (derived from results of Tate & Alexander 1975; and Oliver et al. 1979; Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^{-12} \text{ mL} \pm \text{cell}^{-1} \pm \text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.5\text{--}1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991);

estimated photolysis $t_{1/2} \sim 5$ min, $t_{1/2} = 3$ d for reaction with OH radical and $t_{1/2} > 2$ yr for reaction with O_3 (Tuazon et al. 1984);

photooxidation $t_{1/2} = 25.4\text{--}254$ h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 0.5\text{--}1.0$ h, based on measured rate of photolysis in the vapor phase under sunlight (Hanst et al. 1977; quoted, Howard et al. 1991).

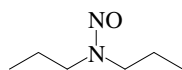
Groundwater: $t_{1/2} = 1008\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: degradation $t_{1/2} \sim 3$ wk in 4 aerobic soils (shake flask-GC, Oliver et al. 1979)

$t_{1/2} = 504\text{--}4320$ h, based on aerobic soil die-away test data (derived from data of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biota:

16.1.6.2 *N*-Nitrosodipropylamine

Common Name: Di-*n*-Propylnitrosoamine

Synonym: N-nitrosodi-*n*-propylamine, N-nitroso-N-propyl-1-propanamine

Chemical Name: di-*n*-propylnitrosoamine, N-nitrosodi-*n*-propylamine

CAS Registry No: 621-64-7

Molecular Formula: $C_6H_{14}N_2O$, $CH_3CH_2CH_2N(NO)CH_2CH_2CH_3$

Molecular Weight: 130.187

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

206 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

176.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9900 (Mirvish et al. 1976)

Vapor Pressure (Pa at $25^{\circ}C$):

53.33 ($37^{\circ}C$, calculated-Troutin's rule, Mabey et al. 1982)

Henry's Law Constant (Pam^3/mol at $25^{\circ}C$):

0.638 (calculated-P/C, Mabey et al. 1982)

0.355 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.31 (calculated as per Leo et al. 1971 from Mirvish et al. 1976 data, Callahan et al. 1979)

1.36 (shake flask-UV, Singer et al. 1977)

1.49 (calculated-f const., Mabey et al. 1982)

2.35 ($30.5^{\circ}C$, shake flask-HPLC, Vera et al. 1992)

2.45 (recommended, Sangster 1993)

1.35 (Kollig 1993)

1.36 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

0.99 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

1.18 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.09 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: both aqueous and atmospheric photolysis $t_{1/2} = 0.17$ – $1.0\ h$, based on measured rate of photolysis in the vapor phase under sunlight (Oliver 1981; quoted, Howard et al. 1991).

Hydrolysis:

Oxidation: rate constants in water for singlet oxygen $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 2.66\text{--}26.6 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 504\text{--}4320 \text{ h}$, based on aerobic soil die-away test data, and aqueous anaerobic $t_{1/2} = 2016\text{--}17280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (derived from results of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biotransformation: rate constant for bacterial biotransformation $k \sim 3 \times 10^{-12} \text{ mL} \pm \text{cell}^{-1} \pm \text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.66\text{--}26.6 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Surface water: $t_{1/2} = 0.17\text{--}1.0 \text{ h}$, based on measured rate of photolysis in the vapor phase under sunlight (Oliver 1981; quoted, Howard et al. 1991).

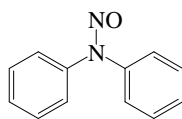
Groundwater: $t_{1/2} = 1008\text{--}8640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: degradation $t_{1/2} \sim 3 \text{ wk}$ in 4 aerobic soils (shake flask-GC, Oliver et al. 1979)

$t_{1/2} = 504\text{--}4320 \text{ h}$, based on aerobic soil die-away test data (derived from results of Tate & Alexander 1975 and Oliver et al. 1979, Howard et al. 1991).

Biota

16.1.6.3 Diphenylnitrosoamine

Common Name: Diphenylnitrosoamine

Synonym: N-nitrosodiphenylamine, N-nitroso-N-phenylbenzamine

Chemical Name: diphenylnitrosoamine, N-nitrosodiphenylamine

CAS Registry No: 86-30-6

Molecular Formula: $C_{12}H_{10}N_2O$, $C_6H_5N(NO)C_6H_5$

Molecular Weight: 198.219

Melting Point ($^{\circ}C$):

66.5 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

151–153 (Windholz 1976; Callahan et al. 1979)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

220.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.392 (mp at $66.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

35.1 (shake flask-LSC, Banerjee et al. 1980)

40.0 (calculated-S, Mabey et al. 1982)

Vapor Pressure (Pa at $25^{\circ}C$):

13.33 (estimated, Mabey et al. 1982)

Henry's Law Constant (Pam^3/mol at $25^{\circ}C$):

66.87 (calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.13 (shake flask-LSC, Banerjee et al. 1980;)

3.13 (recommended, Sangster 1993)

3.13 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.63 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

2.34 (quoted, Isnard & Lambert 1988)

Sorption Partition Coefficient, $\log K_{OC}$:

2.81 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

2.84 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constants in water for singlet oxygen $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ and for peroxy radical $k < 3600 \text{ M}^{-1} \pm \text{h}^{-1}$ at 25°C (Mabey et al. 1982);

photooxidation $t_{1/2} = 0.70 - 7.0 \text{ h}$ in air, based on measured rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 240 - 816 \text{ h}$, based on data from one soil-die-away test; a range was bracketed around the reported $t_{1/2} = 22 \text{ d}$ (Mallik & Tesfai 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 960 - 3264 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant for bacterial transformation $k = 1 \times 10^{-10} \text{ mL} \pm \text{cell}^{-1} \pm \text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.70 - 7.0 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radicals in air (quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 240 - 816 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 480 - 1632 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 240 - 816 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.1.7 HETEROCYCLIC COMPOUNDS

16.1.7.1 Pyrrole



Common Name: Pyrrole

Synonym: 1H-pyrrole

Chemical Name: pyrrole, 1H-pyrrole

CAS Registry No: 109-97-7

Molecular Formula: C_4H_4NH

Molecular Weight: 67.090

Melting Point ($^{\circ}C$):

−23.39 (Lide 2003)

Boiling Point ($^{\circ}C$):

129.79 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9691 (Weast 1982–83; Dean 1985)

0.96985, 0.96565 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

69.2 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

78.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

−4.40 (Perrin 1972)

−3.80 (Riddick et al. 1986)

−4.10 (Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.15, 38.75 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.908 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

47000 (Dean 1985)

45000 (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

358285* ($176.67^{\circ}C$, static-Bourdon gauge, measured range 176.67 – $271.11^{\circ}C$, Kobe et al. 1956)

1102* (ebulliometry, extrapolated-Antoine eq., measured range 65.67 – $166^{\circ}C$, Scott et al. 1967; Osborn & Douslin 1968)

$\log (P/mmHg) = 7.30295 - 1507.015/(t/^{\circ}C + 211.010)$; temp range 65.67 – $166^{\circ}C$ (Antoine eq., ebulliometry, Scott et al. 1967)

$\log [(P/atm) = [1 - 402.914 \pm (T/K)] \times 10^{\{0.870073 - 5.43768 \times 10^{-4} \pm (T/K) + 4.16086 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 65.67 – $166^{\circ}C$ (ebulliometric method, Cox eq., Scott et al. 1967)

$\log (P/mmHg) = 7.30275 - 1506.877/(t/^{\circ}C + 210.995)$, temp range 65.57 – $166^{\circ}C$ (ebulliometric method, Antoine eq., Scott et al. 1967; Osborn & Douslin 1968)

$\log [(P/atm) = [1 - 402.915 \pm (T/K)] \times 10^{\{0.872196 - 5.54923 \times 10^{-4} \pm (T/K) + 4.30369 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 65.57 – $166^{\circ}C$ (ebulliometric method, Cox eq., Osborn & Douslin 1968)

8386* ($60.3^{\circ}C$, isoteniscope method, measured range 60.3 – $100.3^{\circ}C$, Eon et al. 1971)

1136 (calculated-Cox eq., Chao et al. 1983)

$\log (P/atm) = [1 - 402.916/(T/K)] \times 10^{\{0.880256 - 6.05913 \times 10^{-4} \pm (T/K) + 5.02726 \times 10^{-7} \pm (T/K)^2\}}$; temp range: 250.0 – $635.0 K$ (Cox eq., Chao et al. 1983)

- 1100 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.42113 - 1502.586/(129.775 + t/^{\circ}\text{C})$; temp range 65.67–166°C (Antoine eq. from exptl. data of Scott et al. 1967, Boublik et al. 1984)
 1100 (extrapolated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 7.29470 - 1501.56/(210.42 + t/^{\circ}\text{C})$; temp range 66–166°C (Antoine eq., Dean 1985, 1992)
 1100 (quoted lit., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.42765 - 1506.877/(210.995 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 1103 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.42263 - 1504.171/(-62.39 + T/\text{K})$; temp range 338–440 K (Antoine eq., Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 54.1597 - 4.2745 \times 10^3/(T/\text{K}) - 15.873 \cdot \log(T/\text{K}) - 4.5171 \times 10^{-10} \cdot (T/\text{K}) + 4.2338 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 250–640 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 1.640 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C or as indicated

- 0.75 (shake flask-AS, Hansch & Anderson 1967; Leo et al. 1971; Hansch & Leo 1979)
 0.62 (HPLC-RV correlation, Garst 1984)
 0.82 (23°C, shake flask-HPLC, De Voogt et al. 1988)
 0.80 (23°C, TLC-RT correlation, De Voogt et al. 1990)
 0.75 (recommended, Sangster 1989, 1993)
 0.75 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = (1.22 \pm 0.04) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (relative rate method, Atkinson et al. 1984)

$k_{\text{O}_3} = 1.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate of 1.0 d^{-1} , $k_{\text{OH}} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate of 10 d^{-1} and $k_{\text{NO}_3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate of 1000 d^{-1} (review, Atkinson & Carter 1984)

$k_{\text{O}_3} = 1.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate of 1.0 d^{-1} , $k_{\text{OH}} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate of 5.2 d^{-1} and $k_{\text{NO}_3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with loss rate $k = 1000 \text{ d}^{-1}$ (review, Atkinson 1985)

$k_{\text{NO}_3} = (4.9 \pm 1.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 1 \text{ K}$ (relative rate method, Atkinson et al. 1985)

$k_{\text{O}_3} = 1.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime $\tau = 24 \text{ h}$, $k_{\text{OH}} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 2.3 \text{ h}$ during daylight hours, $k_{\text{NO}_3} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $\tau(\text{calc}) = 1.4 \text{ min}$ during nighttime hours at room temp. (Atkinson et al. 1985)

$k_{\text{OH}} = 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 5.2 d^{-1} at room temp. (Atkinson 1985)

$k_{\text{OH}}^* = (1.03 \pm 0.06) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–442 K (flash photolysis-resonance fluorescence, Wallington et al. 1988)

$k_{\text{OH}}^* = 9.31 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–442 K (flash photolysis-resonance fluorescence, Atkinson 1989)

$k_{\text{OH}} = 1.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 287.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated lifetimes of 2.3 h, 1.4 min and 24 h due to gas-phase reactions with OH radical (concn of $1 \times 10^6 \text{ cm}^{-3}$ during daylight hours), NO_3 radical (concn of $2.4 \times 10^6 \text{ cm}^{-3}$ during nighttime hours) and O_3 (clean tropospheric concn of $7.2 \times 10^{11} \text{ molecule cm}^{-3}$), respectively, at room temp. (Atkinson et al. 1985)

TABLE 16.1.7.1.1

Reported vapor pressures of pyrrole at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Kobe et al. 1956		Scott et al. 1967		Eon et al. 1971	
static-Bourdon gauge		ebulliometry		isoteniscope/manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
176.67	358285	65.671	9582	60.3	8386
182.22	399626	68.522	10884	70.3	13025
187.78	454747	71.374	12335	80.3	19732
193.33	509867	77.098	15740	90.3	29198
198.89	571878	79.970	17725	100.3	42263
204.44	647669	82.847	19920	$\Delta H_v/(\text{kJ mol}^{-1}) = 41.84$	
210.00	730351	88.622	25007		
215.56	806142	94.422	31160		
221.11	895713	100.244	38547		
226.67	992174	106.096	47359		
232.22	1081746	111.972	57803		
237.78	1185097	117.875	70109		
243.33	1309119	123.806	84525		
248.89	1440031	129.764	101325		
254.44	1564053	135.753	120798		
260.00	1715635	141.768	143268		
265.56	1867217	147.812	169052		
271.11	2032580	153.884	198530		
		159.984	232087		
		166.109	270110		
		eq. 2	P/mmHg		
		A	7.30295		
		B	1507.015		
		C	210.010		
		bp/°C	129.764		
		$\Delta H_v/(\text{kJ mol}^{-1})$	45.10		

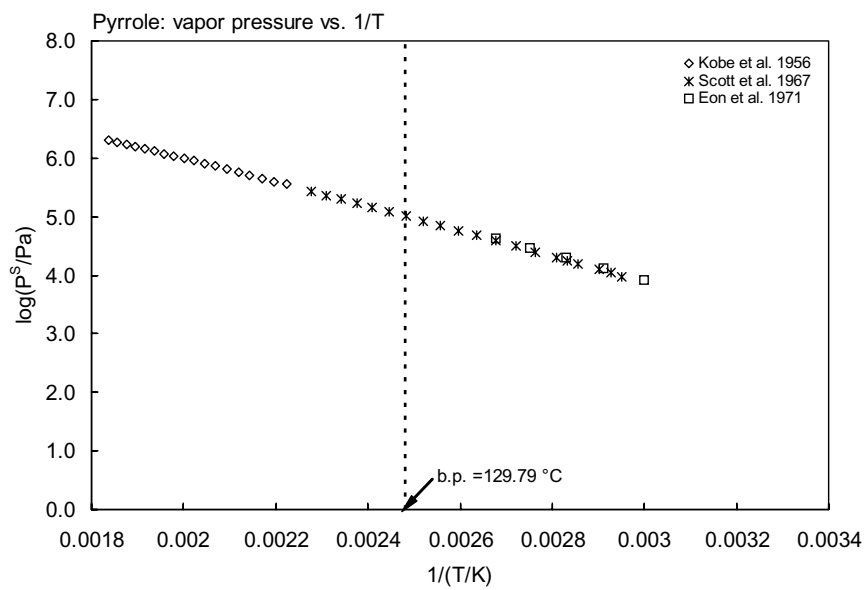
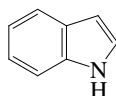


FIGURE 16.1.7.1.1 Logarithm of vapor pressure versus reciprocal temperature for pyrrole.

16.1.7.2 Indole



Common Name: Indole

Synonym: benzo[*b*]pyrrole, 1-benzo[*b*]pyrrole, 1H-indole

Chemical Name: indole

CAS Registry No: 120-72-9

Molecular Formula: C₈H₇N

Molecular Weight: 117.149

Melting Point (°C):

52.5 (Weast 1982–83; Lide 2003)

Boiling Point (°C):

254.0 (Weast 1982–83; Stephenson & Malanowski 1987)

253.6 (Lide 2003)

Density (g/cm³ at 20°C):

1.2200 (Weast 1982–83)

1.0643 (Dean 1985)

Molar Volume (cm³/mol):

133.4 (calculated-Le Bas method at boiling point)

Dissociation Constant, pK_a:

–3.5, –3.62 (Perrin 1972)

–3.17 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} J/mol K:

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.537 (mp at 52.5°C)

Water Solubility (g/m³ or mg/L at 25°C):

3558 (shake flask-GC, Price 1976)

1874 (Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

2.24 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.369 – 1933.005/(254.707 + t/°C); temp range 193.3–254.7°C (Antoine eq., Boublik et al. 1984)

1.565 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P_s/kPa) = 10.3289 – 3916/(T/K); temp range 291–319 K, (solid, Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 94.1625 – 6.9431 × 10³/(T/K) – 30.613 · log (T/K) + 9.928 × 10^{–3} · (T/K) + 1.7461 × 10^{–13} · (T/K)²; temp range 274–790 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pam³/mol at 25°C):

0.14 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, log K_{ow}:

1.14 ± 0.01 (shake flask-UV, Iwasa et al. 1965)

2.14 (shake flask-UV, Hansch & Anderson 1967)

2.25 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)

2.00 (unpublished result, Leo et al. 1971)

2.00, 2.25, 2.13 (Hansch & Leo 1979)

1.66 (RP-HPLC-RT correlation, Veith et al. 1979a)

2.17 (RP-HPLC-RT correlation, Hanai & Hubert 1982)

2.14 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)

1.92	(inter-laboratory studies, HPLC average, Eadsforth & Moser 1983)
2.16 ± 0.03	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
1.81	(HPLC-k' correlation, Eadsforth 1986)
2.16	(HPLC-RT correlation, Minick et al. 1988)
2.14	(recommended, Sangster 1989; 1993)
2.27	(23°C, shake flask-HPLC, De Voogt et al. 1988, 1990)
2.07	(HPLC-RT correlation, De Voogt et al. 1990)
2.19	(HPLC-RT correlation, Ritter et al. 1994)
2.14	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

16.1.7.3 Pyridine



Common Name: Pyridine

Synonym:

Chemical Name: pyridine

CAS Registry No: 110-86-1

Molecular Formula: C_5H_5N

Molecular Weight: 79.101

Melting Point ($^{\circ}C$):

−41.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

115.23 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9819 (Weast 1982–83)

Molar Volume (cm^3/mol):

80.6 (calculated-density, Rohrschneider 1973)

93.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK :

5.23 (pK_a , Leo et al. 1971; Jori et al. 1983; Zachara et al. 1987)

5.198, 5.21, 5.22, 5.229 (Perrin 1972)

5.54 (UV, Yeh & Higuchi 1976)

5.23, 5.16 (quoted, shake flask-TN, Clarke 1984)

5.17 (pK_{BH^+} , Dean 1985; Riddick et al. 1986)

5.21 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.41, 36.39 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.414 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Andon & Cox 1952; Andon et al. 1954; Jori et al. 1983; Riddick et al. 1986)

miscible (Dean 1985; Zachara et al. 1987; Stephenson 1993a)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2666* ($24.8^{\circ}C$, summary of literature data, temp range -18.9 to $115.4^{\circ}C$, Stull 1947)

2520 (interpolated-regression of tabulated data, Stull 1947)

620, 2109 (0 , $20^{\circ}C$, static method-tensimeter, Brown & Barbaras 1947)

2775* (ebulliometry, measured range 47.3 – $115.5^{\circ}C$, extrapolated-Antoine eq., Herington & Martin 1953)

$\log (P/mmHg) = 7.05811 - 1384.991/(216.296 + t/^{\circ}C)$; temp range 47.3 – $115.5^{\circ}C$ (Antoine eq., ebulliometric measurements, Herington & Martin 1953)

2774* (gas saturation, measured range 20 – $40^{\circ}C$, Andon et al. 1954)

461637* ($176.67^{\circ}C$, static-Bourdon gauge, measured range 176.67 – $343.33^{\circ}C$, Kobe et al. 1956)

19920* ($67.299^{\circ}C$, comparative ebulliometry, measured range 67.299 – $152.886^{\circ}C$, McCullough et al. 1957)

$\log (P/mmHg) = 7.04162 - 1374.103/(215.014 + t/^{\circ}C)$; temp range 67.3 – $152.9^{\circ}C$ (Antoine eq. ebulliometry, McCullough et al. 1957)

2763* (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

- log (P/mmHg) = $7.04144 - 1373.990/(t/^{\circ}\text{C} + 215.001)$; temp range 67.3–152.9°C (ebulliometric method, Antoine eq., Osborn & Douslin 1968)
- log [(P/atm) = $[1 - 399.384 \pm (T/K)] \times 10^{\{0.856586 - 6.60597 \times 10^{-4} \pm (T/K) + 5.93625 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 67.3–152.9°C (ebulliometric method, Cox eq., Osborn & Douslin 1968)
- 2789 (calculated-Antoine eq., Cabani et al. 1971)
- log (P/mmHg) = $[-0.2185 \times 9649.4/(T/K)] + 8.347670$; temp range –18.9 to 115.4°C (Antoine eq., Weast 1972–73)
- 2767 (calculated-Cox eq., Chao et al. 1983)
- log (P/atm) = $[1 - 388.399/(T/K)] \times 10^{\{0.848882 - 6.09810 \times 10^{-4} \pm (T/K) + 5.15399 \times 10^{-7} \pm (T/K)^2\}}$; temp range: 235.0–620.0 K (Cox eq., Chao et al. 1983)
- 2775, 2763 (extrapolated-Antoine equations, Boublik et al. 1984)
- log (P/kPa) = $6.18358 - 1385.39/(115.256 + t/^{\circ}\text{C})$; temp range 47.3–115.47°C (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)
- log (P/kPa) = $6.16609 - 1373.826/(115.235 + t/^{\circ}\text{C})$; temp range 67.3–152.9°C (Antoine eq. from reported exptl. data of McCullough et al. 1957, Boublik et al. 1984)
- 2763 (extrapolated-Antoine eq., Dean 1985, 1992)
- log (P/mmHg) = $7.04115 - 1373.80/(214.98 + t/^{\circ}\text{C})$; temp range 67–153°C (Antoine eq., Dean 1985, 1992)
- 2773 (Howard et al. 1986; quoted, Banerjee et al. 1990)
- 2700 (selected, Riddick et al. 1986)
- log (P/kPa) = $6.18595 - 1386.683/(216.469 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
- 2770 (interpolated-Antoine eq. II, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.17372 - 1379.953/(-57.436 + T/K)$; temp range 323–426 K (Antoine eq. I, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.30308 - 1448.781/(-50.948 + T/K)$; temp range 296–353 K (Antoine eq. II, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.16446 - 1373.263/(-58.18 + T/K)$; temp range 348–434 K (Antoine eq. III, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $6.284 - 1455.584/(-48.272 + T/K)$; temp range 431–558 K (Antoine eq. IV, Stephenson & Malanowski 1987)
- log (P_L/kPa) = $7.25663 - 2578.625/(115.604 + T/K)$; temp range 552–620 K (Antoine eq. V, Stephenson & Malanowski 1987)
- 2773, 1653 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
- 2573* (24.82°C, ebulliometry, measured range 23.55–116.23°C, Lencka 1990)
- ln (P/kPa) = $14.1480 - 3132.3/[(T/K) - 59.179]$; temp range 295.7–388.4 K (ebulliometric measurements, Antoine eq., Lencka 1990)
- log (P/mmHg) = $33.5541 - 3.1318 \times 10^3/(T/K) - 8.8646 \cdot \log (T/K) + 7.1293 \times 10^{-12} \cdot (T/K) + 2.2813 \times 10^{-6} \cdot (T/K)^2$; temp range 232–620 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 0.895 (volatility ratio-transpiration method, Andon et al. 1954)
- 0.900 (exptl., Hine & Mookerjee 1975)
- 0.595, 0.766 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 1.114 (modified gas-stripping, Hawthorne et al. 1985)
- 1.120 (computed, Yaws et al. 1991)
- 0.305 (calculated-molecular structure, Russell et al. 1992)
- 27.78 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
- log K_{AW} = $-1.508 - 128/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

- 0.65 (shake flask-UV, Iwasa et al. 1965)
- 0.64 (Gehring et al. 1967)
- 0.65, 0.64 (Leo et al. 1971; Hansch & Leo 1979)
- 0.66 (HPLC-RT correlation, Mirrlees et al. 1976)
- 0.63 ± 0.02 (shake flask at pH 7, Unger et al. 1978)
- 0.63 (shake flask-titration, Clarke 1984; Clarke & Cahoon 1987)

0.63 ± 0.06	(HPLC-RV correlation-ALPM, Garst & Wilson 1984)
0.62	(shake flask-UV at pH 7.4, El Tayar et al. 1984)
0.63	(shake flask-potentiometric titration, Clarke 1984)
0.54	(calculated- activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
1.28	(HPLC- k' correlation, Eadsforth 1986)
0.79	(calculated- γ from UNIFAC, Banerjee & Howard 1988)
0.70	(shake flask-CPC, Berthod et al. 1988)
0.63	(shake flask-HPLC at pH 7, De Voogt et al. 1988, 1990)
0.65	(recommended, Sangster 1989, 1993)
0.70	(RP-TLC-RT correlation, De Voogt et al. 1990)
0.65	(shake flask-UV, Yamagami et al. 1990)
0.60	(pH 7.2, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

-1.805	(estimated of Anvil Points subsurface materials, Zachara et al. 1987)
-2.541	(estimated of Loring subsurface materials, Zachara et al. 1987)
0.340	(calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , Half-Lives, $t_{1/2}$

Volatilization:

Photolysis:

Oxidation: rate constant k ; for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated *data at other temperatures see reference:

photooxidation $t_{1/2} = 14.7\text{--}24.4$ yr in water, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991)

$k_{OH} = (4.9 \pm 0.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes of 46 d in clean troposphere and 23 d in moderately polluted atmosphere; $k_{O_3} < 1.1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with atmospheric lifetimes of > 4 yr in clean troposphere and > 1.3 yr in moderately polluted atmosphere at room temp. (relative rate method, Atkinson et al. 1987)

$k_{OH} = (0.494 - 0.256) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296–297 K (review, Atkinson 1989)

$k_{OH}(\text{calc}) = 0.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated grab sample of aerobic soil (Sims & Sommers 1985; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 168\text{--}672$ h, based on anaerobic acclimated screening test data (Naik et al. 1972; selected, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetimes of 46 d in clean troposphere and 23 d in moderately polluted atmosphere, based on the gas-phase reaction with hydroxyl radical in air at room temp. and > 4 yr in clean troposphere and > 1.3 yr in moderately polluted atmosphere, based on the gas-phase reaction with O_3 (calculated rate constant) in air at room temp. (Atkinson et al. 1987);

photooxidation $t_{1/2} = 128\text{--}1284$ h, based on measured rate data for the reaction with hydroxyl radical in air (selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 14.7\text{--}24.4$ yr, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991);

$t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: disappears in less than 7 d in soil suspensions (Sims & O'Loughlin 1989);

$t_{1/2} = 24\text{--}168$ h, based on unacclimated grab sample of aerobic soil (Sims & Sommers 1985; selected, Howard et al. 1991).

Biota:

TABLE 16.1.7.3.1

Reported vapor pressures of pyridine at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \\ \log P = A[1 - B/(T/K)] & (5) & \text{where } \log A = a - b(T/K) + c(T/K)^2 & \end{array}$$

1.

Stull 1947		Herington & Martin 1953		Andon et al. 1954		Kobe et al. 1956	
summary of literature data		ebulliometry		gas saturation		static-Bourdon gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−18.9	133.3	47.327	8506	20	2109	176.67	461637
2.50	666.6	52.71	10820	25	2774	182.22	502988
13.2	1333	58.349	13806	40	6013	187.78	564988
24.8	2666	68.403	20805			193.33	633889
38.0	5333	75.77	27592			198.89	702790
46.8	7999	82.43	35246			204.44	778581
57.8	13332	82.728	35597			210.00	868153
75.0	26664	88.459	43472			215.56	950834
95.6	53329	92.749	50279			221.11	1047295
115.4	101325	100.994	65759			226.67	1157537
		105.356	75351			232.22	1267778
mp/°C	−42	107.169	79679			237.78	1378020
		110.028	86860			243.33	1495152
		113.222	95488			248.89	1632954
		113.232	95536			254.44	1763866
		113.374	95905			260.00	1908558
		114.015	97713			265.56	2067030
		114.699	99692			271.11	2232392
		115.112	100914			276.67	2397755
		115.287	101402			282.22	2590678
		115.407	101758			287.78	2790491
		115.473	101977			293.33	2997194
						298.89	3183226
		bp/°C	115.256			304.44	3438160
		$\Delta H_v/(\text{kJ mol}^{-1}) = 36.39$				310.00	3672423
		Antoine eq.				315.56	3941137
		eq. 2	P/mmHg			321.11	4216741
		A	7.05811			326.67	4478565
		B	1384.991			332.22	4774839
		C	216.296			337.78	5084894
						343.33	5429399

(Continued)

TABLE 16.1.7.3.1 (Continued)

2.

McCullough et al. 1957		Osborn & Douslin 1968		Lencka 1990	
comparative ebulliometry		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
67.299	19920	67.299	19920	23.55	2394
75.154	25007	73.154	25007	24.82	2573
79.045	31160	79.054	31160	27.0	2902
84.847	38547	84.974	38547	29.26	3290
90.946	47359	90.946	47359	31.63	3720
96.958	57803	96.958	57803	35.86	4626
103.008	70109	103.008	70109	41.0	6035
109.101	84525	109.101	84525	48.51	8525
115.234	101325	115.234	101325	54.17	10999
121.408	120789	121.408	120798	60.65	14321
127.622	143268	127.622	143268	69.25	20650
133.878	169052	133.878	169053	76.97	27794
140.174	198530	140.174	198517	83.45	35213
146.509	232067	146.509	232088	88.70	42359
152.886	270110	152.886	270111	91.76	47951
				96.68	55423
mp/°C	115.23	Antoine eq		100.01	61720
Antoine eq		eq. 2	P/mmHg	102.18	66148
eq. 2	P/mmHg	A	7.04144	106.03	74603
A	7.04162	B	1373.990	112.70	91299
B	1374.103	C	215.001	116.23	101277
C	215.014				
		data also fitted to Cox eq.		eq. 3	cP/kPa
data also fitted to Cox eq.				A	14.1480
eq. 5	P/atm			B	3132.30
A				C	59.719
a	0.858631				
10 ⁻⁴ b	6.7114				
10 ⁻⁷ c	6.0722				
B	388.394				

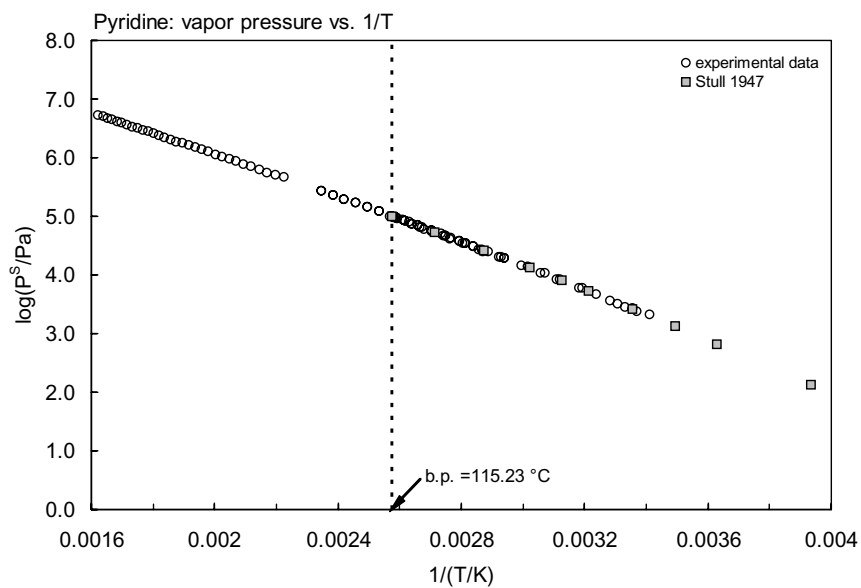


FIGURE 16.1.7.3.1 Logarithm of vapor pressure versus reciprocal temperature for pyridine.

16.1.7.4 2-Methylpyridine



Common Name: 2-Methylpyridine

Synonym: α -picoline, 2-picoline

Chemical Name: 2-methylpyridine, α -picoline

CAS Registry No: 109-06-8

Molecular Formula: $C_5H_4NCH_3$

Molecular Weight: 93.127

Melting Point ($^{\circ}C$):

−66.68 (Lide 2003)

Boiling Point ($^{\circ}C$):

129.38 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9443 (Weast 1982–83)

0.9444, 0.93981 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

98.6 ($20^{\circ}C$, calculated-density)

115.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK :

5.957, 6.06 (Perrin 1972)

5.97 (pK_a , $20^{\circ}C$, Weast 1982–83)

6.00 (pK_{BH^+} , Riddick et al. 1986; quoted, Howard 1990)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

42.919, 36.271 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.724 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 1.0)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Andon & Cox 1952)

miscible (Riddick et al. 1986; Yaws et al. 1990)

miscible (Stephenson 1993a)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1370* (interpolated-regression of tabulated data, temp range -11.0 to $128.8^{\circ}C$, Stull 1947)

308, 1140 (0 , $20.3^{\circ}C$, static method-tensimeter, Brown & Barbaras 1947)

1277 (manometry, calculated-Antoine eq., Hopke & Sears 1951)

1496* (ebulliometry, extrapolated-Antoine eq., measured range 64.3 – $130^{\circ}C$, Herington & Martin 1953)

$\log (P/mmHg) = 7.03450 - 1417.578/(211.874 + t/^{\circ}C)$; temp range 64.3 – $130^{\circ}C$ (ebulliometric measurements, Antoine eq., Herington & Martin 1953)

1496 (calculated-Antoine eq., Andon et al. 1954)

19920* ($79.794^{\circ}C$, comparative ebulliometry, measured range 79.8 – $168^{\circ}C$, Scott et al. 1963a)

$\log (P/mmHg) = 7.03202 - 1415.494/(t/^{\circ}C + 211.589)$; temp range 79.8 – $168^{\circ}C$ (ebulliometric measurements, Antoine eq., Scott et al. 1963a)

1493 (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

$\log (P/mmHg) = 7.03192 - 1415.424/(t/^{\circ}C + 211.589)$; temp range 79.8 – $168^{\circ}C$ (ebulliometric measurements, Antoine eq., Osborn & Douslin 1968)

$\log [(P/atm) = [1 - 402.536 \pm (T/K)] \times 10^{\{0.866637 - 6.80114 \times 10^{-4} \pm (T/K) + 6.00534 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 79.8 – $168^{\circ}C$ (ebulliometric method, Cox eq., Osborn & Douslin 1968)

$\log (P/\text{mmHg}) = [-0.2185 \times 9933.2/(T/K)] + 8.290910$; temp range -11.0 to 128.8°C (Antoine eq., Weast 1972–73)

1500 (calculated-Cox eq., Chao et al. 1983)

$\log (P/\text{atm}) = [1 - 402.320/(T/K)] \times 10^4 \{0.887914 - 7.70705 \times 10^{-4} \pm (T/K) + 6.85261 \times 10^{-7} \pm (T/K)^2\}$; temp range: 215.0 – 620.0 K (Cox eq., Chao et al. 1983)

1067 (20°C , Verschuereen 1983)

1494, 1498 (extrapolated-Antoine equations, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.16509 - 1421.237/(212.286 + t/^\circ\text{C})$; temp range 64.363 – 130.04°C (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.15718 - 1415.663/(211.617 + t/^\circ\text{C})$; temp range 79.79 – 168.36°C (Antoine eq. from reported exptl. data of Scott et al. 1963, Boublik et al. 1984)

1494 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.0324 - 1415.73/(211.63 + t/^\circ\text{C})$, temp range: 80 – 168°C (Antoine eq., Dean 1985, 1992)

1333 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.15940 - 1417.578/(211.874 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

1386 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.2309 - 1164.1/(-71.0 + T/K)$; temp range 209 – 245 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.1558 - 1415.29/(-61.521 + T/K)$; temp range 352 – 442 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15522 - 1414.906/(-61.566 + T/K)$; temp range 352 – 442 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.32356 - 1546.248/(-44.271 + T/K)$, temp range: 429 – 537 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.32144 - 2667.496/(107.978 + T/K)$; temp range 521 – 621 K (Antoine eq.-V, Stephenson & Malanowski 1987)

1500* (ebulliometry, interpolated-Antoine eq., measured range 295.7 – 388.4 K, Ľencka 1990)

$\ln (P/\text{kPa}) = 14.1560 - 3249.15/[T(K) - 61.863]$; temp range 295.7 – 388.4 K (ebulliometric measurements, Antoine eq., Ľencka 1990)

$\log (P/\text{mmHg}) = 34.3728 - 3.2825 \times 10^3/(T/K) - 9.0927 \cdot \log (T/K) - 3.6324 \times 10^{-10} \cdot (T/K) + 2.1425 \times 10^{-6} \cdot (T/K)^2$; temp range 206 – 621 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

1.010 (measured volatility ratio-transpiration method, Andon et al. 1954)

1.010 (exptl., Hine & Mookerjee 1975)

0.821, 0.749 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

2.90 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

30.22 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = -0.700 - 354/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.52 (HPLC-RT correlation, Schultz & Moulton 1985)

1.11 (shake flask, Log P Database, Hansch & Leo 1987)

1.11 (shake flask-UV, Yamagami et al. 1990)

1.11 (recommended, Sangster 1989; 1993)

1.11 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.602 (calculated- K_{OW} , Lyman et al. 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 88$ h for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Howard 1990).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 11.2$ d in air, based on the gas-phase reaction with photochemically produced hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1990).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 11.2$ d, based on the gas-phase reaction with photochemically produced hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1990).

Surface water: estimated $t_{1/2} = 1.0$ d for methylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 16.1.7.4.1

Reported vapor pressures of 2-methylpyridine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Stull 1947	Herington & Martin 1953		Scott et al. 1963(a)	Lencka 1990			
summary of literature data	ebulliometry		comparative ebulliometry	ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-11.1	133.3	64.363	10660	79.794	19920	18.49	1015
12.6	666.6	69.916	13459	85.853	25007	22.09	1264
24.4	1333	76.836	17758	91.942	31160	24.58	1463
37.4	2666	82.362	21954	98.074	38547	26.74	1657
51.2	5333	88.566	27600	104.252	47359	30.60	2062
59.9	7999	93.617	33044	110.472	57803	33.71	2446
71.4	13332	101.283	42906	116.736	70109	40.03	3414
89.0	26664	108.594	54434	123.038	84525	48.69	5258
108.4	53329	114.552	65581	129.387	101325	57.60	7942
128.8	101325	117.647	72020	135.773	120798	71.51	14375
		122.132	82297	142.207	143268	80.35	20380
mp/°C	-70.0	126.992	91140	148.683	169052	87.31	26426
		125.664	94663	155.201	198530	94.31	33920
		127.828	96885	161.761	232087	101.18	42854
		128.591	99021	168.356	270110	104.03	47076
		129.290	100985			109.24	55653
		129.608	101879	bp/°C	129.39	113.01	62604
		130.037	103095	Antoine eq.		115.31	67182

TABLE 16.1.7.4.1 (Continued)

Stull 1947		Herington & Martin 1953		Scott et al. 1963(a)		Lencka 1990	
summary of literature data		ebulliometry		comparative ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		bp/°C	129.408	eq. 2	P/mmHg	119.20	75535
		$\Delta H_v/(\text{kJ mol}^{-1}) = 37.76$		A	7.03202	122.93	84296
		eq. 2	P/mmHg	B	1415.494	125.77	92024
		A	7.03450	C	211.598	129.88	102813
		B	1417.578			Antoine eq.	
		C	211.874			eq. 3	P/kPa
						A	14.1560
						B	3249.15
						C	61.383

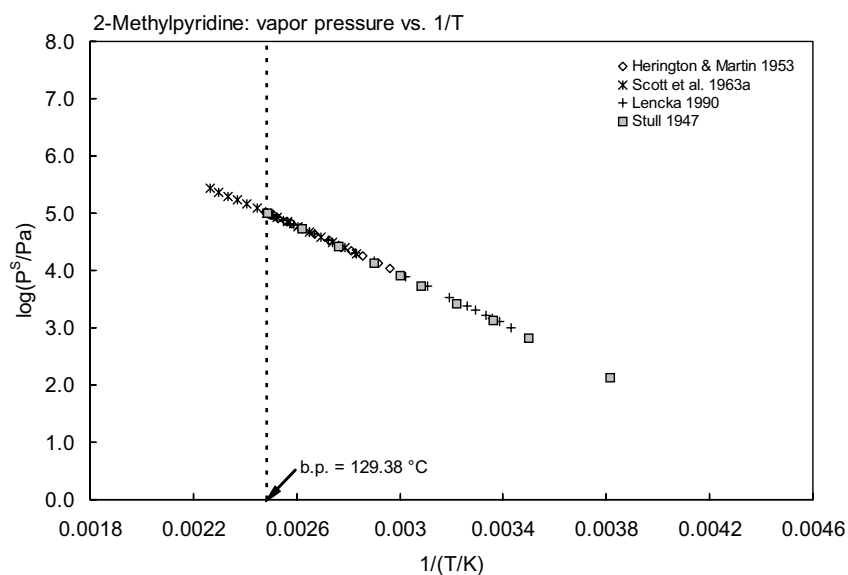


FIGURE 16.1.7.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpyridine.

16.1.7.5 3-Methylpyridine



Common Name: 3-Methylpyridine

Synonym: β -picoline, 3-picoline

Chemical Name: 3-methylpyridine, β -picoline

CAS Registry No: 108-99-6

Molecular Formula: $C_5H_4NCH_3$

Molecular Weight: 93.127

Melting Point ($^{\circ}C$):

-18.14 (Lide 2003)

Boiling Point ($^{\circ}C$):

144.14 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9443 (Weast 1982-83)

0.9566 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

97.35 ($20^{\circ}C$, calculated-density)

115.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:

5.67, 5.703 (Perrin 1972)

5.68 (pK_a , $20^{\circ}C$, Weast 1982-83; pK_a , protonated cation + 1, Dean 1985)

5.75 (pK_{BH^+} , Riddick et al. 1986)

5.65 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.233, 37.323 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.18 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Andon & Cox 1952; Andon et al. 1954; Yaws et al. 1990)

miscible (Riddick et al. 1986; Howard 1993)

miscible (Stephenson 1993a)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

150.7, 594.6 (0, $20^{\circ}C$, static method-tensimeter, Brown & Barbaras 1947)

794* (ebulliometry, extrapolated-Antoine eq., Herington & Martin 1953)

$\log (P/mmHg) = 7.03247 - 1469.894/(209.907 + t/^{\circ}C)$; temp range 81.2 – $145.1^{\circ}C$ (ebulliometric measurements, Antoine eq., Herington & Martin 1953)

794 (calculated-Antoine eq., Andon et al. 1954)

9582* ($74.036^{\circ}C$, comparative ebulliometry, measured range 74.036 – $184.568^{\circ}C$, Scott et al. 1963b)

$\log (P/mmHg) = 7.05375 - 1484.208/(t/^{\circ}C + 211.532)$, temp range 79.8 – $168^{\circ}C$ (ebulliometric measurements, Antoine eq., Scott et al. 1963b)

811 (ebulliometry, calculated-Antoine eq., Osborn & Douslin 1968)

$\log (P/mmHg) = 7.30275 - 1506.877/(t/^{\circ}C + 210.995)$, temp range: 74 – $185^{\circ}C$, (ebulliometric measurements, Antoine eq., Osborn & Douslin 1968)

$\log [(P/atm) = [1 - 417.287 \pm (T/K)] \times 10^{\{0.854256 - 6.02835 \times 10^{-4} \pm (T/K) + 5.00169 \times 10^{-7} \pm (T/K)^2\}}$, temp range: 74 – $185^{\circ}C$ (ebulliometric method, Cox eq., Osborn & Douslin 1968)

806 (calculated-Cox eq., Chao et al. 1983)

$\log (P/\text{atm}) = [1 - 417.217/(T/K)] \times 10^4 \{0.865977 - 6.48542 \times 10^{-4} \pm (T/K) + 5.41256 \times 10^{-7} \pm (T/K)^2\}$; temp range: 255.0–645.0 K (Cox eq., Chao et al. 1983)
 796, 800 (extrapolated-Antoine equations, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.16152 - 1472.639/(210.214 + t/^{\circ}\text{C})$; temp range 81.3–145.1 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data of Herington & Martin 1953, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.17577 - 1482.229/(211.305 + t/^{\circ}\text{C})$; temp range 74.03–184.6 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data of Scott et al. 1963, Boublik et al. 1984)
 800 (extrapolated-Antoine eq., Dean 1985, 1992)
 $\log (P/\text{mmHg}) = 7.05021 - 1481.78/(211.25 + t/^{\circ}\text{C})$; temp range 74–185 $^{\circ}\text{C}$ (Antoine eq., Dean 1985, 1992)
 1333 (Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.15737 - 1469.894/(209.907 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 802 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.245 - 3246.9/(T/K)$; temp range 225–255 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.17593 - 1482.943/(-61.705 + T/K)$; temp range 347–458 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.17791 - 1484.285/(-61.554 + T/K)$; temp range 347–458 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.18988 - 1491.897/(-60.745 + T/K)$; temp range 347–381 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.16648 - 1476.25/(-62.502 + T/K)$; temp range 374–458 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.38586 - 1659.184/(-38.176 + T/K)$; temp range 450–570 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.57549 - 3151.52/(161.352 + T/K)$; temp range 561–645 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 35.2679 - 3.4364 \times 10^3/(T/K) - 9.3555 \cdot \log (T/K) - 1.3286 \times 10^{-10} \cdot (T/K) + 2.0461 \times 10^{-6} \cdot (T/K)^2$; temp range 255–645 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$ or as indicated):

0.788 (volatility ratio-transpiration method, Andon et al. 1954)
 0.784; 0.637; 0.749 (exptl.; calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
 1.836 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 12.69 (20 $^{\circ}\text{C}$, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = -0.826 - 348/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.20 (HPLC-RT correlation, Mirrlees et al. 1976)
 1.20 \pm 0.02 (shake flask at pH 7, Unger et al. 1978)
 1.19 (HPLC-RT correlation, Lewis et al. 1983)
 1.18 \pm 0.01 (HPLC-RV correlation-ALPM, Garst 1984; Garst & Wilson 1984)
 1.20 (shake flask, Log P Database, Hansch & Leo 1985, 1987)
 1.20 (recommended, Sangster 1989, 1993)
 1.20 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.699 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.029 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: estimated photooxidation rate constant $k = 1.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radicals/ cm^3 in air at 25 $^{\circ}\text{C}$ which corresponds to an atmospheric half-life of 11 d (Atkinson 1987; quoted, Howard 1993).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} = 11$ d from estimated photooxidation rate constant $k = 1.43 \times 10^{-12} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radicals/cm³ in air at 25°C (Atkinson 1987; quoted, Howard 1993).

Surface water: estimated $t_{1/2} = 1.0$ d for methylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.7.5.1

Reported vapor pressures of 3-methylpyridine at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^\circ\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^\circ\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Herington & Martin 1953**Scott et al. 1963(b)****ebulliometry****comparative ebulliometry**

$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
81.282	12871	74.036	9582
85.275	15061	77.115	10884
92.059	19478	80.202	12335
97.519	23773	85.303	13949
103.922	29747	86.403	15740
109.006	35349	89.524	17725
115.583	43796	92.658	19920
121.932	53445	98.946	25007
129.368	66822	105.270	31160
132.163	72471	111.640	38547
137.714	84938	118.052	47359
140.871	92693	124.508	57803
142.132	95948	131.008	70109
142.639	97265	137.551	84525
143.293	99017	144.135	101325
143.577	99782	150.767	120798
143.993	100927	157.441	143268
144.320	101791	164.156	169052
144.659	102725	170.918	198530
145.101	103988	177.821	232087
		184.568	270110
bp/ $^\circ\text{C}$	144.143		
$\Delta H_v/(\text{kJ mol}^{-1}) = 37.76$		bp/ $^\circ\text{C}$	144.14
eq. 2	P/mmHg		
A	7.03247	Antoine	
B	1469.894	eq. 2	P/mmHg
C	209.907	A	7.05375
		B	1484.208
		C	211.532

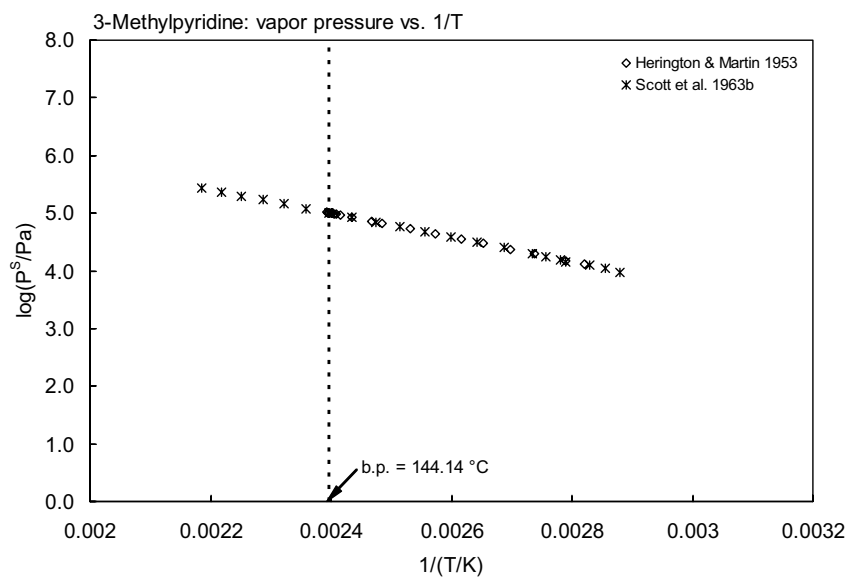


FIGURE 16.1.7.5.1 Logarithm of vapor pressure versus reciprocal temperature for 3-methylpyridine.

16.1.7.6 2,3-Dimethylpyridine



Common Name: 2,3-Dimethylpyridine

Synonym: 2,3-lutidine

Chemical Name: 2,3-dimethylpyridine, 2,3-lutidine

CAS Registry No: 583-61-9

Molecular Formula: C_7H_9N , $C_5H_3N(CH_3)_2$

Molecular Weight: 107.153

Melting Point ($^{\circ}C$):

-15.5 (Stephenson & Malanowski 1987)

Boiling Point ($^{\circ}C$):

161.12 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9461, 0.9421 ($20^{\circ}C$, $25^{\circ}C$, Coulson et al. 1959)

0.9319 ($25^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

115.0 (calculated-density, Stephenson & Malanowski 1987)

135.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:

6.70 ($20^{\circ}C$, Perrin 1972)

6.57 (pK_a , Weast 1982–83)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

104000* ($20^{\circ}C$, shake flask-GC, measured range 16 – $90^{\circ}C$, Stephenson 1993a)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

366.6, 922.6, 7119 (25 , 40 , $81.2^{\circ}C$, calculated-empirical method with bp and Antoine eq., Andon et al. 1954)

346.4* (ebulliometry, extrapolated-Antoine eq., measured range 99.5 – $162.4^{\circ}C$, Coulson et al. 1959)

$\log(P/mmHg) = 7.05075 - 1528.935/(205.499 + t/^{\circ}C)$; temp range 99.5 – $162.4^{\circ}C$ (Antoine eq., ebulliometry, Coulson et al. 1959)

359.0 (calculated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 434.216/(T/K)] \times 10^{0.881714 - 6.74484 \times 10^{-4} \pm (T/K) + 5.55055 \times 10^{-7} \pm (T/K)^2}$; temp range: 260.0 – 655.0 K (Cox eq., Chao et al. 1983)

425.5 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.45509 - 1739.902/(229.887 + t/^{\circ}C)$; temp range 155.3 – $162.4^{\circ}C$ (Antoine eq. from reported exptl. data of Coulson et al. 1959, Boublik et al. 1984)

352.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.18881 - 1538.772/(-66.477 + T/K)$; temp range; 372 – 476 K (Antoine eq., Stephenson & Malanowski 1987)

457 (extrapolated-Antoine eq., Dean 1992)

$\log(P/mmHg) = 7.447 - 1832.6/(240.1 + t/^{\circ}C)$; temp range 155 – $162^{\circ}C$ (Antoine eq., Dean. 1992)

2000* ($54.556^{\circ}C$, comparative ebulliometry, measured range 327.706 – 475.952 K, data fitted to Wagner eq., Steele et al. 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.725 (volatility ratio-transpiration method, Andon et al. 1954)

0.732 (exptl., Hine & Mookerjee 1975)

0.859, 0.732 (calculated.-group contribution, bond contribution, Hine & Mookerjee 1975)
 21.01 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 0.039 - 617/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 13.0$ d for dimethylpyridine in Rhine River in case of a first order reduction process (Zoeteman et al. 1980)

TABLE 16.1.7.6.1
Reported aqueous solubilities and vapor pressures of 2,3-dimethylpyridine at various temperatures

Aqueous solubility		Vapor pressure					
Stephenson 1993a		Coulson et al. 1959		Steele et al. 1995			
shake flask-GC/TC		ebulliometry		comparative ebulliometry			
t/°C	S/g·m ⁻³	t/°C	P/Pa	T/K	P/Pa		
16.0	171500	99.543	14583	327.706	2000		
18.0	121500	107.822	19765	333.396	2666		
20.0	104000	116.337	26607	341.852	3999.9		
25.0	86000	122.909	33113	348.166	5333		
30.0	69100	128.606	39759	357.560	7998.9		
35.0	59900	133.429	46191	364.611	10666		
40.0	53700	137.704	52572	370.315	13332		
50.0	48200	141.757	59255	376.239	16665		
60.0	43700	145.829	66652	381.163	19933		
70.0	43000	148.764	72421	387.649	25023		
80.0	43300	152.203	79677	387.646	25023		
90.0	43500	155.326	86769	394.176	31177		
		157.94	93067	400.749	38565		
		158.603	94703	407.364	47375		
		159.141	96085	414.025	57817		
		160.125	98614	420.729	70120		
		160.668	100030	427.477	84533		
		161.199	101438	434.270	101325		
		161.682	102701	441.106	120790		
		162.077	103788	447.989	143250		
		162.412	104696	454.913	169020		
				461.885	198490		
		mp/°C	−15.22	468.897	232020		
		bp/°C	161.157	475.982	270020		
ΔH _v = 41.07 kJ/mol							
Antoine eq.				Data fitted to Wagner eq.			
log P = A − B/(C + t/°C)							
		P/mmHg					
		A					
		7.05075					
		B					
		1528.935					
		C					
		205.499					

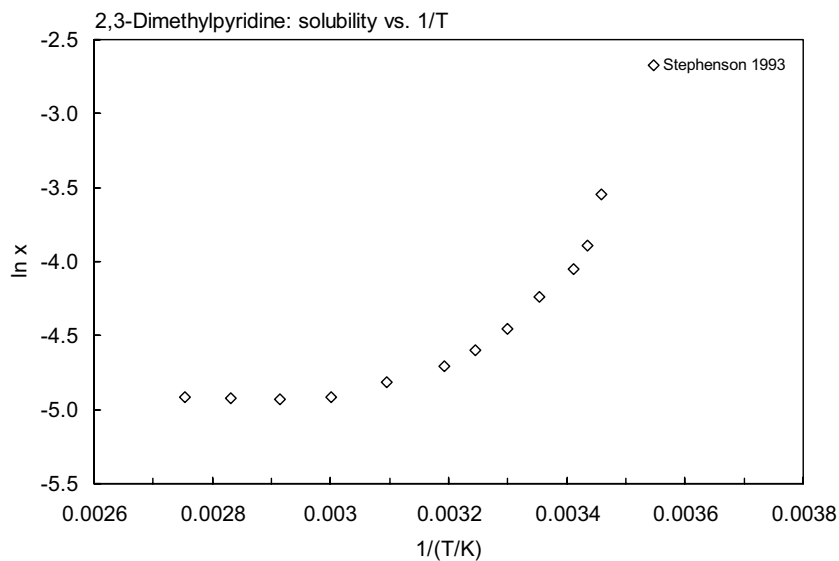


FIGURE 16.1.7.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,3-dimethylpyridine.

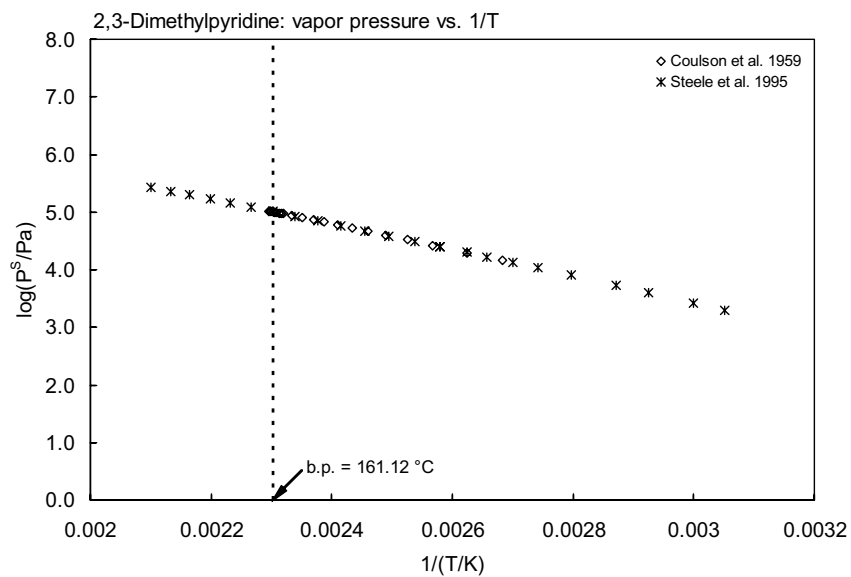
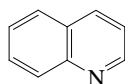


FIGURE 16.1.7.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylpyridine.

16.1.7.7 Quinoline



Common Name: Quinoline

Synonym: benzo[b]-pyridine, 1-benzazine

Chemical Name: quinoline

CAS Registry No: 91-22-5

Molecular Formula: C_9H_7N

Molecular Weight: 129.159

Melting Point (°C):

−14.78 (Lide 2003)

Boiling Point (°C):

237.16 (Lide 2003)

Density (g/cm^3 at 20°C):

1.0929 (Weast 1982–83)

1.09771, 1.08579 (15, 30°C, Riddick et al. 1986)

Molar Volume (cm^3/mol):

118.1 (calculated-density, Rohrschneider 1973)

144.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:

4.90 (pK_a , 20°C, Weast 1982–83; Zachara et al. 1987; Matzner et al. 1991)

4.80 (pK_a , protonated cation + 1, Dean 1985)

4.94 (pK_{BH^+} , Riddick et al. 1986)

4.87 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.71 (at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.79 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6110 (Albersmeyer 1958)

6840 (shake flask-HPLC/UV, Fu & Luthy 1985, 1986)

6386* (20.35°C, equilibrium cell-GC, measured range 20.35–225°C, Leet et al. 1987)

5426 (centrifuge-HPLC at pH 7 and pH 8, Matzner et al. 1991)

8400, 6600 (20°C, 30°C, shake flask-GC, Stephenson 1993a)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

15.51* (extrapolated-regression of tabulated data, temp range 59.7–237.7°C, Stull 1947)

1.213 (extrapolated, Maczynski & Maczynska 1965)

11.20* (25.16°C, gas saturation-IR, measured range 12.62–35.9°C, Van De Rostyne & Prausnitz 1980)

$\ln(P/mmHg) = 20.96 - 6993.2/(T/K)$; temp range 12.62–35.9°C (gas saturation-IR, Van De Rostyne & Prausnitz 1980)

11.14 (calculated-bp, Mackay et al. 1982)

12.83 (calculated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 510.552/(T/K)] \times 10^4 \{0.897177 - 6.73559 \times 10^{-4} \pm (T/K) + 4.69070 \times 10^{-7} \pm (T/K)^2\}$; temp range: 290.0–780.0 K (Cox eq., Chao et al. 1983)

11.04 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 5.94201 - 1668.355/(186.212 + t/^{\circ}\text{C})$, temp range 164.7–237.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

11.05 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.81759 - 1668.73/(186.26 + t/^{\circ}\text{C})$, temp range 164–238°C (Antoine eq., Dean 1985, 1992)

1.216 (recommended, Neely & Blau 1985)

12.8 (Howard et al. 1986)

11.2 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 5.92679 - 1656.30/(184.78 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

42120* (472.85 K, vapor-liquid equilibrium, measured range 472.85–548.05 K, Klara et al. 1987)

$\log (P/\text{kPa}) = 14.4961 - 4390.0/(65.19 + T/\text{K})$; temp range 472.85–548.05 K (vapor-liquid equilibrium, Klara et al. 1987)

$\log (P_L/\text{kPa}) = 5.92679 - 1656.3/(-88.37 + T/\text{K})$; temp range 433–511 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.15102 - 2846.253/(41.795 + T/\text{K})$; temp range 463–794 K (Antoine eq.-II, Stephenson & Malanowski 1987)

6.145 (calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 76.5432 - 5.7748 \times 10^3/(T/\text{K}) - 24.619 \cdot \log (T/\text{K}) + 8.4666 \times 10^{-3} \cdot (T/\text{K}) + 3.5586 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 258–782 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.0253 (calculated-P/C, Smith & Bomberger 1980)

0.026 (calculated-P/C, Mackay 1985)

0.168 (calculated-P/C, Meylan & Howard 1991)

0.0697 (estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.03 (shake flask-UV, Iwasa et al. 1965)

2.06 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)

2.03 (Schultz et al. 1970)

2.04 (HPLC-RT correlation, Mirrlees et al. 1976)

2.04 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

2.02 (Hansch & Leo 1979)

2.01 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)

1.88 (HPLC- k' correlation, Haky & Young 1984)

2.20 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

2.10 (shake flask-HPLC, De Voogt et al. 1988, 1990)

2.09 (28°C, shake flask-UV at pH 7.4, Go & Ngiam 1988)

2.03 (recommended, Sangster 1989, 1993)

2.10, 2.15 (HPLC-RT correlation, shake flask-electrometric titration, Slater et al. 1994)

2.03 (recommended, Hansch et al. 1995)

2.17 ± 0.66, 2.33 ± 0.56 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

1.91 (microemulsion electrokinetic chromatography-retention factor correlation, Jia et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.04 (Coyote Creek sediment with organic content of 1.9%, Smith et al. 1978)

1.96, 2.10, 1.67, 1.72 (estimated- K_{ow} , Karickhoff 1985)

1.42, 1.62 (estimated-S, Karickhoff 1985)

2.20 (best estimate, Karickhoff 1985)

0.251 (estimated Anvil Points subsurface materials, Zachara et al. 1987)

−1.516 (estimated Loring subsurface materials, Zachara et al. 1987)

2.89; 3.05 (humic acid, HPLC- k' correlation; quoted lit., Nielsen et al. 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 7000$ h in stream, $t_{1/2} = 35000$ h in eutrophic pond and $t_{1/2} = 28000$ h in eutrophic lake and oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978).

Photolysis:

$k = 7.8 \times 10^{-7} \text{ s}^{-1}$, assuming exposed to 12-h sunlight per day in June, photolysis $t_{1/2} = 1200$ h in stream, $t_{1/2} = 3000$ h in eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978)

$k(\text{aq.}) = 3.6 \times 10^{-7} \text{ s}^{-1}$ for summer with $t_{1/2} = 535$ h and $k = 5.0 \times 10^{-8} \text{ s}^{-1}$ for winter with $t_{1/2} = 3851$ h both at pH 6.9 and under sunlight at 40°N (Mill et al. 1981; quoted, Howard et al. 1991)

photolytic $t_{1/2} = 550$ h in aquatics (Haque et al. 1980)

$t_{1/2} = 5\text{--}12$ d for disappearance via direct photolysis in aqueous media (Harris 1982)

Oxidation:

$k = 2.8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical with $t_{1/2} > 10^4$ h in stream, eutrophic pond and lake and oligotrophic lake, based on RO_2 concentration of 10^{-9} M on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978)

$k(\text{aq.}) = 3.5 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 548$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N ; $k(\text{aq.}) = 2.8 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 8$ yr for free-radical oxidation in air-saturated water (NRCC 1983) photooxidation $t_{1/2} = 10\text{--}99$ h in air, based on an estimated rate constant for vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991)

first-order photodegradation $k = 8.0 \times 10^{-6} \text{ s}^{-1}$ at 313 nm of in organic-free water with $t_{1/2} = 24.0$ h and $k = 8.4 \times 10^{-6} \text{ s}^{-1}$ in lake water with $t_{1/2} = 23$ h both saturated with air (Kochany & Maguire 1994)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

$t_{1/2} = 0.5$ h in stream, eutrophic lake and pond and $t_{1/2} = 10000$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

Biodegradation $k = 7.4 \times 10^{-5} \text{ mL cell}^{-1} \text{ d}^{-1}$ in enrichment culture (Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 72\text{--}240$ h, based on an acclimated fresh water grab sample data (Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 288\text{--}960$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 10\text{--}99$ h, based on an estimated rate constant for vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: half-life for all processes, except for dilution: $t_{1/2} = 0.5$ h in stream, eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

half-life for all processes, including for dilution: $t_{1/2} = 0.28$ h in stream, $t_{1/2} = 0.5$ h in eutrophic lake and pond and $t_{1/2} = 600$ h in oligotrophic lake, based on transformation and transport of quinoline predicted by the one-compartment model (Smith et al. 1978);

$t_{1/2} = 5\text{--}12$ d for direct photolysis in aqueous media (Harris 1982);

$t_{1/2} = 72\text{--}240$ h, based on an acclimated fresh water grab sample data (Rogers et al. 1984; quoted, Howard et al. 1991);

degrade readily in sunlight in near surface lake water at 40°N latitude in summer with a $t_{1/2} \sim 14$ calendar-d while its $t_{1/2}(\text{calc}) \sim 123$ calendar-d in winter (Kochany & Maguire 1994).

Groundwater: $t_{1/2} = 144\text{--}480$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 72\text{--}240$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Complete mineralization within 7–10 d in batch experiments independent of pH (5.8 and 7.2) (Thomsen et al. 1999)

Biota:

TABLE 16.1.7.7.1

Reported aqueous solubilities and vapor pressures of quinoline at various temperatures and the coefficients for the vapor pressure equations:

Vapor pressure				Aqueous solubility			
Stull 1947		Van De Rostyne & Prausnitz		Klara et al. 1987		Leet et al. 1987	
summary of literate data		gas saturation-IR (1980)		vapor-liquid equilibrium		equilibrium cell-GC	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	S/g·m ⁻³
59.7	133.3	12.62	3.853	472.85	42120	20.35	6386
89.6	666.6	16.71	5.963	504.95	90990	40.05	6458
103.8	1333	21.35	8.159	514.35	112400	64.85	8252
119.8	2666	22.42	9.56	534.35	170300	80.25	10620
136.7	5333	25.16	11.20	548.05	222600	100.05	13920
148.1	7999	28.25	14.80			120.65	20163
163.2	13332	29.10	14.93	eq. 3	P/kPa	145.85	31285
186.2	26664	35.90	24.26	log P = A – B/(C + T/K)		159.65	43555
212.3	53329			A	14.4961	179.85	69602
237.7	101325	eq. 1a	P/mmHg	B	4390.0	199.25	126288
		ln P = A – B/(T/K)		C	65.19	209.05	171494
mp/°C	–15.0	A	20.96			220.25	324333
		B	6993.2			225.05	498697

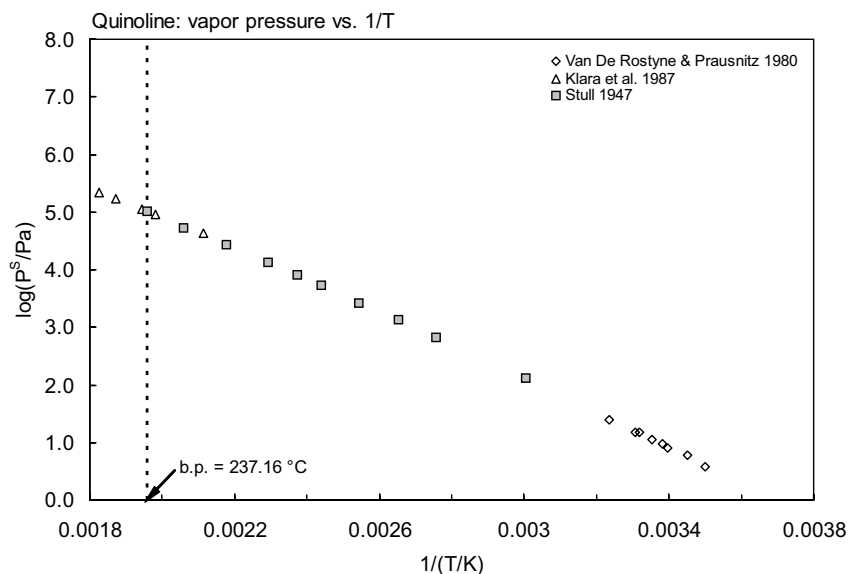
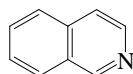


FIGURE 16.1.7.7.1 Logarithm of vapor pressure versus reciprocal temperature for quinoline.

16.1.7.8 Isoquinoline



Common Name: Isoquinoline

Synonym: leucoline

Chemical Name: isoquinoline

CAS Registry No: 119-65-3

Molecular Formula: C_9H_7N

Molecular Weight: 129.159

Melting Point ($^{\circ}C$):

26.47 (Lide 2003)

Boiling Point ($^{\circ}C$):

243.22 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0986 (Weast 1982–83)

1.0910 (Dean 1985)

Molar Volume (cm^3/mol):

118.4 ($30^{\circ}C$, Stephenson & Malanowski 1987)

144.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK :

5.40 (pK_a , Perrin 1972)

5.42 (pK_a , $20^{\circ}C$, Weast 1982–83)

5.40 (pK_a , protonated cation + 1, Dean 1985)

5.38 (pK_{BH}^{+} , Riddick et al. 1986)

5.39 (pK_a , Sangster 1989)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

48.96 (bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.448 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F : 0.967 (mp at $26.47^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4520 (Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11.8* (extrapolated-regression of tabulated data, temp range 63.5 – $240.5^{\circ}C$, Stull 1947)

7.80 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 516.182/(T/K)] \times 10^4 \{0.91210 - 6.33889 \times 10^{-4} \pm (T/K) + 4.267359 \times 10^{-7} \pm (T/K)^2\}$; temp range: 300.0 – $800.0\ K$ (Cox eq., Chao et al. 1983)

6.33 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.03709 - 1723.459/(184.268 + t/^{\circ}C)$; temp range 166 – $244^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6.35 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 6.9122 - 1723.4/(184.3 + t/^{\circ}C)$; temp range 167 – $244^{\circ}C$ (Antoine eq., Dean 1992)

6.70 (Riddick et al. 1986)

$\log(P_L/kPa) = 6.03203 - 1719.5/(-89.12 + T/K)$; temp range 439 – $517\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 45.5737 - 4.4715 \times 10^3/(T/K) - 13.308 \cdot \log(T/K) + 4.0186 \times 10^{-3} \cdot (T/K) - 6.4589 \times 10^{-14} \cdot (T/K)^2$; temp range 299 – $803\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

19.14 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.08 (shake flask-UV, Hansch & Anderson 1967)

2.09 (HPLC-RT correlation, Mirrlees et al. 1976)

2.08 (recommended, Sangster 1989, 1993)

2.30 ± 0.15 , 2.17 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)

2.08 (recommended, Hansch et al. 1995)

2.21 ± 0.66 , 2.26 ± 0.56 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.09 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 82.0 \text{ h}^{-1}$, $k_2 = 34.2 \text{ h}^{-1}$ (*daphnia pulex*, 21°C , Southworth et al. 1978)

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 1 \text{ min}$ (*daphnia pulex*, Southworth et al. 1978).

TABLE 16.1.7.8.1
Reported vapor pressures of isoquinoline at
various temperatures

Stull 1947

summary of literature data

$t/^\circ\text{C}$	P/Pa
63.5	133.3
92.7	666.6
107.8	1333
123.7	2666
141.6	5333
152.0	7999
167.6	13332
190.0	26664
214.5	53329
240.5	101325
mp/ $^\circ\text{C}$	24.5

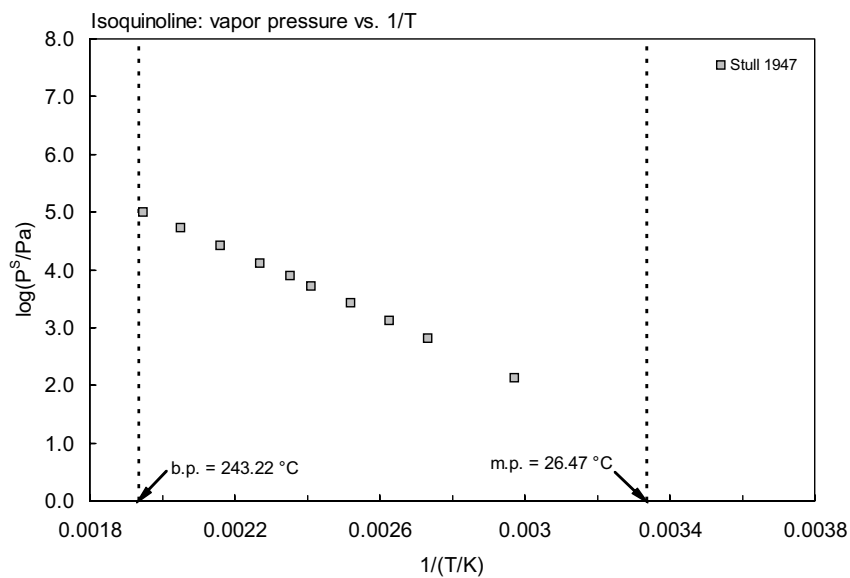
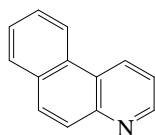


FIGURE 16.1.7.8.1 Logarithm of vapor pressure versus reciprocal temperature for isoquinoline.

16.1.7.9 Benzo[f]quinoline



Common Name: Benzo[f]quinoline

Synonym: 5,6-benzoquinoline, naphthopyridine

Chemical Name: 5,6-benzoquinoline, benzo(f)quinoline

CAS Registry No: 85-02-9

Molecular Formula: $C_{13}H_9N$

Molecular Weight: 179.217

Melting Point ($^{\circ}C$):

94 (Lide 2003)

Boiling Point ($^{\circ}C$):

352 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

196.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK:

5.15 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.210 (mp at $94^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

76.1 (shake flask-GC, Smith et al. 1978)

77.1 (Mill et al. 1981)

176.0 (Steen & Karickhoff 1981)

78.7 (average literature value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00747* ($25.05^{\circ}C$, gas saturation, measured range 288.26–323.15 K, McEachern et al. 1975)

$\log (P/mmHg) = 4339.977/(T/K) + 10.2555$; temp range 288.26–323.15 K (Antoine eq., gas saturation, McEachern et al. 1975)

0.00670 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 9.37682 - 4338.411/(T/K)$; temp range 288–323 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0096 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.20 (Steen & Karickhoff 1981)

3.40 (TLC-RT correlation, De Voogt et al. 1988)

3.25 ($23^{\circ}C$, shake flask-HPLC, pH 7, De Voogt et al. 1990)

3.25, 3.40 (lit. values; Sangster 1993)

3.46 ± 0.64 , 3.51 ± 0.53 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.18 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.11 (Coyote Creek sediment, Smith et al. 1978)
 4.64, 4.32 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 4.07 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} > 10000$ h in river, $t_{1/2} > 100000$ h in eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis:

$k = (1.4 \pm 0.7) \times 10^{-4} \text{ s}^{-1}$ for transformation and transport when exposed to 12 h sunlight in mid-June with estimated $t_{1/2} = 2.8$ h in river, $t_{1/2} = 7.0$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 1.4$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978)

photolytic $t_{1/2} = 0.52$ h in aquatics (Haque et al. 1980)

$t_{1/2} = 1$ h for disappearance via direct photolysis in aqueous media (Harris 1982)

Oxidation:

laboratory studied $k < 2.8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with the RO_2 radicals and estimated $t_{1/2} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

$k(\text{aq.}) = 3.7 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 0.5$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N ; $k(\text{aq.}) < 2.8 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} > 8$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated $t_{1/2} = 190$ h in river, eutrophic pond, eutrophic lake and $t_{1/2} > 10^6$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: $t_{1/2} = 0.5$ h in river water, $t_{1/2} = 6.9$ h in pond water, $t_{1/2} = 7.0$ h in eutrophic lake and $t_{1/2} = 1.4$ h in oligotrophic lake predicted by one-compartment for all processes including dilution (Smith et al. 1978)
 $t_{1/2} = 1$ h for disappearance via direct photolysis in aqueous media (Harris 1982).

TABLE 16.1.7.9.1
Reported vapor pressures of benzo[f]quinoline at various temperatures

McEachern et al. 1975

gas saturation	
T/K	P/Pa
288.26	0.00213
293.10	0.00333
298.20	0.00747
303.13	0.0116
308.23	0.0199
313.17	0.0324
318.24	0.0560
323.15	0.0901
P/mmHg	
$\log P = A - B/(T/K)$	
A	10.2555
B	4399.977
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 83.094$	
$\Delta S_{\text{subl}}/(\text{J mol}^{-1} \text{ K}^{-1}) = 196.36$	

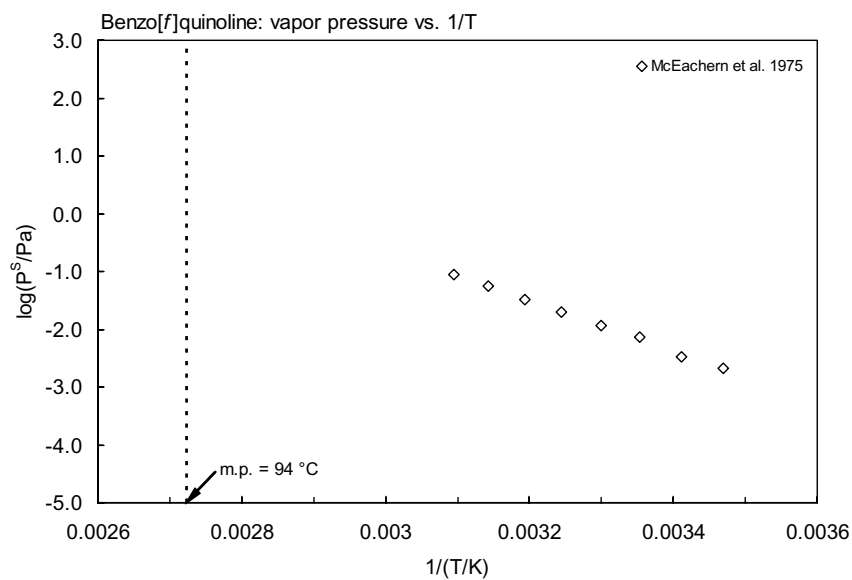
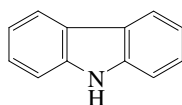


FIGURE 16.1.7.9.1 Logarithm of vapor pressure versus reciprocal temperature for benzo[f]quinoline.

16.1.7.10 Carbazole



Common Name: Carbazole

Synonym: 9H-carbazole, dibenzopyrrole

Chemical Name: carbazole

CAS Registry No: 86-74-8

Molecular Formula: $C_{12}H_9N$, $C_6H_4NHC_6H_4$

Molecular Weight: 167.206

Melting Point ($^{\circ}C$):

246.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

354.69 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.260 ($25^{\circ}C$, Jiménez et al. 1990)

Molar Volume (cm^3/mol):

192.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.00674 (mp at $246.3^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.03 ± 0.05 ($20^{\circ}C$, shake flask-GC, Smith et al. 1978)

1.037 (Mill et al. 1981)

0.428 ($20^{\circ}C$, shake flask-fluorophotometry, Hashimoto et al. 1982)

1.67, 1.03, 0.908; 1.204 (quoted values; lit. average, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7999* ($248.2^{\circ}C$, summary of literature data, temp range: 248.2 – $354.8^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 15421.6/(T/K)] + 8.251923$; temp range: 248.2 – $354.8^{\circ}C$ (Antoine eq., Weast 1972–73)

0.0933 ($20^{\circ}C$, Smith et al. 1978)

$\log(P/atm) = [1 - 627.897/(T/K)] \times 10^{[0.924810 - 5.18974 \times 10^{-4} \pm (T/K) + 2.68415 \times 10^{-7} \pm (T/K)^2]}$; temp range: 518.0 – 631.0 K (Cox eq., Chao et al. 1983)

0.00424 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.20101 - 2169.73/(162.465 + t/^{\circ}C)$; temp range 252.6 – $357.3^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 7.0863 - 2179.4/(163.5 + t/^{\circ}C)$; temp range 253 – $368^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.0012 (Antoine eq.-I, Stephenson & Malanowski 1987)

0.0045 (liquid, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.1069 - 4780/(T/K)$; temp range not specified (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.21123 - 2179.424/(-109.636 + T/K)$; temp range 525 – 631 K (liquid, Antoine eq.-II., Stephenson & Malanowski 1987)

0.0002* (extrapolated-Antoine eq., Knudsen effusion, measured range 73.43 – $90.80^{\circ}C$, Jiménez et al. 1990)

$\log(P/Pa) = 14.64 - 5288.4/(T/K)$; temp range 73.43 – $90.80^{\circ}C$ (Knudsen effusion, Jiménez et al. 1990)

$\log(P/mmHg) = -119.857 - 3.2537 \times 10^3/(T/K) + 52.568 \cdot \log(T/K) - 4.6797 \times 10^{-2} \cdot (T/K) + 1.4113 \times 10^{-5} \cdot (T/K)^2$; temp range 518 – 899 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

16.0 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.29 (shake flask-UV at pH 7.4, Rogers 1969)
 3.01 (HPLC- k' correlation, Eadsforth 1986)
 3.50 (calculated, Eadsforth 1986)
 3.72 (recommended, Sangster 1989, 1993)
 3.59 (HPLC-RT correlation, Jenke et al. 1990)
 3.84 (shake flask-HPLC at pH 7, De Voogt et al. 1988)
 3.47 ± 0.63 , 3.22 ± 0.53 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)
 3.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.24 (Coyote Creek sediment, Smith et al. 1978)
 4.74 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)
 3.80 (soil-pore water partition coeff., Askov soil - a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis:

$k = 6.6 \times 10^{-5} \text{ s}^{-1}$ for transformation and transport when exposed to midday sunlight in late January with estimated $t_{1/2} = 6.0$ h in river, $t_{1/2} = 15.0$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 3.0$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978)

photolytic $t_{1/2} = 1.0$ h in aquatics (Haque et al. 1980)

$t_{1/2} = 3$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

Oxidation:

laboratory investigated $k = 29 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radicals and estimated $t_{1/2} > 240$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)

$k(\text{aq.}) = 1.9 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 1.0$ h under natural sunlight conditions for midday, midsummer at a latitude of 40°N ; $k(\text{aq.}) = 29 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 280$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated half-lives of 14 h in river, eutrophic pond, eutrophic lake and $> 10^3$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated $t_{1/2} = 6.0$ h in river, $t_{1/2} = 15.0$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 3.0$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978);

photolytic $t_{1/2} = 1.0$ h in aquatics (Haque et al. 1980); $t_{1/2} = 3$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

TABLE 16.1.7.10.1

Reported vapor pressures of carbazole at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

Stull 1947		Jiménez et al. 1990	
summary of literature data		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
248.2	7999	73.43	0.0610
265.0	13332	78.72	0.101
292.5	26664	81.0	0.129
323.0	53329	83.59	0.167
354.8	101325	86.67	0.219
		87.13	0.227
mp/°C	244.8	90.80	0.329
		ρ (at 25°C)	1.26 g/cm ³
		eq. 1	P/Pa
		A	14.04
		B	5288.4
		enthalpy of sublimation:	
		$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 103.3$	
		at 25°C	

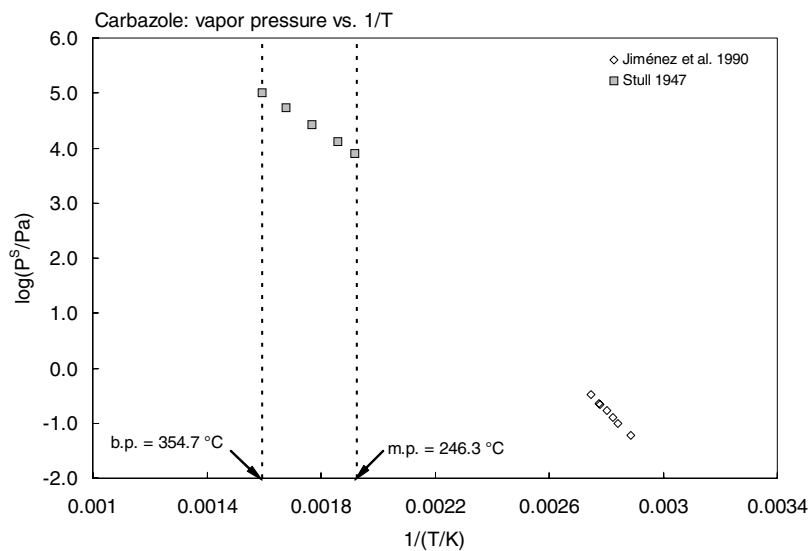
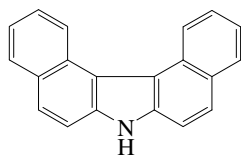


FIGURE 16.1.7.10.1 Logarithm of vapor pressure versus reciprocal temperature for carbazole.

16.1.7.11 Benzo[c,g]carbazole



Common Name: Benzo[c,g]carbazole

Synonym: 7H-dibenzo[c,g]carbazole

Chemical Name: 7H-dibenzo[c,g]carbazole

CAS Registry No: 194-59-2

Molecular Formula: $C_{20}H_{13}N$, $C_{10}H_6NHC_{10}H_6$

Molecular Weight: 267.324

Melting Point ($^{\circ}C$):

158 (Lide 2003)

Boiling Point ($^{\circ}C$)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

296.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.0496 (mp at $158^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.063 ± 0.003 (shake flask-GC, Smith et al. 1978)

0.064 (Mill et al. 1981)

0.064 (Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$):

1.33×10^{-7} (estimated by comparison with benzo[a]pyrene, Smith et al. 1978)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.00048 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.75 (calculated-S, Steen & Karickhoff 1981)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

4.93 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, $\log K_{OC}$:

4.31 (Coyote Creek sediment, Smith et al. 1978)

6.03, 6.16 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 15000$ h in river, $t_{1/2} = 37000$ h in eutrophic pond, $t_{1/2} = 73000$ h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: rate constant

$k = 5.2 \times 10^{-4} s^{-1}$ for transformation and transport when exposed to midday sunlight in mid-January with estimated $t_{1/2} = 1.0$ h in river, $t_{1/2} = 1.5$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 0.5$ h in oligotrophic lake assuming winter insulation by the one compartment model (Smith et al. 1978)
photolytic $t_{1/2} = 0.35$ h in aquatics (Haque et al. 1980).

Oxidation:

laboratory studied $k = 830 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with the RO_2 radicals and estimated $t_{1/2} > 700 \text{ h}$ in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)
 $k = 5.5 \times 10^{-4} \text{ s}^{-1}$ with $t_{1/2} = 0.4 \text{ d}$ under natural sunlight conditions for midday, midsummer at a latitude of 40°N ; $k = 830 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 10 \text{ d}$ for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated half-life to be very long in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model with no acclimated cultures obtained during the screening studies (Smith et al. 1978).

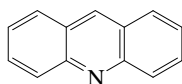
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: $t_{1/2} = 0.36 \text{ h}$ in river water, $t_{1/2} = 1.5 \text{ h}$ in pond water, $t_{1/2} = 1.5 \text{ h}$ in eutrophic lake and $t_{1/2} = 0.5 \text{ h}$ in oligotrophic lake for all processes predicted by one-compartment model (Smith et al. 1981);
 $t_{1/2} = 10 \text{ d}$ for free-radical oxidation in air-saturation water (NRCC 1983).

16.1.7.12 Acridine



Common Name: Acridine

Synonym: 2,3,5,6-dibenzopyridine

Chemical Name: acridine, 2,3,5,6-dibenzopyridine

CAS Registry No: 260-94-6

Molecular Formula: $C_{13}H_9N$

Molecular Weight: 179.217

Melting Point ($^{\circ}C$):

110 (Lide 2003)

Boiling Point ($^{\circ}C$):

344.86 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.005 (Weast 1982–83)

Molar Volume (cm^3/mol):

196.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

5.60 (Albert 1966; Matzner et al. 1991; Matzner & Bales 1994)

5.58 ($20^{\circ}C$, Weast 1982–83)

5.60 (protonated cation + 1, Dean 1985)

10.65 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.58 ± 0.38 (McEachern et al. 1975)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.147 (mp at $110^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

57.4 (Albert 1966)

38.4 ($24^{\circ}C$, shake flask-LSC, Means et al. 1980)

46.6 (literature average, Pearlman et al. 1984)

54.8 (centrifuge-HPLC at pH 8, Matzner et al. 1991)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($129.4^{\circ}C$, summary of literature data, temp range 129.4 – $346^{\circ}C$, Stull 1947)

$\log (P/mmHg) = [-0.2185 \times 15174.6/(T/K)] + 8.251980$; temp range 129.4 – $346^{\circ}C$ (Antoine eq., Weast 1972–73)

0.0065* (Langmuir free evaporation, measured range 7.96 – $50^{\circ}C$, McEachern et al. 1975)

$\log (P/mmHg) = 27.076 - 11021.64/(T/K)$; measured range 281.2 – $323.3 K$ (Langmuir free evaporation, McEachern et al. 1975)

0.0075 (extrapolated-Cox eq., Chao et al. 1983)

$\log (P/atm) = [1 - 618.827/(T/K)] \times 10^4 \{0.839996 - 4.19344 \times 10^{-4} \pm (T/K) + 3.63487 \times 10^{-7} \pm (T/K)^2\}$; temp range: 402.6 – $619.2 K$ (Cox eq., Chao et al. 1983)

0.2066 (static apparatus-extrapolated from Chebyshev polynomials, Sivaraman & Kobayashi 1983)

0.0065 (Interpolated-Antoine eq.-I, Stephenson & Malanowski 1987; quoted, Ma et al. 1990)

$\log (P_S/kPa) = 8.30838 - 3365.943/(-48.723 + T/K)$; temp range 293–367 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.73664 - 2699.39/(-48.611 + T/K)$; temp range 402–619 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.030 (calculated-P/C, Ma et al. 1990)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.40 (shake flask-UV, Hansch & Fujita 1964)
 3.39 (HPLC-RT correlation, Mirreles et al. 1976)
 3.39 (shake flask at pH 7.4, Unger et al. 1978)
 3.62 (shake flask-LSC, Means et al. 1980)
 3.29 (shake flask-AS at pH 7.4, Unger & Chiang 1981)
 3.31 ± 0.03 (HPLC-RV correlation-ALPM, Garst 1984)
 3.35 ± 0.02 (HPLC-RV correlation-ALPM, Garst & Wilson 1984)
 3.32 (shake flask-GC at pH 7.0, Haky & Leja 1986)
 3.40 (recommended, Sangster 1989, 1993)
 3.40 (recommended, Hansch et al. 1995)
 $3.18 \pm 0.64, 3.27 \pm 0.53$ (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

2.40 (selected, Ma et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

4.69 (average of sediments and soil samples, equilibrium sorption isotherm, Means et al. 1980)
 3.32 (calculated, Means et al. 1980)
 -0.157 (estimated of Loring subsurface material, Zachara et al. 1987)
 0.610 (estimated of Anvil Points subsurface material, Zachara et al. 1987)
 3.09–3.41 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987)
 3.16–3.33 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987)
 2.36–2.52 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987)
 2.98–3.30 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987)
 2.19–2.48 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987)
 4.22, 4.26 (soil, quoted, calculated-MCI χ , Sabljic 1987)
 4.11, 3.32 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
 4.11, 4.31 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 4.00 (HPLC- k' correlation, Nielsen et al. 1997)
 4.79 (soil-pore water partition coeff., Askov soil - a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 109 \text{ h}^{-1}$, $k_2 = 3.68 \text{ h}^{-1}$ (*daphnia pulex*, 21°C , Southworth et al. 1978)

Half-Lives in the Environment:

Biota: elimination $t_{1/2} = 11.3 \text{ min}$ (*daphnia pulex*, Southworth et al. 1978).

TABLE 16.1.7.12.1

Reported vapor pressures of acridine at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		McEachern et al. 1975			
summary of literature data		Langmuir free evaporation			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
129.4	133.3	7.96	0.000653	eq. 1a	P/mmHg
165.8	666.6	12.02	0.001027	A	27.076
184.0	1333	16.08	0.002413	B	11021.64
203.5	2666	19.95	0.00329	temp range: 281.2–323.2 K	
224.2	5333	25.05	0.00652	enthalpy of fusion:	
238.7	7999	25.05	0.00656	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.58$	
256.0	13332	29.98	0.01145	enthalpy of sublimation:	
284.0	26664	35.08	0.0213	$\Delta H_{\text{sub}}/(\text{kJ mol}^{-1}) = 121.75$	
314.3	53329	40.02	0.0380	temp range: 281.2–323.3 K	
345.0	101325	45.09	0.0640	enthalpy of vaporization:	
		50.0	0.1074	$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 72.59$	
mp/°C	110.5				

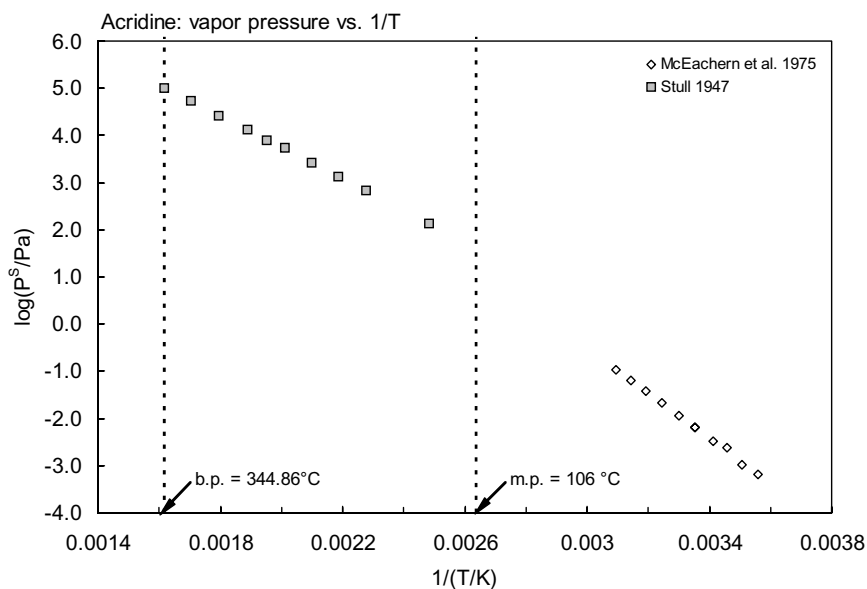


FIGURE 16.1.7.12.1 Logarithm of vapor pressure versus reciprocal temperature for acridine.

16.1.8 SULFUR COMPOUNDS

16.1.8.1 Carbon disulfide



Common Name: Carbon disulfide

Synonym: carbon disulphide

Chemical Name: carbon disulfide

CAS Registry No: 75-15-0

Molecular Formula: CS_2

Molecular Weight: 76.141

Melting Point ($^{\circ}\text{C}$):

−112.1 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

46 (Lide 2003)

Density (g/cm^3):

1.2632 (20 $^{\circ}\text{C}$, Weast 19820–83)

1.26311, 1.2555 (20 $^{\circ}\text{C}$, 25 $^{\circ}\text{C}$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

66.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_{V} (kJ/mol):

27.522, 26.736 (25 $^{\circ}\text{C}$, bp, Riddick et al. 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.389 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25 $^{\circ}\text{C}$ (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}\text{C}$):

2100 (20 $^{\circ}\text{C}$, selected, Riddick et al. 1986)

Vapor Pressure (Pa at 25 $^{\circ}\text{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

53329* (28 $^{\circ}\text{C}$, summary of literature data, temp range −73.8 to 46.5 $^{\circ}\text{C}$, Stull 1947)

47359* (24.582 $^{\circ}\text{C}$, comparative ebulliometry, measured range 3.6–80 $^{\circ}\text{C}$, Waddington et al. 1962)

$\log (P/\text{mmHg}) = 6.94194 - 1168.623/(241.534 + t/^{\circ}\text{C})$; temp range 3.6–80 $^{\circ}\text{C}$ (Antoine eq., comparative ebulliometry, Waddington et al. 1962)

49704* (25.931 $^{\circ}\text{C}$, temp range −17.76 to 45.142 $^{\circ}\text{C}$, Boublik & Aim 1972; quoted, Boublik et al 1984)

$\log (P/\text{kPa}) = 6.86752 - 1169.022/(241.582 + t/^{\circ}\text{C})$, temp range 3.6–80 $^{\circ}\text{C}$ (Antoine eq. derived from exptl. data of Waddington et al. 1949, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.03385 - 1151.908/(239.748 + t/^{\circ}\text{C})$, temp range −17.76 to 45.14 $^{\circ}\text{C}$ (Antoine eq. derived from exptl. data, Boublik et al. 1984)

48210 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.06694 - 1168.623/(t/^{\circ}\text{C} + 241.534)$ temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_{\text{L}}/\text{kPa}) = 6.03694 - 1153.5/(-33.22 + T/\text{K})$; temp range 256–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 6.07588 - 1174.112/(-30.896 + T/\text{K})$; temp range 260–353 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 6.19814 - 1231.307/(-26.024 + T/\text{K})$; temp range 338–408 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 6.80466 - 1278.903/(43.404 + T/\text{K})$; temp range 388–497 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_{\text{L}}/\text{kPa}) = 7.58592 - 2639.181/(165.312 + T/\text{K})$; temp range 490–533 K (Antoine eq.-V, Stephenson & Malanowski 1987)

39597 (20°C, Howard 1990)

$\log (P/\text{mmHg}) = 25.1475 - 2.0349 \times 10^3/(T/K) - 6.7794 \cdot \log (T/K) + 3.4828 \times 10^{-3} \cdot (T/K) - 1.0105 \times 10^{-14} \cdot (T/K)^2$;
temp range 162–552 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

142 (calculated-P/C, Howard 1990)

1946 (calculated-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

1577 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 3.485 - 1077/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.70–4.60 (Hansch & Leo 1985)

2.14 (recommended, Sangster 1993)

1.94 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

0.90 (calculated-solubility, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.80 (calculated-solubility, Howard 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 2.6$ h in a model river (Howard 1990)

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 1.1$ yr at pH 9 in alkaline solution (Howard 1990)

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: $t_{1/2} = 9$ d degraded by reacting with atomic oxygen and photochemically produced OH radicals (Howard 1990)

TABLE 16.1.8.1.1

Reported vapor pressures of carbon disulfide at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Waddington et al. 1962		Boublik & Aim 1972	
summary of literature data		comparative ebulliometry		in Boublik et al. 1984	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
-73.8	133.3	3.588	19920	-17.76	6967
-54.3	666.6	8.772	25007	-12.358	9306
-44.7	1333	13.999	31168	-7.204	12046
-34.3	2666	19.269	38547	-3.286	14549
-22.5	5333	24.582	47359	1.223	17921
-15.3	7999	29.927	57803	5.076	21314

TABLE 16.1.8.1.1 (Continued)

Stull 1947		Waddington et al. 1962		Boublik & Aim 1972	
summary of literature data		comparative ebulliometry		in Boublik et a. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−5.1	13332	35.318	70109	9.448	25780
10.4	26664	40.751	84525	12.981	29923
28.0	53329	46.225	101325	17.168	35493
46.5	101325	51.744	120798	21.087	41470
		57.295	143268	25.931	49704
mp/°C	−110.8	62.885	169052	31.522	61295
		68.531	198530	38.041	77125
		74.218	232087	45.142	97853
		79.927	270110		
				bp/°C	46.217
		bp/°C	46.22		
		Antoine eq.		eq. 2	P/kPa
		eq. 2	P/mmHg	A	6.03385
		A	6.94194	B	1151.908
		B	1168.623	C	239.748
		C	241.534		
		data also fitted to Cox eq.			
		see ref.			

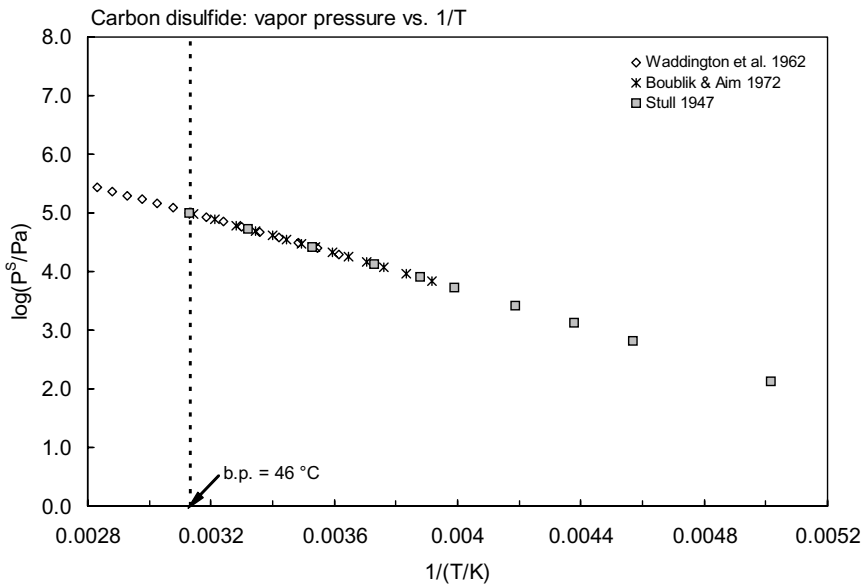


FIGURE 16.1.8.1.1 Logarithm of vapor pressure versus reciprocal temperature for carbon disulfide.

16.1.8.2 Dimethyl sulfide



Common Name: Dimethyl sulfide

Synonym: DMS, methyl sulfide, thiobismethane, 2-thiapropene

Chemical Name: dimethyl sulfide

CAS Registry No: 75-18-3

Molecular Formula: C_2H_6S , $(CH_3)_2S$

Molecular Weight: 62.134

Melting Point ($^{\circ}C$):

−98.24 (Lide 2003)

Boiling Point ($^{\circ}C$):

37.33 (Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

0.84825, 0.84230 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1961)

0.8423 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

73.2 (Kamlet et al. 1986)

73.8 ($20^{\circ}C$, calculated-density)

77.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_{BH+} :

−6.99 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.49, 26.82 ($25^{\circ}C$, bp, Dreisbach 1961)

27.65, 27.0 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.99 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

15606 (Hine & Mookerjee 1975)

6300 (Verschueren 1983)

22000 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)

20000 (Riddick et al. 1986)

19600 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

53174* ($20.087^{\circ}C$, static method, measured range -22.547 to $20.087^{\circ}C$, Osborn et al. 1942)

$\log (P/mmHg) = 16.51798 - 1876.370/(T/K) - 3.04727 \pm \log (T/K)$; temp range -22.547 to $20.087^{\circ}C$ (static method, Osborn et al. 1942)

53329* ($18.7^{\circ}C$, summary of literature data, temp range -75.6 to $36^{\circ}C$, Stull 1947)

64650 (calculated from determined data, Dreisbach 1961)

$\log (P/mmHg) = 6.93138 - 1081.587/(229.746 + t/^{\circ}C)$, temp range -50 to $130^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1961)

64501* (interpolated-Antoine eq., temp range -47.4 to $58.319^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.94879 - 1090.755/(230.799 + t/^{\circ}C)$; temp range -47.4 to $58.319^{\circ}C$ (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

70300 (Hine & Mookerjee 1975)

$\log (P/mmHg) = [-0.2185 \times 6742.3/(T/K)] + 7.589204$; temp range -75 to $224.5^{\circ}C$ (Antoine eq., Weast 1972–73)

56000 ($20^{\circ}C$, Verschueren 1983)

64443 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

64460 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.27843 - 1196.875/(242.81 + t/^{\circ}\text{C})$, temp range -22.55 to 20.09°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

64470 (extrapolated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.1509 - 1195.58/(242.68 + t/^{\circ}\text{C})$; temp range -22 to 20°C (Antoine eq., Dean 1985, 1992)

64650 (quoted, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.07369 - 1090.755/(230.799 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)

64520 (interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.07043 - 1088.851/(-42.594 + T/\text{K})$; temp range 268–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.13042 - 1124.998/(-37.961 + T/\text{K})$; temp range 307–379 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.42655 - 1344.329/(-7.456 + T/\text{K})$; temp range 372–453 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.36327 - 2293.043/(130.243 + T/\text{K})$; temp range 447–503 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 37.2604 - 2.4251 \times 10^3/(T/\text{K}) - 11.384 \cdot \log (T/\text{K}) + 5.8122 \times 10^{-3} \cdot (T/\text{K}) + 8.5893 \times 10^{-14} \cdot (T/\text{K})^2$; temp range 175–503 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence. Additional data at other temperatures designated * are compiled at the end of this section):

278.1 ($1/K_{\text{AW}}$, exptl., Hine & Mookerjee 1975)

298, 366.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

165 (20°C , headspace-GC, Vitenberg et al. 1975)

180.4, 184.7, 173.5 (headspace-GC, concn. of 10, 1.0, 0.1 ppm by weight, Przyjazny et al. 1983)

180.4, 184.7, 173.5 (headspace-GC, concn. of 10, 1.0 and 0.1 ppm by weight, measured range 25 – 70°C , data presented in graph, Przyjazny et al. 1983)

$\log (1/K_{\text{AW}}) = 1637.3/(T/\text{K}) - 4.354$; temp range 25 – 70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)

$\log (1/K_{\text{AW}}) = 1635.6/(T/\text{K}) - 4.358$; temp range 25 – 70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)

$\log (1/K_{\text{AW}}) = 1598.2/(T/\text{K}) - 4.205$; temp range 25 – 70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983)

163.4 (quoted, Gaffney et al. 1987)

184, 1271 (quoted, calculated-molecular structure, Russell et al. 1992)

138 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)

233.0* (equilibrium headspace-GC, in seawater, measured range 18 – 44°C , Wong & Wang 1997)

61.97 (equilibrium headspace-GC, Marin et al. 1999)

155 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 3.556 - 1394/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}^* = (9.80 \pm 1.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299.9 K, measured range 299.9–426.5 K (flash photolysis-resonance fluorescence, Atkinson et al. 1978)

$k_{\text{OH}}^* = (8.28 \pm 0.87) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 273–400 K by flash photolysis-resonance fluorescence, Kurylo 1978)

$k_{\text{O}(^3\text{P})}^* = 57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas-phase reaction with $\text{O}(^3\text{P})$ atom at 296 K, measured range 252–493 K (Slagle et al. 1978)

$k_{\text{OH}}^* = (4.26 \pm 0.56) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 248–363 K (flash photolysis-resonance fluorescence, Wine et al. 1981)

$k_{\text{OH}} = (1.0 \pm 0.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated lifetime $\tau \sim 30$ h in the daytime, $k_{\text{NO}_3} = (5.4 \pm 0.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated $\tau \sim 3$ h in the nighttime hours at 296 ± 2 K (Atkinson et al. 1984)

$k_{\text{O}_3} < 8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.05 \text{ d}^{-1}$, $k_{\text{OH}} = 9.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.8 d^{-1} , and $k_{\text{NO}_3} = 9.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 20 d^{-1} at room temp. (review, Atkinson & Carter 1984)

$k_{\text{O}_3} < 8 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.004 \text{ d}^{-1}$, $k_{\text{OH}} = 6.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.27 d^{-1} , and $k_{\text{NO}_3} = 9.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 20 d^{-1} at room temp. (review, Atkinson 1985)

$k_{\text{OH}}^* = (4.09, 4.44) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 267–397 K (flash photolysis-resonance fluorescence, Hynes et al. 1986)

$k_{\text{OH}}^* = (3.60 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 297–440 K by flash photolysis-resonance fluorescence; $k_{\text{OH}} = 9.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative rate to *n*-hexane, $k_{\text{OH}} = 5.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ relative rate to cyclohexane at 296 K (Wallington et al. 1986a)

$k_{\text{NO}_3}^* = (8.1 \pm 1.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 280–350 K (flash photolysis-visible absorption, Wallington et al. 1986b)

$k_{\text{OH}}^* = (5.50 \pm 1.0) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 260–393 K (discharge flow-resonance fluorescence, Hsu et al. 1987)

$k_{\text{OH}} = (8.0 \pm 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Relative rate method, Barnes et al. 1989)

$k_{\text{OH}} = 3.60 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 3.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{\text{NO}_3}^* = (10.6 \pm 1.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 256–376 K (flow tube-laser induced fluorescence, Dlugokencky & Howard 1988)

$k_{\text{OH}}^* = 4.56 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 4.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 9.77 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljić & Güsten 1990; Müller & Klein 1991)

$k_{\text{NO}_3}^* = 1.07 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetime $\tau \sim 30$ h due to reaction with OH radical in the daytime and $\tau \sim 3$ h due to reaction at night with NO_3 radical (Atkinson et al. 1984);

calculated lifetimes, $\tau > 20$ d due to reaction with O_3 in 24-h, $\tau = 28$ h with OH radical during daytime and $\tau = 120$ min with NO_3 radical during nighttime in “clean” atmosphere; $\tau > 3$ d due to reaction with O_3 in 24-h, $\tau = 420$ min with OH radical in daytime and $\tau = 13$ min with NO_3 in nighttime in “moderately polluted” atmosphere (Winer et al. 1984)

estimated tropospheric chemical lifetimes, $\tau = 2$ d, 2 d and > 15 d for reactions with OH, NO_3 and O_3 , respectively, under typical remote tropospheric conditions (Falbe-Hansen et al. 2000)

TABLE 16.1.8.2.1

Reported vapor pressures and Henry's law constants of dimethyl sulfide at various temperatures

Vapor pressure						Henry's law constant	
Osborn et al. 1942		Stull 1947		Zwolinski & Wilhoit 1971		Wong & Wang 1997	
static method-manometer		summary of literature data		selected values		equilibrium headspace-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
							in seawater
-22.547	6994	-75.6	-133.3	47.4	1333	18	164.6
-10.028	13699	-58.0	666.6	-37.7	2666	25	233.0
0.096	22437	-49.2	1333	-31.5	4000	35	381.7
4.943	28042	-39.4	2666	-26.9	5333	44	556.4
15.138	43512	-28.4	5333	-23.03	6666		
20.087	53174	-21.4	7999	-19.85	7999	log K _{AW} = A - B/(T/K)	
		-12.0	13332	-14.62	10666		
mp/K	174.855	2.60	26664	-10.39	13332	A	K _{AW} 4.806
bp/K	310.49	18.7	53329	-2.258	19998	B	1735
		36.0	101325	3.885	26664		
log P = A - B/(T/K) - C·log (T/K)				8.883	33331		
	P/mmHg	mp/°C	-83.2	13.127	39997		
A	16.51798			20.138	53329		
B	1876.370			25.860	66661		
C	3.04727			30.733	79993		
				35.000	93326		
$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 7.985$				35.794	95992		
$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) = 27.98$				36.572	98659		
at 291.06 K				37.333	101325		
				25	64501		
				Antoine eq.			
				log P = A - B/(C + t/°C)			
					P/mmHg		
				A	6.94879		
				B	1090.755		
				C	230.799		
				bp/°C	37.333		
				$\Delta H_{\text{v}}/(\text{kJ mol}^{-1}) =$			
				at 25°C	27.65		
				at bp	26.92		

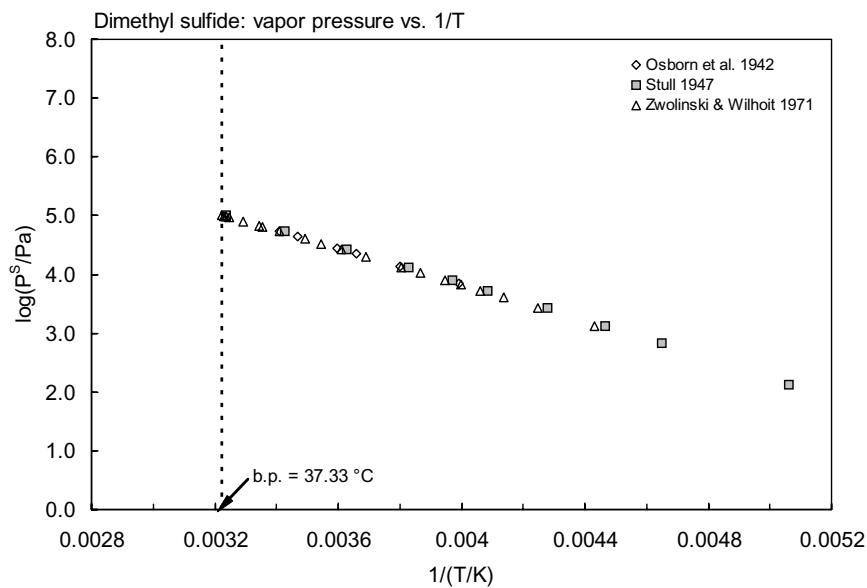


FIGURE 16.1.8.2.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl sulfide.

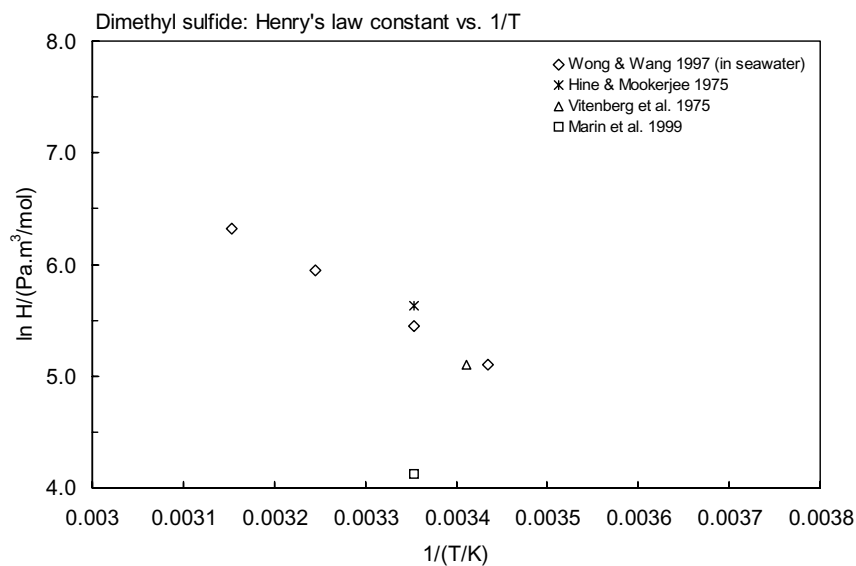


FIGURE 16.1.8.2.2 Logarithm of Henry's law constant versus reciprocal temperature for dimethyl sulfide.

16.1.8.3 Dimethyl disulfide



Common Name: Dimethyl disulfide

Synonym: 2,3-dithiabutane

Chemical Name: dimethyl disulfide

CAS Registry No: 624-92-0

Molecular Formula: $C_2H_6S_2$, CH_3SSCH_3

Molecular Weight: 94.199

Melting Point ($^{\circ}C$):

-84.67 (Lide 2003)

Boiling Point ($^{\circ}C$):

109.74 (Lide 2003)

Density (g/cm^3):

1.6025 ($20^{\circ}C$, Weast 1982-83)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

103.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

38.37, 33.68 (25, bp, Zwolinski & Wilhoit 1971)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3400 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3825* (static method, measured range $0-60^{\circ}C$, Scott et al. 1950)

3813* (interpolated-Antoine eq., temp range $5.356-109.745^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.97792 - 1396.342/(218.863 + t/^{\circ}C)$; temp range $5.356-109.745^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

3850 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

$\log(P/kPa) = 6.18000 - 1389.151/(223.184 + t/^{\circ}C)$, temp range $0-60^{\circ}C$ (Antoine eq. derived from Scott et al. 1950 data, Boublik et al. 1984)

$\log(P/kPa) = 6.08703 - 1336.665/(217.767 + t/^{\circ}C)$, temp range $61.4-128.6^{\circ}C$ (Antoine eq. derived from Scott et al. 1950 data, Boublik et al. 1984)

$\log(P_L/kPa) = 6.10018 - 1349.006/(-54.389 + T/K)$, temp range 297-402 K, (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 36.232 - 3.1241 \times 10^3/(T/K) - 9.9328 \cdot \log(T/K) + 2.2831 \times 10^{-11} \cdot (T/K) + 3.1730 \times 10^{-6} \cdot (T/K)^2$; temp range 125-499 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated):

121 ($20^{\circ}C$, headspace-GC, Vitenberg et al. 1975)

112, 101 (headspace-GC, concn. of 10 and 1.0 ppm by weight, measured range $25-70^{\circ}C$, data presented in graph, Przyjazny et al. 1983)

$\log(1/K_{AW}) = 1657.1/(T/K) - 4.211$; temp range $25-70^{\circ}C$ (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)

$\log(1/K_{AW}) = 1854.4/(T/K) - 4.828$; temp range $25-70^{\circ}C$ (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)

77.5 ($20^{\circ}C$, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.828 - 1384/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.77 (shake flask, Log P Database, Hansch & Leo 1987)
- 1.77 (recommended, Sangster 1993)
- 1.77 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 2.40 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at 297 K (relative rate method, Cox & Sheppard 1980)

$k_{OH}^* = (1.84 - 19.8) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at 298 K, measured range 255–377 K (flask photolysis-resonance fluorescence, Wine et al. 1984)

$k_{OH}^* = 2.05 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at 298 K (tentative recommended, Atkinson 1985)

$k_{NO_3}^* = 4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 280–350 K (flash photolysis-optical absorption, Wallington et al. 1986)

$k_{NO_3}^* = (7.3 \pm 1.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured range 334–382 K (flow tube-laser induced fluorescence, Dlugokencky & Howard 1988)

$k_{NO_3} = 7.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range ~300–380 K (recommended, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 16.1.8.3.1

Reported vapor pressures of dimethyl disulfide at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

Scott et al. 1950				Zwolinski & Wilhoit 1971			
static method-manometer		ebulliometric method		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	904	61.411	19920	5.356	1333	106.905	93326
15	2230	67.301	25007	18.299	2666	107.872	95992
20	2936	73.234	31160	25.891	4000	108.819	98659
25	3825	79.201	38547	31.579	5333	109.745	101325
30	4930	85.218	47359	36.177	6666	25.0	3813
35	6301	91.283	57803	40.060	7999	Antoine eq.	
40	7975	97.393	70109	46.435	10666	eq. 2	P/mmHg
45	10007	103.54	84525	51.600	13332	A	6.97792
50	12448	109.738	101325	61.518	19998	B	1396.342
55	15359	115.984	120798	69.008	26664	C	218.863
60	18813	122.273	143268	75.099	33331	bp/°C	109.745
		128.611	169052	80.271	39997	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
				88.812	53329	at 25°C	38.37
				95.780	66661	at bp	33.68
				101.712	79993		

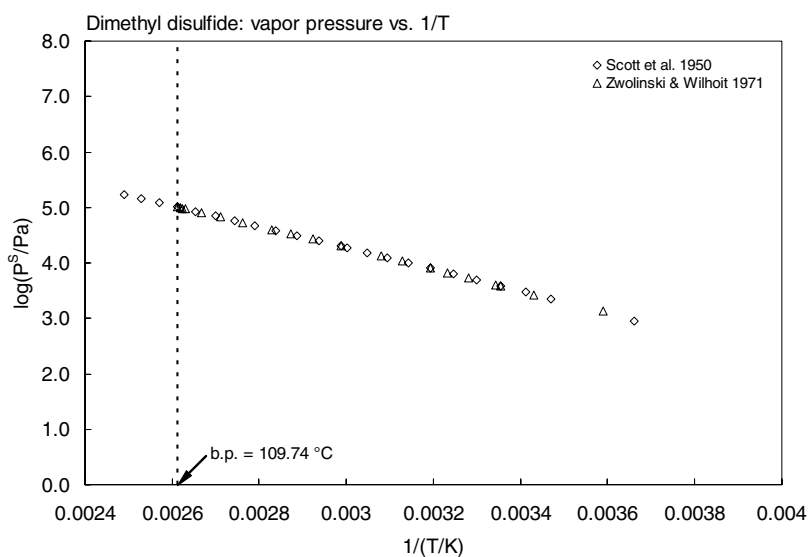


FIGURE 16.1.8.3.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl disulfide.

16.1.8.4 Dimethyl sulfoxide (DMSO)



Common Name: Dimethyl sulfoxide

Synonym: DMSO, sulfinylbismethane, methyl sulfoxide, methylsulfinylmethane, SQ 9453, DMS-70, DMS-90, Deltan, Demasorb, Demavet, Demeso, Dermasorb, Dolicur, Domoso, Dromisol, Gamasol 90, Hyadur, Rimso-50, Sclerosol, Somipront, Somtexan, Topsym

Chemical Name: dimethyl sulfoxide

CAS Registry No: 67-68-5

Molecular Formula: C_2H_6OS , $(CH_3)_2SO$

Molecular Weight: 78.133

Melting Point ($^{\circ}C$):

17.89 (Lide 2003)

Boiling Point ($^{\circ}C$):

189.0 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

1.1014 (Weast 1982–83)

Molar Volume (cm^3/mol):

85.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

1.4 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

52.88, 43.14 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.368 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

253000 (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

80.0* (gas saturation, measured range 20 – $50^{\circ}C$, Douglas 1948)

$\log (P/mmHg) = 26.49588 - 3539.32/(T/K) - 6.000 \pm \ln (T/K)$; temp range 20 – $50^{\circ}C$ (gas saturation, Douglas 1948)

460* ($52.35^{\circ}C$, Hg manometer, measured range 325.5 – $442.1 K$, Jakli & van Hook 1972)

$\ln (P/mmHg) = 17.4922 - 4517.79/(T/K - 47.2583)$; temp range 291.7 – $463 K$ (Hg manometer, Antoine eq. with literature data, Jakli & van Hook 1972)

56.0 ($20^{\circ}C$, Verschueren 1983)

80.9 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.64816 - 1922.32/(223.353 + t/^{\circ}C)$; temp range 52.4 – $168.95^{\circ}C$ (Antoine eq. from reported exptl. data of Jakli & von Hook 1972, Boublik et al. 1984)

80.0 (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.72161 - 1962.06/(225.892 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

79.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.72167 - 1962.05/(-47.258 + T/K)$; temp range 305 – $464 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/mmHg) = 45.4653 - 4.0439 \times 10^3/(T/K) - 13.21 \cdot \log (T/K) + 1.0981 \times 10^{-7} \cdot (T/K) + 6.4155 \times 10^{-6} \cdot (T/K)^2$; temp range 292 – $465 K$ (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.35 (shake flask, Hansch & Leo 1979, 1987)
- 0.85 (calculated-UNIFAC activity coefficients, Banerjee & Howard 1988)
- 1.35 (recommended, Sangster 1989)
- 1.35 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 4.96 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (6.2 \pm 2.2) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{NO_3} = (1.7 \pm 0.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{O_3} < 5.0 \times 10^{-19} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ at room temp (Barnes et al. 1989)

$k_{OH} = (62 \pm 25) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson 1989)

$k_{OH} = (1.0 \pm 0.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp (Hynes & Wine 1996)

$k_{OH} = (8.7 \pm 1.6) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Urbanski et al. 1998)

$k_{OH} = (5.9 \pm 1.5) \times 10^{-11} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ with tropospheric lifetime $\tau = 5 \text{ h}$, $k_{NO_3} = (5.0 \pm 3.8) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with tropospheric lifetime $\tau = 3 \text{ d}$; $k_{O_3} < 1.0 \times 10^{-19} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$ with tropospheric lifetime $\tau > 150 \text{ d}$ and $k_{Cl} = (7.4 \pm 1.0) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with Cl atoms with tropospheric lifetime $\tau = 62 \text{ d}$ at room temp and 740 torr (Relative rate method, Falbe-Hansen et al. 2000)

Hydrolysis: $k = 6.60 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ (Buxton et al. 1986)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated tropospheric chemical lifetimes, $\tau = 5 \text{ h}$, 3 d and $> 150 \text{ d}$ for reactions with OH, NO_3 and O_3 , respectively, under typical remote tropospheric conditions (Falbe-Hansen et al. 2000)

TABLE 16.1.8.4.1

Reported vapor pressures of dimethyl sulfoxide at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)		
$\log P = A - B/(C + T/K)$	(3)	$\log P = A - B/(C + T/K)$	(3a)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)	$\ln P = A - B/(T/K) - C \cdot \ln(T/K)$	(4a)		
Douglas 1948	Jakli & van Hook 1972				
gas saturation	mercury manometer				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	55.6	52.35	460	140.15	22905
25	80.0	56.25	573	148.05	29471
30	113.7	61.45	767	162.15	47036
35	159.3	66.15	993	168.95	56342
40	220.8	74.85	1560	eq. 3	P/mmHg
45	302.6	79.95	2000	A	17.4922
50	409.3	85.65	2653	B	4517.79
		90.26	3293	C	47.2583
eq. 4	P/mmHg	96.05	4226		
A	29.49558	100.45	5106		
B	3539.32	100.55	5133		
C	6.0000	104.95	6246		
		111.95	8359		
bp/°C	192	117.95	10452		
$\Delta H_v = 52.89 \text{ kJ/mol}$		127.45	14745		

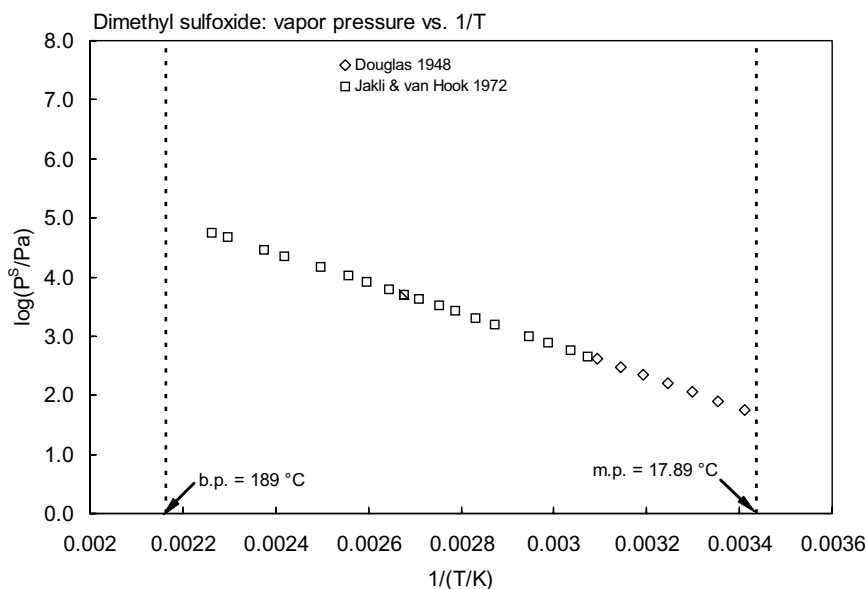
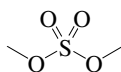


FIGURE 16.1.8.4.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl sulfoxide.

16.1.8.5 Dimethyl sulfate



Common Name: Dimethyl sulfate

Synonym: sulfuric acid dimethyl ester, DMS

Chemical Name: dimethyl sulfate

CAS Registry No: 77-78-1

Molecular Formula: $C_2H_6O_4S$, $CH_3O-SO_2-OCH_3$

Molecular Weight: 126.132

Melting Point ($^{\circ}C$):

-27 (Lide 2003)

Boiling Point ($^{\circ}C$):

188 (decomposes, Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.3322 (Dean 1985)

Molar Volume (cm^3/mol):

95.0 ($20^{\circ}C$, Stephenson & Malanowski 1987)

109.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

28000 (hydrolyzes, Verschueren 1983; Dean 1985)

28000 ($18^{\circ}C$, Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

< 133 ($20^{\circ}C$, Verschueren 1983)

128 (extrapolated, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.28235 - 2437.54/(T/K)$, temp range 340–470 K, (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 33.9406 - 3.853 \times 10^3/(T/K) - 8.5921 \cdot \log(T/K) - 1.1705 \times 10^{-10} \cdot (T/K) + 8.226 \times 10^{-7} \cdot (T/K)^2$; temp range 241–758 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2}$ = of 36.5–365 h, based on estimated rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first order hydrolysis rate constant $k = 1.6 \times 10^{-4} s^{-1}$ at pH 7 and $25^{\circ}C$ with $t_{1/2} = 1.2 h$ (Mabey & Mill 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} \sim 168\text{--}672$ h and aqueous anaerobic biodegradation $t_{1/2} \sim 672\text{--}2688$ h (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 36.5\text{--}365$ h, based on photooxidation half-life in air from estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime (reaction with liquid water) estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 1.2\text{--}12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991) and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Lee et al. 1980; quoted, Howard et al. 1991).

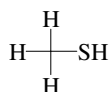
Groundwater: $t_{1/2} = 1.2\text{--}12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991) and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Lee et al. 1980; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 1.2\text{--}12$ h, based on overall hydrolysis rate constant for pH 7 at 25°C and for complete hydrolysis in neutral, slightly basic, and acidic aqueous solutions (Howard et al. 1991).

Biota:

16.1.8.6 Methanethiol



Common Name: Methanethiol

Synonym: methyl mercaptan

Chemical Name: methanethiol

CAS Registry No: 74-93-1

Molecular Formula: CH_4S , CH_3SH

Molecular Weight: 48.108

Melting Point ($^{\circ}\text{C}$):

−123 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

5.9 (Lide 2003)

Density (g/cm^3):

0.8665 (20°C , Weast 1982–83)

Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

55.3 (20°C , Stephenson & Malanowski 1987)

55.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

23.8, 24.57 (25, bp, Zwolinski & Wilhoit 1971)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F: 1.0)

Water Solubility (g/m^3 or mg/L at 25°C):

39000 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

101410* (5.977°C , static method-Hg manometer, measured range -51.3 to 5.977°C , Russell et al. 1942)

$\log(P/\text{mmHg}) = 18.27429 - 1769.05/(T/\text{K}) - 3.70248 \pm \log(T/\text{K})$; temp range 221.88–279.137 K (static method, Russell, et al. 1942)

101325* (8.7°C , summary of literature data, temp range -90.7 to 7.8°C , Stull 1947)

202117* (extrapolated, summary of literature data, temp range -70.3 to 5.956°C , Zwolinski & Wilhoit 1971)

$\log(P/\text{mmHg}) = 7.03163 - 1015.547/(238.706 + t/^{\circ}\text{C})$; temp range -70.3 to 24.694°C (Antoine eq., Zwolinski & Wilhoit 1971)

202346 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

$\log(P/\text{kPa}) = 6.18991 - 1030.496/(248.330 + t/^{\circ}\text{C})$, temp range -51.28 to 5.977°C , (Antoine eq. derived from Russell et al. 1942 data, Boublik et al. 1984)

$\log(P_L/\text{kPa}) = 6.19283 - 1031.216/(-32.916 + T/\text{K})$, temp range 221–283 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.19219 - 1030.918/(-32.845 + T/\text{K})$, temp range 222–279 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.13699 - 1006.199/(-35.529 + T/\text{K})$, temp range 267–359 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.53487 - 1278.361/(5.318 + T/\text{K})$, temp range 345–424 K, (Antoine eq.-IV, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

- 247 (distilled water, headspace-GC/FID, measured range $25\text{--}70^\circ\text{C}$, data in graph, Przyjazny et al. 1983)
 $\text{Log}(1/K_{\text{AW}}) = 1347.1/(T/K) - 3.537$; temp range $25\text{--}70^\circ\text{C}$ (headspace-GC, Przyjazny et al. 1983)
 187 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)
 300 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 3.249 - 1219/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}^* = 3.39 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299.8 K , measured range $300\text{--}423 \text{ K}$ (flash photolysis-resonance fluorescence, Atkinson et al. 1977)

$k_{\text{OH}}^* = 3.37 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , measured range $244\text{--}366 \text{ K}$ (flash photolysis-resonance fluorescence, Wine et al. 1981)

$k_{\text{OH}} = 9.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K (relative rate method, Cox & Sheppard 1980)

$k_{\text{OH}} = 2.01 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 293 K (discharge flow-EPR, Mac Leod et al. 1983)

$k_{\text{OH}} = 2.56 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-RF, Lee & Tang 1983)

$k_{\text{OH}}^* = (3.04 - 32.5) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , measured range $254\text{--}430 \text{ K}$ ((flash photolysis-resonance fluorescence, Wine et al. 1984)

$k_{\text{OH}}^* = 3.31 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{\text{NO}_3} = 9.2 \times 10^{-13} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range $250\text{--}370 \text{ K}$ (IUPAC recommended, Atkinson et al. 1989)

$k_{\text{NO}_3} = 9.3 \times 10^{-13} \text{ cm}^3 \pm \text{molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range $254\text{--}367 \text{ K}$ (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

TABLE 16.1.8.6.1
Reported vapor pressures of methanethiol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Russell et al. 1942		Stull 1947		Zwolinski & Wilhoit 1971			
static-Hg manometer		summary of literature data		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–53.28	5484	–90.7	133.3	–70.3	1333	3.869	93326
–23.872	26859	–75.3	666.6	–61.5	2666	4.580	95992
–9.474	53235	–67.5	1333	–55.9	4000	5.275	98659
0.029	79913	–58.8	2666	–51.7	5333	5.956	101325
5.977	101410	–49.2	5333	–48.3	6666	25.0	202117
		–43.1	7999	–45.4	7999	eq. 2	P/mmHg
bp/K	279.12	–34.8	13332	–40.7	10666	A	7.03163
		–22.1	26664	–36.87	13332	B	1015.547
eq. 4	P/mmHg	–7.80	53329	–29.55	19998	C	238.706
A	18.27429	8.70	101325	–24.03	26664	bp/°C	5.956
B	1769.05			–19.54	33331	ΔH _v /(kJ mol ^{–1}) =	
C	3.70248	mp/°C	–	–15.73	39997	at 25°C	23.8
				–9.44	53329	at bp	24.57
				–4.31	66661		
				0.051	79993		

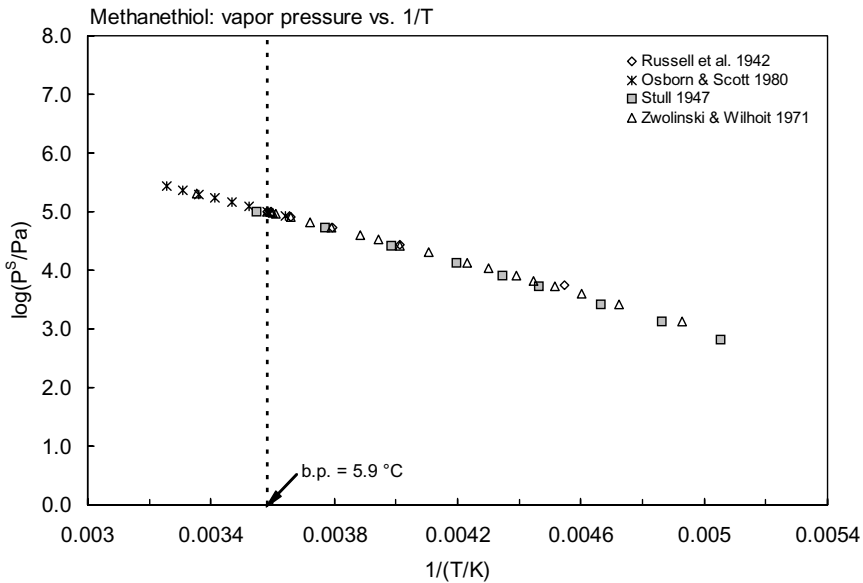


FIGURE 16.1.8.6.1 Logarithm of vapor pressure versus reciprocal temperature for methanethiol.

16.1.8.7 Ethanethiol



Common Name: Ethanethiol

Synonym: ethyl mercaptan, thioethyl alcohol, ethylhydrosulfide

Chemical Name: ethanethiol

CAS Registry No: 75-08-1

Molecular Formula: C_2H_6S , C_2H_5SH

Molecular Weight: 62.134

Melting Point (C):

−147.88 (Lide 2003)

Boiling Point (°C):

35.0 (Stull 1947; Dreisbach 1961; Weast 1982–83; Boublik et al. 1984; Dean 1985; Lide 2003)

Density (g/cm³ at 20°C):

0.83914, 0.83316 (20°C, 25°C, Dreisbach 1961)

0.8391 (Weast 1982–83)

0.8315 (25°C, Dean 1985)

Molar Volume (cm³/mol):

74.0 (20°C, calculated-density)

77.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

27.30, 26.78 (25°C, bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

15600 (Hine & Mookerjee 1975)

12000 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)

15000 (Verschueren 1983)

6800 (Dean 1985)

6760 (20°C, Budavari 1989)

14800 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

74630* (interpolated-regression of tabulated data, temp range −76.7 to 35°C, Stull 1947)

70110* (24.933°C, ebulliometric method, measured range 0.405–66.14°C, McCullough et al. 1952)

$\log(P/\text{mmHg}) = 6.95206 - 1084.531/(231.385 + t/^\circ\text{C})$; temp range 0.405–66.14°C (Antoine eq., ebulliometric method, McCullough et al. 1952)

70300 (calculated from determined data, Dreisbach 1961)

$\log(P/\text{mmHg}) = 6.95206 - 1084.531/(231.385 + t/^\circ\text{C})$; temp range −40 to 100°C (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/\text{mmHg}) = 6.95205 - 1084.531/(T/K + 231.385)$ (Antoine eq., Osborn & Douslin 1966)

66660*, 70290 (23.613°C, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/\text{mmHg}) = 6.95026 - 1084.531/(231.385 + t/^\circ\text{C})$; temp range −49.2 to 55.83°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

70320 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

58660 (20°C, Verschueren 1983)

70290 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.0768 - 1084.455/(231.374 + t/^\circ\text{C})$, temp range 0.405–66.115°C (Antoine eq. from reported exptl. data of McCullough et al. 1952, Boublik et al. 1984)

70300 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.95206 - 1084.531/(231.39 + t/^{\circ}\text{C})$; temp range -49 to 56°C (Antoine eq., Dean 1985, 1992)
 $\log (P_L/\text{kPa}) = 6.07243 - 1081.984/(-42.085 + T/\text{K})$, temp range 273 – 340 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.08253 - 1086.982/(-41.517 + T/\text{K})$, temp range 273 – 313 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.10279 - 1099.374/(-39.807 + T/\text{K})$, temp range 303 – 375 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.42565 - 1328.598/(-6.231 + T/\text{K})$, temp range 365 – 448 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.84948 - 2874.377/(200.657 + T/\text{K})$, temp range 442 – 499 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 29.2763 - 2.2725 \times 10^3/(T/\text{K}) - 7.7769 \cdot \log (T/\text{K}) - 3.8954 \times 10^{-11} \cdot (T/\text{K}) + 3.517 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 125 – 499 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

278.1 (exptl., Hine & Mookerjee 1975)
 298, 366.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 451 (20°C , headspace-GC, Vitenberg et al. 1975)
 360.3 (distilled water, headspace-GC/FID, measured range 25 – 70°C , data in graph, Przyjazny et al. 1983)
 $\log (1/K_{\text{AW}}) = 1486.1/(T/\text{K}) - 4.147$; temp range 25 – 70°C (headspace-GC, Przyjazny et al. 1983)
 292.4 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 278, 96.44 (quoted, calculated-molecular structure, Russell et al. 1992)
 292.5 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 4.147 - 1486/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and the Arrhenius expression see reference:

$k_{\text{O}(3\text{P})}^* = 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas-phase reaction with $\text{O}(^3\text{P})$ atom at 298 K, measured range 257 – 495 K (Slagle et al. 1978)

$k_{\text{OH}} = 3.67 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (discharge flow-RF, Lee & Tang 1983)

$k_{\text{OH}} = 2.70 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 293 K (discharge flow-EPR, Mac Leod et al. 1984)

$k_{\text{OH}}^* = 4.26 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 252 – 425 K (flash photolysis-resonance fluorescence, Wine et al. 1984)

$k_{\text{OH}}^* = 4.65 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{\text{OH}} = 4.65 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Barnes et al. 1986)

$k_{\text{OH}}^* = 4.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{NO}_3} = (1.21 \pm 0.28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298K (relative rate method, Mac Leod et al. 1986; quoted, Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 16.1.8.7.1

Reported vapor pressures of ethanethiol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		McCullough et al. 1952		Zwolinski & Wilhoit 1971			
summary of literature data		ebulliometry		selected values			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–76.7	133.3	0.405	25007	–49.2	1333	eq. 2	P/mmHg
–59.1	666.6	5.236	31160	–39.5	2666	A	6.95206
–50.2	1333	10.111	38547	–33.3	4000	B	1084.531
–40.7	2666	15.017	47359	–28.7	5333	C	231.385
–29.8	5333	19.954	57803	–24.9	6666	bp/°C	35.003
–22.4	7999	24.933	70109	–21.77	7999	ΔH _v /(kJ mol ^{–1}) =	
–13.0	13332	29.944	84525	–16.58	10666	at 25°C	27.30
1.50	26664	35.000	101325	–12.38	13332	at bp	26.78
17.7	53329	40.092	120798	–4.304	19998		
35.0	101325	45.221	142368	1.796	26664		
		50.390	169052	6.758	33331		
mp/°C	–121	55.604	198530	10.972	39997		
		60.838	232087	17.932	53329		
		66.115	270110	23.613	66661		
				28.451	79993		
		Antoine eq.		32.686	93326		
		eq. 2	P/mmHg	33.475	95992		
		A	6.95206	34.247	98659		
		B	1084.531	35.003	101325		
		C	231.385	25.0	70288		

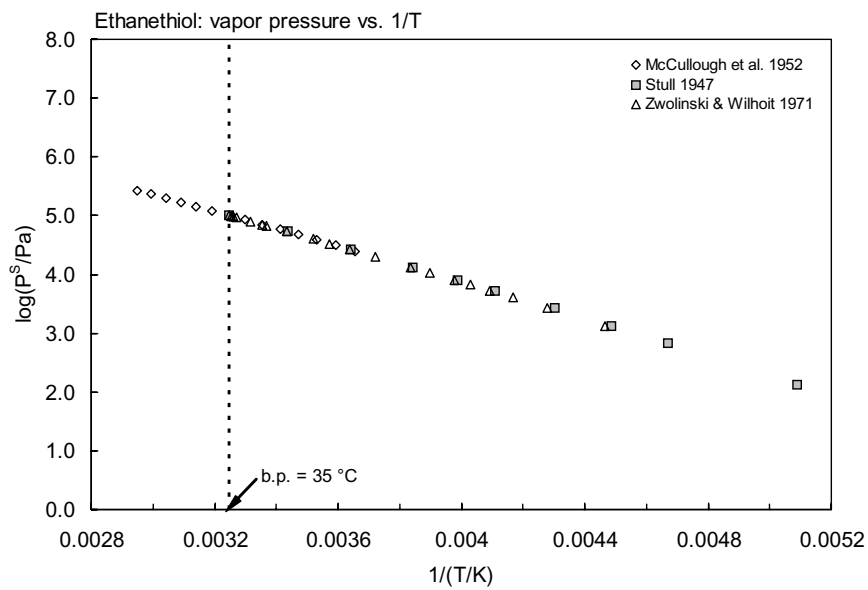
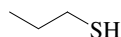


FIGURE 16.1.8.7.1 Logarithm of vapor pressure versus reciprocal temperature for ethanethiol.

16.1.8.8 1-Propanethiol



Common Name: 1-Propanethiol

Synonym: *n*-propyl mercaptan, 1-mercaptopropane

Chemical Name: 1-propanethiol

CAS Registry No: 107-03-9

Molecular Formula: C₃H₈S, CH₃CH₂CH₂SH

Molecular Weight: 76.171

Melting Point (°C):

−113.13 (Lide 2003)

Boiling Point (°C):

67.8 (Lide 2003)

Density (g/cm³):

0.8411 (20°C, Weast 1982–83)

Dissociation Constant, pK_a:

Molar Volume (cm³/mol):

99.6 (calculated-density, Stephenson & Malanowski 1987)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.88, 29.53 (25°C, bp, Zwolinski & Wilhoit 1971)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

3800 (estimated-activity coefficient by headspace-GC/FID, Przyjazny et al. 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

13332* (15.3°C, summary of literature data, temp range −56.0 to 67.4°C, Stull 1947)

19920* (24.275°C, ebulliometry, measured range 24.3–102.088°C, Pennington et al. 1956)

log (P/mmHg) = 6.92846 − 1183.307/(T/K + 224.624); temp range 24.3–102.088°C (Antoine eq., ebulliometry, Pennington et al. 1956; Osborn & Douslin 1966)

20558* (interpolated-Antoine eq., temp range −25 to 90.73°C, Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.92846 − 1183.307/(224.624 + t/°C); temp range −25 to 90.73°C (Antoine eq., Zwolinski & Wilhoit 1971)

20569 (calculated-Antoine eq. of Boublik et al. 1973, Przyjazny et al. 1983)

log (P/kPa) = 6.05331 − 1183.265/(224.618 + t/°C), temp range 24.27–102.088°C (Antoine eq. derived from Pennington et al. 1956 data, Boublik et al. 1984)

log (P_L/kPa) = 6.05019 − 1181.703/(−48.687 + T/K), temp range 296–376 K, (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 6.92846 − 1183.307/(224.62 + t/°C), temp range −25 to 91°C (Antoine eq., Dean 1992)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

414 (distilled water, headspace-GC/FID, measured range 25–70°C, data in graph, Przyjazny et al. 1983)

log (1/K_{AW}) = 1552.2/(T/K) − 4.428; temp range 25–70°C (headspace-GC, Przyjazny et al. 1983)

331 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log K_{AW} = 4.428 − 1552/(T/K), (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW}:

1.81 (shake flask, Log P Database, Hansch & Leo 1987)

1.81 (recommended, Sangster 1993)

1.81 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO₃ radical and k_{O3} with O₃ or as indicated, *data at other temperatures see reference:

k_{OH}* = (4.18–4.56) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K, measured range 257–419 K (flash photolysis-resonance fluorescence, Wine et al. 1984)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):

Half-Lives in the Environment:

TABLE 16.1.8.8.1
Reported vapor pressures of 1-propanethiol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)
log P = A – B/(C + T/K)		(3)			
log P = A – B/(T/K) – C·log (T/K)		(4)			
Stull 1947		Pennington et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–56.0	133.3	24.275	18820	–25.0	1333
–36.3	666.6	29.563	25007	–14.3	2666
–26.3	1333	34.891	31160	–7.60	4000
–15.4	2666	40.254	38547	–2.50	5333
–3.20	5333	45.663	47359	1.65	6666
4.60	7999	51.113	57803	5.13	7999
15.3	13332	56.605	70109	10.84	10666
31.5	26664	62.139	84525	15.47	13332
49.2	53329	67.719	101325	24.369	19998
67.4	101325	73.341	120798	31.092	26664
		79.004	143268	36.562	33331
mp/°C	–112	84.710	169052	41.208	39997
		90.464	198543	48.884	53329
		96.225	232087	55.151	66661
		102.088	270110	60.489	79993
				65.163	93326
		bp/°C	67.72	66.034	95992
		Antoine eq.		66.886	98659

TABLE 16.1.8.8.1 (Continued)

Stull 1947		Pennington et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		eq. 2	P/mmHg	67.720	101325
		A	6.92846	25.0	20558
		B	1183.307		
		C	224.824	eq. 2	P/mmHg
				A	6.92846
				B	1193.307
				C	224.624
				bp/°C	67.72
				ΔH_v /(kJ mol ⁻¹) =	
				at 25°C	31.88
				at bp	29.53

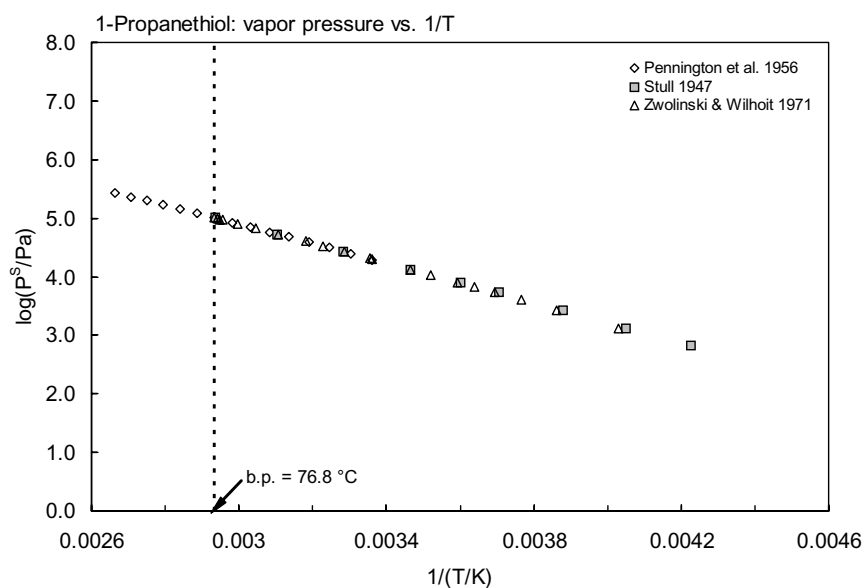
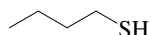


FIGURE 16.1.8.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1-propanethiol.

16.1.8.9 1-Butanethiol (Butyl mercaptan)



Common Name: 1-Butanethiol

Synonym: butyl mercaptan, *n*-butyl mercaptan

Chemical Name: 1-butanethiol

CAS Registry No: 109-79-5

Molecular Formula: $C_4H_{10}S$, $CH_3(CH_2)_3SH$

Molecular Weight: 90.187

Melting Point ($^{\circ}C$):

−115.7 (Weast 1982–83; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

98.5 (Lide 2003)

Density (g/cm^3 at $25^{\circ}C$):

0.8337 ($20^{\circ}C$, Weast 1982–83)

0.84159, 0.83674 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

107.8 (calculated-density, Stephenson & Malanowski 1987)

121.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

36.53, 32.225 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.46 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

597 (Riddick et al. 1986)

600 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19920* ($51.409^{\circ}C$, ebulliometry, measured range 51.4 – $135.7^{\circ}C$, Scott et al. 1957)

$\log(P/mmHg) = 6.92754 - 1281.018/(T/K + 218.100)$ (Antoine eq., Osborn & Douslin 1966)

5330*, 6070 ($22.4^{\circ}C$, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.92754 - 1281.018/(218.10 + t/^{\circ}C)$; temp range -2.0 to $123.37^{\circ}C$ (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.05296 - 1281.344/(218.139 + t/^{\circ}C)$, temp range 51.409 – $135.7^{\circ}C$ (Antoine eq. derived from Scott et al. 1957 data, Boublik et al. 1984)

6070 (Riddick et al. 1986)

$\log(P/kPa) = 6.05244 - 1281.018/(218.10 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.05011 - 1279.95/(-55.132 + T/K)$, temp range 323 – 409 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 6.92754 - 1281.018/(218.10 + t/^{\circ}C)$, temp range -2 to $123^{\circ}C$ (Antoine eq., Dean 1992)

$\log(P/mmHg) = 36.2672 - 3.0452 \times 10^3/(T/K) - 9.9743 \cdot \log(T/K) - 9.1432 \times 10^{-11} \cdot (T/K) + 3.2087 \times 10^{-6} \cdot (T/K)^2$; temp range 157 – 569 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

460.7 (distilled water, headspace-GC/FID, measured range 25 – $70^{\circ}C$, data in graph, Przyjazny et al. 1983)

$\log(1/K_{AW}) = 1655.9/(T/K) - 4.823$; temp range 25 – $70^{\circ}C$ (headspace-GC, Przyjazny et al. 1983)

911.4 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

363 ($20^{\circ}C$, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.823 - 1656/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.28 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.28 (recommended, Sangster 1989)
- 2.28 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 4.21 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{OH} = 4.55 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wine et al. 1984)

$k_{OH} = 5.82 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Barnes et al. 1986)

$k_{OH} = 5.11 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 16.1.8.9.1

Reported vapor pressures of 1-butanethiol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)		
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)		
$\log P = A - B/(C + T/K)$	(3)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)				
Scott et al. 1957	Zwolinski & Wilhoit 1971				
ebulliometry	selected values				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.409	19920	-2.0	1333	95.687	93326
57.130	25007	9.60	2666	96.630	95992
62.897	31169	16.9	4000	97.553	98659
68.710	38547	22.4	5333	98.456	101325
74.567	47359	26.9	6666	25.0	7399
80.472	57803	30.67	7999	eq. 2	P/mmHg
86.418	70109	36.86	10666	A	6.92854
92.414	84525	41.87	13332	B	1281.018
98.454	101325	51.506	19998	C	218.100
104.544	120798	58.786	26664	bp/°C	98.456
110.682	143268	64.170	33331	$\Delta H_v/(kJ\ mol^{-1}) =$	
116.863	169052	69.742	39997	at 25°C	36.53
123.088	198530	78.056	53329	at bp	32.23
129.362	232087	84.844	66661		
135.678	170110	90.625	79993		

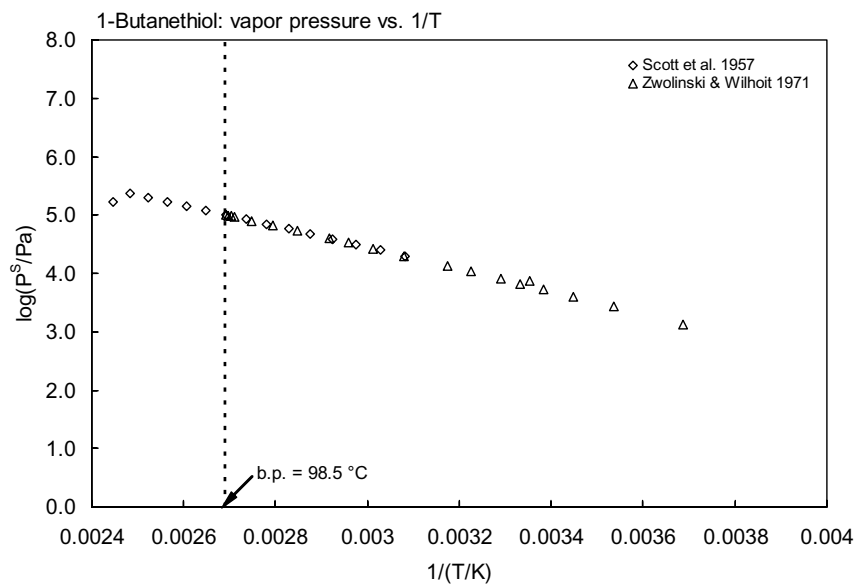
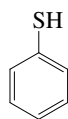


FIGURE 16.1.8.9.1 Logarithm of vapor pressure versus reciprocal temperature for 1-butanethiol.

16.1.8.10 Benzenethiol



Common Name: Benzenethiol

Synonym: thiophenol, phenyl mercaptan, mercaptobenzene

Chemical Name: benzenethiol

CAS Registry No: 108-98-5

Molecular Formula: C_6H_6S , C_6H_5SH

Molecular Weight: 110.177

Melting Point ($^{\circ}C$):

-14.93 (Lide 2003)

Boiling Point ($^{\circ}C$):

169.1 (Lide 2003)

Density (g/cm^3):

1.0766 ($20^{\circ}C$, Weast 1982-83)

Dissociation Constant, pK_a :

6.615 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

102.7 (calculated-density, Stephenson & Malanowski 1987)

106.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

45.35, 36.97 ($25^{\circ}C$, bp, Riddick et al 1986)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.45 (calorimetry at triple pt $258.27\ K$, Scott et al. 1956)

11.447 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133* ($18.6^{\circ}C$, summary of literature data, temp range 18.6 – $168^{\circ}C$, Stull 1947)

1333* ($51.5^{\circ}C$, ebulliometry, measured range 51.5 – $167.0^{\circ}C$, Vonterres et al. 1955)

19920* ($114.543^{\circ}C$, ebulliometry, measured range 114.543 – $7212.160^{\circ}C$, Scott et al. 1956)

$\log(P/mmHg) = 6.99019 - 1529.454/(230.048 + t/^{\circ}C)$; temp range 114.5 – $212^{\circ}C$ (comparative ebulliometry, data fitted to Antoine eq., Scott et al. 1956)

$\log(P/mmHg) = A \pm [1 - 442.298/(T/K)]$, where $\log A = 0.87370 - 6.4975 \times 10^{-4} \pm (T/K) + 5.2309 \times 10^{-7} \pm (T/K)^2$; measured range 114.5 – $212^{\circ}C$ (data fitted to Cox eq., comparative ebulliometry, Scott et al. 1956)

1333* ($52.28^{\circ}C$, derived from compiled data, temp range 52.3 – $198^{\circ}C$, Zwolinski & Wilhoit 1971)

$\log(P/mmHg) = 6.99019 - 1529.454/(230.048 + t/^{\circ}C)$; temp range 52.3 – $198^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log(P/kPa) = 6.11539 - 1529.668/(203.074 + t/^{\circ}C)$, temp range 114.54 – $212.16^{\circ}C$ (Antoine eq. derived from Scott et al. 1956 data, Boublik et al. 1984)

397 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.11509 - 1529.46/(t/^{\circ}C + 258.21)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.11531 - 1530.286/(-69.948 + T/K)$; temp range 385 – $486\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -5.4919 - 2.8549 \times 10^3/(T/K) + 8.1770 \cdot \log(T/K) - 1.9494 \times 10^{-2} \cdot (T/K) + 9.2817 \times 10^{-6} \cdot (T/K)^2$; temp range 258 – $69\ K$ (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

- 2.52 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.52 (recommended, Sangster 1989)
- 2.52 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

TABLE 16.1.8.10.1

Reported vapor pressures of benzenethiol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Vonterres et al. 1955		Scott et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		comparative ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
18.6	133.3	51.5	1333	114.543	19920	52.28	1333
43.7	666.6	71.5	5333	121.191	25007	65.79	2666
56.0	1333	87.8	6666	127.897	31160	74.38	4000
69.7	2666	97.4	9999	134.649	38547	80.81	5333
84.2	5333	105.5	13332	141.447	47359	86.01	6666
93.9	7999	116.3	19998	148.294	57803	90.40	7999
106.6	13332	124.5	26664	155.194	70109	97.61	10666
125.8	26664	131.3	33330	162.140	84525	103.444	13332
146.7	53329	136.5	39997	176.188	120789	114.655	19998
168.0	101325	141.5	46663	183.278	143268	123.120	26664
mp/°C	-	146.0	53329	190.426	169052	130.003	33331
		149.7	59995	197.623	198530	135.847	39997
		153.0	66661	204.867	232087	145.496	53329
		156.0	73327	212.160	270110	153.367	66661
		159.0	79993			160.067	79993
		162.0	86659	mp/K	258.27	165.932	93326
		165.0	93325	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 11.447$		167.024	95992
		167.0	101325	bp/K	416.9	168.092	98659
				169.138	101325		

(Continued)

TABLE 16.1.8.10.1 (Continued)

Stull 1947		Vonterres et al. 1955		Scott et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		ebulliometry		comparative ebulliometry		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				eq. 2	P/mmHg	169.653	102658
				A	6.99019	170.163	103991
				B	1529.454	171.167	106658
				C	203.048		
				temp range 114–212°C		eq. 2	P/mmHg
						A	6.99019
						B	1529.454
						C	203.048
						bp/°C	
						$\Delta H_v/(\text{kJ mol}^{-1}) = 40.6$	
						at normal bp	

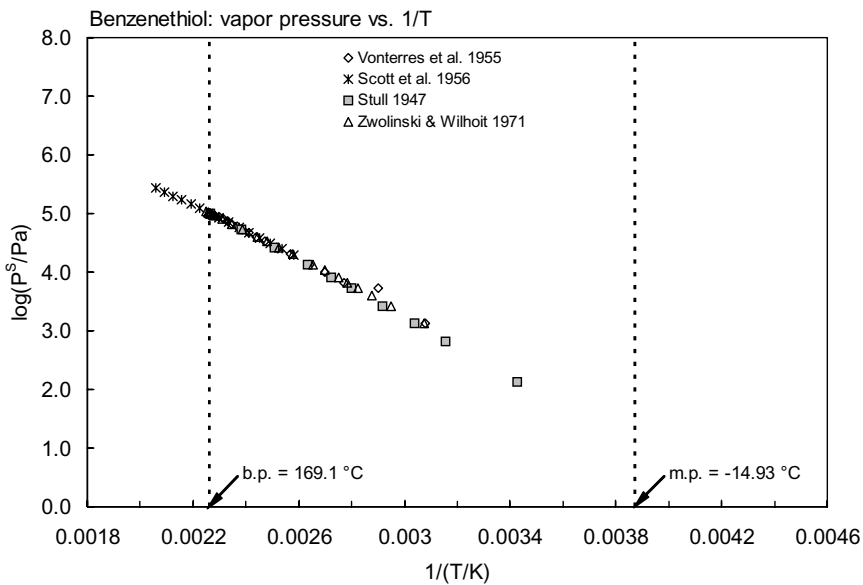


FIGURE 16.1.8.10.1 Logarithm of vapor pressure versus reciprocal temperature for benzenethiol.

16.1.8.11 Thiophene



Common Name: Thiophene

Synonym: thiofuran

Chemical Name: thiophene, thiofuran

CAS Registry No: 110-02-1

Molecular Formula: C_4H_4S

Molecular Weight: 84.140

Melting Point ($^{\circ}C$):

−38.21 (Lide 2003)

Boiling Point ($^{\circ}C$):

84.0 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.06485, 1.05887 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.0649 (Weast 1982–83)

1.06482, 1.05884 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

79.0 ($20^{\circ}C$, calculated from density)

88.10 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

34.6, 31.472 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.088 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3015 (shake flask-GC, Price 1976)

3900 (estimated-activity coefficient by headspace-GC, Przyjazny et al. 1983)

3600 ($18^{\circ}C$, Verschueren 1983)

3020 (selected, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9670* (interpolated-regression of tabulated data, temp range -40.7 to $81.4^{\circ}C$, Stull 1947)

7998 ($20.1^{\circ}C$, Stull 1947)

10622* (ebulliometry and manometry, measured range 0 – $84.155^{\circ}C$, Waddington et al. 1949)

10620 (calculated from determined data, Dreisbach 1955)

$\log (P/mmHg) = 6.95926 - 1246.038/(221.354 + t/^{\circ}C)$, temp range 5 – $155^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

482307* ($148.89^{\circ}C$, static-Bourdon gauge, measured range 148.89 – $304.44^{\circ}C$, Kobe et al. 1956)

44930* ($60.3^{\circ}C$, isoteniscope/manometry, measured range 60.3 – $100.3^{\circ}C$, Eon et al. 1971)

10670, 10660* ($25.09^{\circ}C$, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = 6.95926 - 1246.01/(221.35 + t/^{\circ}C)$; temp range -12.3 to $108.1^{\circ}C$ (Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/mmHg) = [-0.2185 \times 8748.3/(T/K)] + 8.273276$; temp range -40.7 to $84.4^{\circ}C$ (Antoine eq., Weast 1972–73)

2450 (calculated-Cox eq., Chao et al. 1983)

$\log (P/atm) = [1 - 394.395/(T/K)] \times 10^4 \{0.901276 - 10.3229 \times 10^{-4} \pm (T/K) + 21.9193 \times 10^{-7} \pm (T/K)^2\}$; temp range: 278.35 – $443.60\ K$ (Cox eq., Chao et al. 1983)

7998, 13330 (20°C, 30°C, quoted, Verschueren 1983)
 10622, 10620 (quoted exptl., calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.1336 - 1260.606/(222.787 + t/^\circ\text{C})$, temp range 0–40°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.0723 - 1138.803/(220.477 + t/^\circ\text{C})$, temp range 39.9–119.79°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 10620 (calculated-Antoine eq., Dean 1985, 1992)
 $\log(P/\text{mmHg}) = 6.95926 - 1246.02/(221.35 + t/^\circ\text{C})$, temp range –12 to 108°C (Antoine eq., Dean 1985, 1992)
 10620 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.08416 - 1246.02/(221.35 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 10600 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_S/\text{kPa}) = 9.84733 - 2447.236/(T/\text{K})$, temp range 195–228 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.06132 - 1232.35/(-53.438 + T/\text{K})$, temp range 311–393 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 36.6016 - 2.9794 \times 10^3/(T/\text{K}) - 10.104 \cdot \log(T/\text{K}) + 1.1445 \times 10^{-9} \cdot (T/\text{K}) + 3.2472 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 235–579 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

224, 236, 230 (headspace-GC, concn. of 10, 1.0 and 0.1 ppm by weight, measured range 25–70°C, data presented in graph, Przyjazny et al. 1983)
 $\log(1/K_{AW}) = 1563.6/(T/\text{K}) - 4.199$; temp range 25–70°C (headspace-GC, concn of 10 ppm by weight, Przyjazny et al. 1983)
 $\log(1/K_{AW}) = 1580.0/(T/\text{K}) - 4.277$; temp range 25–70°C (headspace-GC, concn of 1.0 ppm by weight, Przyjazny et al. 1983)
 $\log(1/K_{AW}) = 1661.9/(T/\text{K}) - 4.542$; temp range 25–70°C (headspace-GC, concn of 0.1 ppm by weight, Przyjazny et al. 1983)
 223.3 (calculated-P/C with selected values)
 296 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 182 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 4.542 - 1662/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.81 ± 0.01 (shake flask-UV, Iwasa et al. 1965)
 1.79 (calculated-f const., Rekker 1977)
 1.74 (HPLC-RV correlation, Garst 1984)
 1.82 (shake flask, Log P Database, Hansch & Leo 1987)
 1.81 (recommended, Sangster 1989, 1993)
 1.82 (shake flask-UV, Yamagami & Takao 1992)
 1.81 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and the Arrhenius expression see reference:

$k_{\text{OH}} = (9.58 \pm 0.38) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with calculated atmospheric lifetime $\tau \sim 28 \text{ h}$; and $k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ and $k_{\text{O}(^3\text{P})} = 4.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with $\text{O}(^3\text{P})$ atom at room temp. (relative rate method, Atkinson et al 1983)

$k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.004 \text{ d}^{-1}$, $k_{\text{OH}} = 9.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.8 d^{-1} ; $k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.7 d^{-1} at room temp. (review, Atkinson & Carter 1984)

$k_{\text{OH}}^* = (9.37, 9.57) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K , measured range $255\text{--}425 \text{ K}$ (flash photolysis-resonance fluorescence, Wine & Thompson 1984)

$k_{\text{OH}} = 9.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.004 \text{ d}^{-1}$, $k_{\text{OH}} = 9.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.4 d^{-1} , and $k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.7 d^{-1} at room temp. (review, Atkinson 1985)

$k_{\text{NO}_3} = (3.2 \pm 0.7) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 36 h and a loss rate of 0.7 d^{-1} assuming $2.4 \times 10^8 \text{ NO}_3 \text{ radicals/cm}^3$ in nighttime air at $295 \pm 1 \text{ K}$ in the atmosphere (relative rate technique, Atkinson et al. 1985)

$k_{\text{O}_3} < 6 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau > 270 \text{ d}$, $k_{\text{OH}} = 9.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 29 h during daytime hours, and $k_{\text{NO}_3} = 3.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated lifetime of 36 h at room temp. (review, Atkinson 1985)

$k_{\text{OH}}^* = 9.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{NO}_3} = 3.93 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range $272\text{--}296 \text{ K}$ (recommended, Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 14.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (molecular orbital calculations, (Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetime of $\sim 28 \text{ h}$ due to reactions with OH radical (Atkinson et al. 1983);

calculated gas-phase lifetime of 29 h for the reaction with OH radical during daytime hours, calculated lifetime of 36 h for reaction with NO_3 radical and a calculated lifetime $> 270 \text{ d}$ for reaction with O_3 at room temp. (Atkinson et al. 1985)

TABLE 16.1.8.11.1

Reported vapor pressures of thiophene at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Stull 1947	Waddington et al. 1949	Kobe et al. 1956	Zwolinski & Wilhoit 1971				
summary of literature data	manometry and ebulliometry	static-Bourdon gauge	selected values				
t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa
static method							
-40.7	133	0	2858	148.89	482307	-12.3	1333
-20.8	666.6	15	6497	154.44	585659	-1.10	2666
-10.9	1333	20	8355	160.00	620109	5.94	4000
0.0	2666	25	10627	165.56	730351	11.24	5333
12.5	5333	30	13398	171.11	813032	15.52	6666
20.1	7999	35	16733	176.67	895713	19.14	7999

(Continued)

TABLE 16.1.8.11.1 (Continued)

Stull 1947		Waddington et al. 1949		Kobe et al. 1956		Zwolinski & Wilhoit 1971	
summary of literature data		manometry and ebulliometry		static-Bourdon gauge		selected values	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
30.5	13332	40	20736	182.22	992174	25.09	10666
46.5	26664	ebulliometric method		187.78	1088636	29.90	13332
64.7	53329	39.061	19920	193.33	1198877	39.15	19998
81.4	101325	44.560	25007	198.89	1316009	46.14	26664
		50.094	31160	204.44	1440031	51.82	33331
mp/°C	-38.3	55.663	38547	210.00	1584723	56.65	39997
		61.276	47359	215.56	1722525	64.62	53329
		66.931	57903	221.11	1874107	71.12	66661
		72.629	70109	226.67	2039470	76.66	79993
Eon et al. 1971		78.370	84525	232.22	2211722	81.51	93326
isoteniscope-manometer		84.155	101325	237.78	2397755	82.41	95992
t/°C	P/Pa			243.33	2590678	83.30	98659
60.3	44930	mp/°C	-38.1	248.89	2797381	84.16	101325
70.3	64795	bp/°C	84.16	254.44	3010974		
80.3	91459			260.00	3238347	bp/°C	84.16
90.3	126790	eq. 2	P/mmHg	265.56	3472610		
100.3	172519	A	6.95926	271.11	3727544	eq. 2	P/mmHg
		B	1246.038	276.67	3996258	A	6.95926
		C	221.354	282.22	4251192	B	1246.02
$\Delta H_v/(kJ\ mol^{-1}) = 34.77$				287.78	4540576	C	221.35
		$\Delta H_v/(kJ\ mol^{-1}) =$		293.33	4836850		
		at 45.36°C	33.61	298.89	5146905	$\Delta H_v/(kJ\ mol^{-1}) =$	
		at 63.08°C	32.67	304.44	5463849	at 25°C	34.60
		at bp	31.47			at bp	31.47

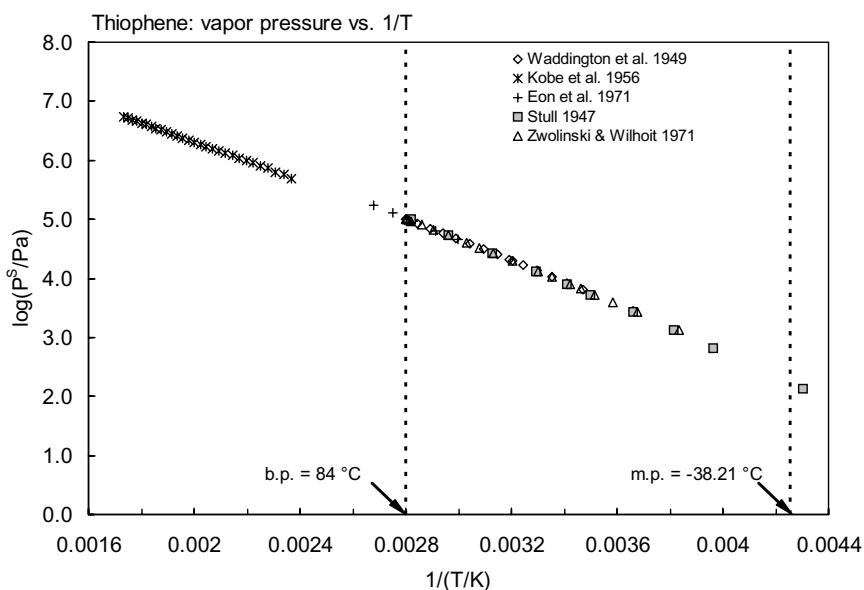
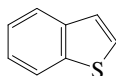


FIGURE 16.1.8.11.1 Logarithm of vapor pressure versus reciprocal temperature for thiophene.

16.1.8.12 Benzo[b]thiophene



Common Name: Benzo[b]thiophene

Synonym: thianaphthene, thionaphthene, 1-benzothiophene

Chemical Name:

CAS Registry No: 95-15-8

Molecular Formula: C_8H_6S

Molecular Weight: 134.199

Melting Point ($^{\circ}C$):

32 (Lide 2003)

Boiling Point ($^{\circ}C$):

221 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1500 (Verschuereen 1983)

Molar Volume (cm^3/mol):

139.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.854 (mp at $32^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

130.0 ($20^{\circ}C$, shake flask, Smith et al. 1978)

130.2 (Mill et al. 1981)

216* ($59.05^{\circ}C$, equilibrium cell-GC, measured range 332.2 – $490.5 K$, Leet et al. 1987)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

26.7 ($20^{\circ}C$, estimated from naphthalene, Smith et al. 1978)

14.80 (calculated-bp, Mackay et al. 1982)

$\log(P/mmHg) = -9.5352 - 2.6947 \times 10^3/(T/K) + 8.8858 \cdot \log(T/K) - 1.5478 \times 10^{-2} \cdot (T/K) + 6.5159 \times 10^{-6} \cdot (T/K)^2$;
temp range 305 – $754 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

28.0 (calculated-P/C, Smith & Bomberger 1980)

24.1 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.09 (shake flask-UV, pH 7.4, Rogers & Cammarata 1969)

3.05 (HPLC-RT correlation, De Voogt et al. 1988)

3.12 (recommended, Sangster 1989, 1993)

3.26 (shake flask-HPLC, De Voogt et al. 1990)

3.18 (HPLC-RT correlation, Ritter et al. 1994)

3.17 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.08 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, $\log K_{oc}$:

1.77 (Coyote Creek sediment, Smith et al. 1978)

2.30 (lab. mixture of microorganisms, Smith et al. 1978)

3.49, 3.0 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 45$ h in river, $t_{1/2} = 230$ h in eutrophic pond, $t_{1/2} = 180$ hours in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: rate constant of transformation and transport of $(6.9 \pm 0.7) \times 10^{-7} \text{ s}^{-1}$ exposed to 12 h sunlight per day in late May with estimated $t_{1/2} = 1200$ h in river, $t_{1/2} = 2900$ h in eutrophic pond, $t_{1/2} = 3500$ h in eutrophic lake and $t_{1/2} = 600$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

Oxidation:

laboratory investigated $k = 83 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical and estimated $t_{1/2} = 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978)
 $k = 5.7 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 34$ h under natural sunlight conditions, $k = 83 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 96$ d for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: estimated $t_{1/2} > 20$ h in river, $t_{1/2} < 20$ h in eutrophic pond, $t_{1/2} = 20$ h in eutrophic lake and very long half-life in oligotrophic lake, based on the biodegradation rate in the presence of alternative carbon sources will be one-half the biodegradation rate of quinoline when quinoline is the only carbon source by the one compartment model (Smith et al. 1978).

Biotransformation:

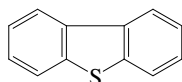
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: estimated volatilization $t_{1/2} = 45$ h in river, $t_{1/2} = 230$ h in eutrophic pond, $t_{1/2} = 180$ h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978);

photolysis rate constant of transformation and transport of $(6.9 \pm 0.7) \times 10^{-7} \text{ s}^{-1}$ exposed to 12 h sunlight per day in late May with estimated photolysis $t_{1/2} = 1200$ h in river, $t_{1/2} = 2900$ h in eutrophic pond, $t_{1/2} = 3500$ h in eutrophic lake and $t_{1/2} = 600$ h in oligotrophic lake by the one compartment model (Smith et al. 1978).

16.1.8.13 Dibenzothiophene



Common Name: Dibenzothiophene

Synonym:

Chemical Name: dibenzothiophene

CAS Registry No: 132-65-0

Molecular Formula: $C_{12}H_8S$

Molecular Weight: 184.257

Melting Point ($^{\circ}C$):

98.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

332.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

191.3 (calculated-Le Bas method at normal boiling point)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.191 (mp at $98.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.11 \pm 0.09 ($28^{\circ}C$, measured, Smith et al. 1978)

1.470 ($24^{\circ}C$, shake flask-LSC, Means et al. 1980)

1.106 (Mill et al. 1981)

1.500 (Steen & Karickhoff 1981)

1.032 (literature average, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.267 ($20^{\circ}C$, estimated, Aubry et al. 1975)

$\log(P/mmHg) = 22.90 - 10910/(T/K)$, temp range $60-00^{\circ}C$ (solid, gas saturation, Edward & Prausnitz 1981)

$\log(P/mmHg) = 21.10 - 8353/(T/K)$, temp range $100-130^{\circ}C$ (liquid, gas saturation, Edward & Prausnitz 1981)

0.263, 0.0083 ($20^{\circ}C$, quoted, calculated-bp, Mackay et al. 1982)

0.893 (static apparatus-extrapolated from Chebyshev polynomials, Sivaraman & Kobayashi 1982)

0.586 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/atm) = [1 - 605.160/(T/K)] \times 10^4 \{0.865373 - 5.51221 \times 10^{-4} \pm (T/K) + 6.05701 \times 10^{-7} \pm (T/K)^2\}$; temp range: $424.81-607.53$ K (Cox eq., Chao et al. 1983)

$\log(P_L/kPa) = 7.18577 - 3140.15/(T/K)$, temp range $385-574$ K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

44.3 (calculated-P/C, Smith & Bomberger 1980)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.38 (shake flask-LSC, Means et al. 1980)

4.33 (HPLC-RT correlation, De Voogt et al. 1988)

4.38 (recommended, Sangster 1989, 1993)

4.49 (shake flask-HPLC, De Voogt et al. 1990)

4.38 (recommended, Hansch et al. 1995)

4.41 ± 0.19 , 4.43 ± 0.61 (HPLC- k' correlation: ODS-65 column, Diol-35 column, Helweg et al. 1997)

4.36 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

3.20 (mixed microbial populations, Steen & Karickhoff 1981)

Sorption Partition Coefficient, log K_{OC} :

3.14 (Coyote Creek sediment, Smith et al. 1978)
 4.05 (soil, Hassett et al. 1980)
 4.05 (average of 3 sediment/soil samples, equilibrium sorption isotherm, Means et al. 1980)
 4.00 (soil, calculated-MCI χ , Sabljic 1987)
 4.00 (soil, calculated-MCI χ , Sabljic 1987)
 4.17 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987)
 3.75 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987)
 2.92 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987)
 4.00 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987)
 3.60 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987)
 4.59 (humic acid, HPLC- k' correlation, Nielsen et al. 1997)
 3.87 (soil: organic carbon OC $\geq 0.1\%$, average, Delle Site 2001)
 4.02, 4.04 (sediments: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)
 4.07 (Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 140$ h in river, $t_{1/2} = 720$ h in eutrophic pond, $t_{1/2} = 580$ h in eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978).

Photolysis: solar photolysis $k = 1.5 \times 10^{-8} \text{ s}^{-1}$ over 24-h day; rate constant of transformation and transport of $(2.04 \pm 0.08) \times 10^{-6} \text{ s}^{-1}$ exposed to 12 h sunlight per day in early March with estimated $t_{1/2} = 380$ h in river, $t_{1/2} = 950$ h in eutrophic pond and eutrophic lake and $t_{1/2} = 190$ h in oligotrophic lake from average photolysis rates on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978); $t_{1/2} = 4\text{--}8$ h for disappearance via direct photolysis in aquatic media (Harris 1982).

Oxidation: laboratory investigated $k < 7.5 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical and estimated $t_{1/2} > 10^5$ h in river, eutrophic pond, eutrophic lake and oligotrophic lake by the one compartment model (Smith et al. 1978). $k = 1.5 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 128$ h under natural sunlight conditions, $k < 7.5 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} > 3.5$ yr for free-radical oxidation in air-saturated water (NRCC 1983)

Hydrolysis:

Biodegradation: $k = 5.3 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ and the estimated $t_{1/2} = 13$ h in river, eutrophic pond, and eutrophic lake and $t_{1/2} > 10^4$ h in oligotrophic lake by the one compartment model (Smith et al. 1978)

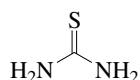
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: $t_{1/2} = 0.5$ h from river water, $t_{1/2} = 13$ h from pond water, $t_{1/2} = 13$ h from eutrophic lake and $t_{1/2} = 140$ h from oligotrophic lake predicted by one-compartment model for all processes; estimated volatilization $t_{1/2} = 140$ h in river, $t_{1/2} = 720$ h in eutrophic pond, $t_{1/2} = 580$ h in eutrophic lake and oligotrophic lake; photolysis rate constant of transformation and transport $k = (2.04 \pm 0.08) \times 10^{-6} \text{ s}^{-1}$ exposed to 12 h sunlight per day in early March with estimated photolysis $t_{1/2} = 380$ h in river, 950 h in eutrophic pond and eutrophic lake and $t_{1/2} = 190$ h in oligotrophic lake; biodegradation $t_{1/2} = 13$ h in river, eutrophic pond water and $t_{1/2} = 140$ h in oligotrophic lake (Smith et al. 1978); $t_{1/2} = 4\text{--}8$ h for disappearance via direct photolysis in aqueous media (Harris 1982).

16.1.8.14 Thiourea



Common Name: Thiourea

Synonym: thiocarbamide

Chemical Name: thiourea

CAS Registry No: 62-56-6

Molecular Formula: $\text{CH}_4\text{N}_2\text{S}$, H_2NCSNH_2

Molecular Weight: 76.121

Melting Point ($^{\circ}\text{C}$):

178 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

decomposes (Verschuereen 1983)

Density (g/cm^3 at 20°C):

1.045 (Weast 1982–83; Verschuereen 1983, Dean 1992)

Dissociation Constant, pK :

2.03 (pK_1 , Dean 1985)

Molar Volume (cm^3/mol):

76.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.42 (Donnelly et al. 1990)

12.55 (Kim et al. 1994)

15.64, 14.92, 15.17 (differential scanning calorimetry in three types of crucibles, Gatta et al. 2000)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

35.2, 33.7, 34.1 (Gatta et al. 2000)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F : 0.0315 (mp at 178°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

91000 (20 – 25°C , shake flask-gravimetric, Dehn 1917)

91800 (13°C , Verschuereen 1983)

89800 (Windholz 1983)

110000 (Budavari 1989)

90000 (Dean 1985)

Vapor Pressure (Pa at 25°C):

Henry's Law Constant (Pa m^3/mol at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

−1.02 (Leo et al. 1971)

−0.95 (shake flask, Cornford 1982)

−2.38, −0.95 (calculated, Verschuereen 1983)

−1.17 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)

−1.08, −1.03 (pH 6.5, pH 12, shake flask-HPLC, Govers et al. 1986)

−1.14, −1.02 (shake flask, Log P Database, Hansch & Loe 1987)

−0.99 (recommended, Sangster 1993)

−1.02 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.73 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)

−0.699 (alga *Chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 1.6\text{--}16$ h in air, based on rate constant for the vapor-phase reaction with OH radical and photooxidation $t_{1/2} = 2048\text{--}81927$ h in water, based on estimated rate data for reaction with OH radical in aqueous solution (Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 24\text{--}168$ h, based on aqueous aerobic screening test data and aqueous anaerobic biodegradation $t_{1/2} = 96\text{--}672$ h, based on aqueous aerobic degradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: $t_{1/2} = 1.6\text{--}16$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

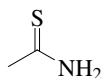
Ground water: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biota:

16.1.8.15 Thioacetamide



Common Name: Thioacetamide

Synonym: ethanethioamide, acetothioamide

Chemical Name: thioacetamide

CAS Registry No: 62-55-5

Molecular Formula: C_2H_5NS , CH_3CSNH_2

Molecular Weight: 75.133

Melting Point ($^{\circ}C$):

115.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

84.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.129 (mp at $115.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

163000 (Dean 1985)

163000 (Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

-0.46, 0.36 (Verschuere 1983)

-0.26 (shake flask, Log P Database, Hansch & Leo 1987)

-0.26 (recommended, Sangster 1993)

-0.26 (recommended, Hansch & Leo 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric $t_{1/2} = 3.2\text{--}31.7$ h, based on estimated rate data for OH radical in air (Howard et al. 1991).

Hydrolysis: first-order rate constant $k = 8.6 \times 10^{-1} h^{-1}$ at pH 7 and $25^{\circ}C$ (Ellington et al. 1987), corresponding to a $t_{1/2} = 8064$ h (Howard et al. 1991);

acid rate constant $k = 6.0 \times 10^{-2} M^{-1} \pm h^{-1}$, corresponding to a $t_{1/2} = 333$ d and base rate constant $k = 1.4 M^{-1} \pm h^{-1}$, corresponding to a $t_{1/2} = 289$ d (Howard et al. 1991).

Biodegradation: aerobic biodegradation $t_{1/2} = 24\text{--}168$ h, based on aqueous aerobic screening test data and anaerobic biodegradation $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 3.2\text{--}31.7$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 24\text{--}268$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

16.2 SUMMARY TABLES

TABLE 16.2.1
Summary of physical properties of nitrogen and sulfur containing compounds

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol		pK _a or pK _b
							MW/ ρ at 20°C	Le Bas	
Nitriles:									
Acetonitrile	75-05-8	CH ₃ CN	41.052	−43.82	81.65	1	52.25	56.3	
Propionitrile	107-12-0	C ₂ H ₅ CN	55.079	−92.78	97.14	1	70.45	78.5	
Butyronitrile	109-74-0	C ₃ H ₇ CN	69.106	−111.9	117.6	1	87.35	100.7	
Acrylonitrile (2-Propenitrile)	107-13-1	C ₂ H ₃ CN	53.063	−83.48	77.3	1	65.83	71.1	
Benzonitrile	100-47-0	C ₆ H ₅ CN	103.122	−13.99	191.1	1		107.9	
Adiponitrile	111-69-3	CN(CH ₂) ₄ CN	108.141	1	295	1		149.6	
Aliphatic amines:									
Methylamine	74-89-5	CH ₃ NH ₂	31.058	−93.5	−6.32	1		43.8	
Dimethylamine	124-40-3	(CH ₃) ₂ NH	45.084	−92.18	6.88	1	68.77	67.5	10.77
Trimethylamine	75-50-3	(CH ₃) ₃ N	59.110	−117.1	2.87	1	93.00	93.3	9.8
Ethylamine	75-04-7	CH ₃ CH ₂ NH ₂	45.084	−80.5	16.5	1	66.02	66.0	10.63
Diethylamine	109-89-7	(C ₂ H ₅) ₂ NH	73.137	−49.8	55.5	1	103.45	111.9	10.8
Triethylamine	121-44-8	(C ₂ H ₅) ₃ N	101.910	−114.7	89	1		154.8	10.78
<i>n</i> -Propylamine	107-10-8	C ₃ H ₇ NH ₂	59.110	−84.75	47.22	1	82.41	88.2	10.568
Dipropylamine	142-84-7	(C ₃ H ₇) ₂ NH	101.190	−63	109.3	1			
Diisopropylamine	108-18-9	<i>i</i> (C ₃ H ₇) ₂ NH	101.190	−61	83.9	1			
Tripropylamine	102-69-2	(C ₃ H ₇) ₃ N	143.270	−93.5	156	1			10.66
<i>n</i> -Butylamine	109-73-9	C ₄ H ₉ NH ₂	73.137	−49.1	77.0	1	98.94	110.4	10.64
Isobutylamine	78-81-9	<i>i</i> C ₄ H ₉ NH ₂	73.137	−86.7	67.75	1		110.4	10.41
<i>tert</i> -Butylamine	75-64-9	(CH ₃) ₃ CNH ₂	73.137	−66.94	44.04	1		110.4	1.685
Di- <i>n</i> -butylamine	111-92-2	(C ₄ H ₉) ₂ NH	129.244	−62	159.6	1		199.2	11.25
Tributylamine	102-82-9	(C ₄ H ₉) ₃ N	185.349	−70	216.5	1		288	9.93
Ethylenediamine	107-15-3	H ₂ NCH ₂ CH ₂ NH ₂	60.098	11.14	117	1			
Ethanolamine	141-43-5	HOCH ₂ CH ₂ NH ₂	61.098	10.5	171	1	60.21	73.4	9.48
Diethanolamine	111-42-2	(HOCH ₂ CH ₂) ₂ NH	105.136	28	268.8	0.934	95.87	126.7	8.88
Triethanolamine	102-71-6	(HOCH ₂ CH ₂) ₃ N	149.188	20.5	335.4	1	132.71	182.1	7.76
Cyclohexylamine	108-91-8	C ₆ H ₁₂ NH	99.174	−17.8	134	1		117.4	10.66

(Continued)

TABLE 16.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol		pK _a or pK _b
							MW/ ρ at 20°C	Le Bas	
Aromatic amines:									
Aniline	62-53-3	C ₆ H ₅ NH ₂	93.127	−6.02	184.17	1	91.15	110.2	4.596
2-Chloroaniline	95-51-2	Cl(C ₆ H ₄)NH ₂	127.572	−1.9	208.8	1	105.21	131.1	2.661
3-Chloroaniline	108-42-9	Cl(C ₆ H ₄)NH ₂	127.572	−10.28	230.5	1	104.91	131.1	3.5
4-Chloroaniline	106-47-8	Cl(C ₆ H ₄)NH ₂	127.572	70.5	232	0.358		131.1	3.982
3,4-Dichloroaniline	95-76-1	Cl ₂ C ₆ H ₃ NH ₂	162.017	72	272	0.346		152.0	
2,4,6-Trichloroaniline	634-93-5	C ₆ H ₄ Cl ₃ N	196.462	78.5	262	0.299		172.9	
<i>o</i> -Toluidine	95-53-4	CH ₃ C ₆ H ₄ NH ₂	107.153	−14.41	200.3	1	107.32	132.4	4.45
<i>m</i> -Toluidine	108-44-1	CH ₃ C ₆ H ₄ NH ₂	107.153	−31.3	203.3	1	108.36	132.4	4.71
<i>p</i> -Toluidine	106-49-0	CH ₃ C ₆ H ₄ NH ₂	107.153	43.6	200.4	0.657	111.40	132.4	5.08
N,N′-Dimethylaniline	121-69-7	C ₆ H ₅ N(CH ₃) ₂	121.180	2.42	194.15	1	126.80	154.6	5.15
2,4-Xylidine	95-68-1	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.180	−14.3	214	1		154.6	4.89
2,5-Xylidine	95-78-3	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.180	15.5	214	1		154.6	4.54
2,6-Xylidine	87-62-7	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.180	11.2	215	1	123.12	154.6	3.95
2-Ethylaniline	578-54-1	C ₂ H ₅ C ₆ H ₄ NH ₂	121.180	−43	209.5	1		139.6	4.42
3-Ethylaniline	587-02-0	C ₂ H ₅ C ₆ H ₄ NH ₂	121.180	−64	214	1		139.6	4.70
4-Ethylaniline	589-16-2	C ₂ H ₅ C ₆ H ₄ NH ₂	121.180	−2.4	217.5	1		139.6	5.00
N,N′-Diethylaniline	91-66-7	C ₆ H ₅ N(C ₂ H ₅) ₂	149.233	−38.8	216.3	1		199.0	6.56
Diphenylamine	122-39-4	(C ₆ H ₅) ₂ NH	169.222	53.2	302	0.529	145.88	200.3	0.90
4-Aminobiphenyl	92-67-1	C ₆ H ₅ C ₆ H ₄ NH ₂	169.222	53.5	302	0.525		168.8	4.27
Benzidine	92-87-5	NH ₂ (C ₆ H ₄) ₂ NH ₂	184.236	120	401	0.117		213.0	4.66
3,3′-Dichlorobenzidine	91-94-1	C ₁₂ H ₁₀ Cl ₂ N ₂	253.126	132.5		0.0882		254.8	11.7
α-Naphthylamine	134-32-7	C ₁₀ H ₇ NH ₂	143.185	49.2	300.7	0.579		161.8	3.92
β-Naphthylamine	91-59-8	C ₁₀ H ₇ NH ₂	143.185	113	306.2	0.137		161.8	4.15
N,N′-Bianiline	122-66-7	(C ₆ H ₅) ₂ (NH) ₂	184.236	131		0.0912		213.0	13.2
2-Nitroaniline	88-74-4	C ₆ H ₆ N ₂ O ₂	138.124	71.0	284	0.354		138.7	−0.28
3-Nitroaniline	99-09-2	C ₆ H ₆ N ₂ O ₂	138.124	113.4	306 dec	0.136		138.7	2.46
4-Nitroaniline	100-01-6	C ₆ H ₆ N ₂ O ₂	138.124	147.5	332	0.0628	97.00	138.7	1.01
2,4-Dinitroaniline	97-02-9	(O ₂ N) ₂ C ₆ H ₃ NH ₂	183.122	180.0		0.0301		167.2	−4.25
2,6-Dinitroaniline	606-22-4	(O ₂ N) ₂ C ₆ H ₃ NH ₂	183.122	141		0.0728		167.2	−5.23
3,5-Dinitroaniline	618-87-1	(O ₂ N) ₂ C ₆ H ₃ NH ₂	183.122	163		0.0443		167.2	0.229

Nitroaromatic compounds:

Nitrobenzene	98-95-3	$C_6H_5NO_2$	123.110	5.7	210.8	1	102.28	112.0
1,2-Dinitrobenzene	528-29-0	$C_6H_4(NO_2)_2$	168.107	116.5	318	0.127		149.4
1,3-Dinitrobenzene	99-65-0	$C_6H_4(NO_2)_2$	168.107	90.3	291	0.229		149.4
1,4-Dinitrobenzene	100-25-4	$C_6H_4(NO_2)_2$	168.107	173.5	297	0.0349		149.4
2-Nitrotoluene	88-72-2	$CH_3C_6H_4NO_2$	137.137	-10.4	222	1	117.93	153.0
3-Nitrotoluene	99-08-1	$CH_3C_6H_4NO_2$	137.137	15.5	232	1		153.0
4-Nitrotoluene	99-99-0	$CH_3C_6H_4NO_2$	137.137	51.63	238.3	0.548		153.0
2,4-Dinitrotoluene (DNT)	121-14-2	$CH_3C_6H_3(NO_2)_2$	182.134	70.5	300 dec	0.358		175.2
2,6-Dinitrotoluene	606-20-2	$CH_3C_6H_3(NO_2)_2$	182.134	66.0	285	0.396		175.2
2,4,6-Trinitrotoluene (TNT)	118-96-7	$CH_3C_6H_2(NO_2)_3$	227.131	80.5	240 exp	0.285	137.32	203.7
1-Nitronaphthalene	86-57-7	$C_{10}H_7NO_2$	173.169	61	304	0.443		176.1
2-Nitronaphthalene	581-89-5	$C_{10}H_7NO_2$	173.169	79	314	0.295		176.1
4-Nitrobiphenyl	92-93-3	$C_{12}H_9NO_2$	199.205	114	340	0.134		211.3
5-Nitro-acenaphthene	602-87-9	$C_{12}H_9NO_2$	199.205	103		0.172		211.3

Amide and ureas:

Acetamide	60-35-5	CH_3CONH_2	59.067	80.16	222	0.288		66.9	7.62
Acrylamide	79-06-1	$H_2C=CHCONH_2$	71.078	84.5	192.5	0.261		80.8	
Benzamide	55-21-0	$C_6H_5CONH_2$	121.137	127.3	290	0.0992		132.4	
Urea	57-13-6	H_2NCONH_2	60.055	133	dec	0.0872	45.39	58.0	

Nitrosoamines:

<i>N</i> -Nitrosodimethylamine	62-75-9	$(CH_3)_2NNO$	74.081		152			87.7	
<i>N</i> -Nitrosodiethylamine	55-18-5	$(C_2H_5)_2NNO$	120.134		176.9			130.6	
Di- <i>n</i> -propyl nitrosamine	621-64-7	$(C_3H_7)_2NNO$	130.187		206			176.5	
Diphenylnitrosamine	86-30-6	$(C_6H_5)_2NNO$	198.219	66.5	152	0.392		220.5	

Heterocyclic compounds:

1 <i>H</i> -Pyrrole	109-97-7	C_4H_5N	67.090	-23.39	129.79	1	69.18	78.2	
1-Methylpyrrole	96-54-8	C_5H_7N	81.117	-56.32	112.81	1		104.0	
Pyrrolidine	123-75-1	C_4H_8NH	71.121	-57.79	86.56	1		96.6	4.453
Imidazole	288-32-4	$C_3H_4N_2$	68.077	89.5	257	0.233		78.9	11.305
Indazole	271-44-3	$C_7H_6N_2$	118.136	148	269	0.0621		130.5	
Indole	120-72-9	C_8H_7N	117.149	52.5	253.6	0.537		133.4	
Indoline	496-15-1	C_8H_9N	119.164		229			140.8	
Pyridine	110-86-1	C_5H_5N	79.101	-41.70	115.23	1	80.56	93.0	5.17
2-Methylpyridine	109-06-8	C_6H_7N	93.127	-66.68	129.38	1	98.61	115.2	5.96
3-Methylpyridine	108-99-6	C_6H_7N	93.127	-18.14	144.14	1	97.35	115.2	5.68
4-Methylpyridine	108-89-4	C_6H_7N	93.127	3.67	145.36	1		115.2	6.00

(Continued)

TABLE 16.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol		pK _a or pK _b
							MW/ ρ at 20°C	Le Bas	
2,3-Dimethylpyridine	583-61-9	C ₇ H ₉ N	107.153	-15.5	161.12	1		135.9	6.6
2,4-Dimethylpyridine	108-47-4	C ₆ H ₉ N	107.153	-64	158.38	1		135.9	
2,6-Dimethylpyridine	108-48-5	C ₇ H ₉ N	107.153	-6.1	144.01	1		135.9	6.72
2,4,6-Trimethylpyridine	108-75-8	C ₈ H ₁₁ N	121.180	-46	170.6	1		158.1	7.43
Quinolines:									
Quinoline	91-22-5	C ₉ H ₇ N	129.159	-14.78	237.16	1		144.7	4.90
Isoquinoline	119-65-3	C ₉ H ₇ N	129.159	26.47	243.22	0.967		144.7	5.4
3-Methyl-isoquinoline	1125-80-0	C ₁₀ H ₉ N	143.185	68	249	0.379		166.9	
2,7-Dimethylquinoline	93-37-8	C ₁₁ H ₁₁ N	157.212	61	264.5	0.443		189.1	
Benzo[f]quinoline	85-02-9	C ₁₃ H ₉ N	179.217	94	352	0.210		196.3	
Benzo[h]quinoline	230-27-3	C ₁₃ H ₉ N	179.217	52	339	0.543		196.3	
9H-Carbazole	86-74-8	C ₆ H ₄ NHC ₆ H ₄	167.206	246.3	354.69	0.00674		192.9	
7H-Dibenzo[c,g]carbazole	194-59-2	(C ₁₀ H ₆) ₂ NH	267.324	158		0.0496		296.1	
Acridine	260-94-6	C ₁₃ H ₉ N	179.217	110	344.86	0.147		196.3	5.60
Benz[a]acridine	225-11-6	C ₁₇ H ₁₁ N	229.276					244.8	
Benz[c]acridine	225-51-4	C ₁₇ H ₁₁ N	229.276	132		0.0892		244.8	
Dibenz[a,h]acridine	53-70-3	C ₂₂ H ₁₄	278.346	269.5	524	0.00399		300.0	
Sulfur compounds:									
Carbon disulfide	75-15-0	CS ₂	76.141	-112.1	46	1	60.28	66.0	
Dimethyl sulfate	77-78-1	(CH ₃ O) ₂ SO ₂	126.132	-27	188 dec	1		109.7	
Diethyl sulfate	64-67-5	(C ₂ H ₅ O) ₂ SO ₂	154.185	-24	208	1		138.4	
Dimethyl sulfite	616-42-2	(CH ₃ O) ₂ SO	110.132		126			100.5	
Dimethyl sulfoxide (DMSO)	67-68-5	(CH ₃) ₂ SO	78.133	17.89	189	1		85.7	
Dimethyl sulfone	67-71-0	(CH ₃) ₂ SO ₂	94.133	108.9	238	0.150		94.0	
Dimethyl sulfide	75-18-3	(CH ₃) ₂ S	62.134	-98.24	37.33	1	73.77	77.4	
Dimethyl disulfide	624-92-0	C ₂ H ₆ S ₂	94.199	-84.67	109.74	1	58.78	103.0	
Diethyl sulfide	352-93-2	C ₄ H ₁₀ S	90.187	-103.91	92.1	1		128.1	
Diethyl disulfide	110-81-6	C ₄ H ₁₀ S ₂	122.252	-101.5	154.0	1		147.4	
Thiols:									
Methanethiol	74-93-1	CH ₃ SH	48.108	-123	5.9	1	55.52	55.2	10.7
Ethanethiol	75-08-1	C ₂ H ₅ SH	62.134	-147.88	35.0	1	74.05	77.4	10.61
Propanethiol	107-03-9	C ₃ H ₇ SH	76.161	-113.13	67.8	1	90.55	99.6	
1-Butanethiol (Butyl mercaptan)	109-79-5	CH ₃ (CH ₂) ₃ SH	90.187	-115.7	98.5	1	107.16	121.8	

2-Butanethiol	513-53-1	C ₄ H ₇ SH	90.187	-165	85.0	1		121.8	
Benzenethiol	108-98-5	C ₆ H ₅ SH	110.177	-14.93	169.1	1	102.34	106.8	6.5
2-Methylbenzenethiol	137-06-4	C ₇ H ₈ S	124.204	15	195	1		129.0	
3-Methylbenzenethiol	108-40-7	C ₇ H ₈ S	124.204	-20	195	1		129.0	
4-Methylbenzenethiol	106-45-6	C ₇ H ₈ S	124.204	43	195	0.666		129.0	
Thiophenes:									
Thioazole	288-47-1	C ₃ H ₃ NS	85.128	-33.62	118	1		85.2	
Thiophene	110-02-1	C ₄ H ₄ S	84.140	-38.21	84.0	1	79.02	88.1	
2-Methylthiophene	554-14-3	C ₅ H ₆ S	98.167	-63.4	112.6	1		110.3	
3-Methylthiophene	616-44-4	C ₅ H ₆ S	98.167	-69	115.5	1		110.3	
Benzo[<i>b</i>]thiophene	95-15-8	C ₈ H ₆ S	134.199	32	221	0.854		139.7	
Dibenzothiophene	132-65-0	C ₁₂ H ₈ S	184.257	98.2	332.5	0.191		191.3	
Thianthrene	92-85-3	(C ₆ H ₄) ₂ S ₂	216.322	159.3	365	0.0481		210.9	
Thiobenzamide	2227-79-4	C ₆ H ₅ CSNH ₂	137.203	117		0.125		135.8	
Thiourea	62-56-6	H ₂ NCSNH ₂	76.121	178		0.0315	72.84	76.2	2.03
Thioacetamide	62-55-5	CH ₃ CSNH ₂	75.133	115.5		0.129		84.2	

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$

TABLE 16.2.2

Summary of selected physical-chemical properties of nitrogen and sulfur containing compounds at 25°C.

Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility			log K _{OW}	H/(Pa·m ³ /mol)	
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		calcd P/C	exptl
Nitriles:								
Acetonitrile	11840	11840	miscible			−0.34		2.75
Propionitrile	5950	5950	103000	1870.0	1870.0	0.16	3.182	3.8
Butyronitrile	2546	2546	33000	477.5	477.5			5.263
Benzonitrile	100	100	2000	19.39	19.39	1.55	5.156	
Acrylonitrile (2-Propenitrile)	11000	11000	75500	1423	1423	0.25	7.731	11.14
Adiponitrile	0.3066	0.3066	8000	73.96	73.96	−0.32	0.0041	
Aliphatic amines:								
Methylamine	357300	357300	miscible			−0.57		1.125
Dimethylamine	206200	206200	miscible			−0.38		1.8
Trimethylamine	219300	219300	miscible			0.27		6.67
Ethylamine	141650	141650	miscible			−0.13		1.012
Diethylamine	31490	31490	miscible			0.43		2.60
Triethylamine	7610	7610	55000	540	540	1.64	14.099	
<i>n</i> -Propylamine	40740	40740	miscible			0.48		1.274
Dipropylamine			53000	520	520			
Diisopropylamine			12390	122				
Tripropylamine			220	1.536	1.54	2.79		
<i>n</i> -Butylamine	13650	13650	miscible			0.97		1.526
Isobutylamine	18760	18760	miscible			0.73		
<i>t</i> -Butylamine	48260	48260	miscible			0.4		
Di- <i>n</i> -butylamine	304	304	4700	36.37	36.37	2.83	8.359	
Tributylamine	5330	5330	40	0.216	0.216		2.47 × 10 ⁴	
Ethanolamine	34.66	34.66	miscible			−1.31		
Diethanolamine	0.0373	0.0399	miscible			−1.43		
Triethanolamine	4.79 × 10 ^{−4}	4.79 × 10 ^{−4}	miscible			−1.59		
Cyclohexylamine	1173	1173	miscible			1.49		
Diphenylamine	0.0612	0.115	300	1.773	3.338	3.45	0.035	
α-Naphthylamine	0.254	0.45				2.23		
β-Naphthylamine	0.035	0.248	6.4	0.045	0.317	2.34		
4-Aminobiphenyl						2.83		

Aromatic amines:

Aniline	65.19	65.19	36070	387.4	387.35	0.90	0.168	12.16
2-Chloroaniline	22.66	22.66	3800	29.79	29.79	1.90	0.761	
3-Chloroaniline	9.53	9.530	5440	42.64	42.64	1.88	0.223	
4-Chloroaniline	2.33	6.873	3000	23.52	69.37	1.83	0.099	
3,4-Dichloroaniline	1.3	3.746	92.05	0.568	1.637	2.67	2.289	
2,4,6-Trichloroaniline	0.00626	0.021				3.694		
<i>o</i> -Toluidine	13.3	13.30	15000	139.98	139.98		0.095	
<i>m</i> -Toluidine	36	36.0	15030	140.26	140.26	1.44	0.257	
<i>p</i> -Toluidine	45	61.48	7350	68.59	93.70	1.4	0.656	
N,N'-Dimethylaniline	107	107.0	1105	9.119	9.119	2.31	11.734	
2,4-Xylidine	20.5	20.50	5900	48.69	48.69		0.421	
2,5-Xylidine			5000	41.26	41.26			
2,6-Xylidine	670	670.0	4700	38.79	38.79	1.94	17.275	
2-Ethylaniline			7500	61.89	61.89	1.93		
4-Ethylaniline	13.5	13.50	5100	42.09	42.09	1.96	0.321	
N,N'-Diethylaniline	9.7	9.70	670	4.49	4.49		2.161	
Benzidine	1.0×10^{-6}	1.06×10^{-5}	400	2.17	23.1	1.81	4.61×10^{-7}	
3,3'-Dichlorobenzidine	5.6×10^{-5}	6.41×10^{-4}	3.1	0.0122	0.140	3.51	0.005	
N,N'-Bianiline	0.0035		0.252	0.0014	0.0154	3.82	3.45×10^{-4}	
2-Nitroaniline	0.62	1.851	1200	8.687	25.93	1.78		
4-Nitroaniline	0.035	0.589	800	5.792	97.50	1.31		
2,4-Dinitroaniline						4.1		

Nitroaromatic compounds:

Nitrobenzene	20	20.0	1900	15.43	15.43	1.85	1.296	
1,2-Dinitrobenzene	0.0052	0.0433						
1,3-Dinitrobenzene	0.0081	0.0348	546	3.25	13.94	1.49	0.002	
1,4-Dinitrobenzene	13.3	386.63	442	2.63	76.43	2.37	5.059	
2-Nitrotoluene	17.9	17.90	651.42	4.75	4.75	2.30	3.768	
3-Nitrotoluene	27.2	27.20	499.19	3.64	3.64	2.45	7.473	
4-Nitrotoluene	0.653	1.2004	254.4	1.86	3.41	2.37	0.352	
2,4-Dinitrotoluene (DNT)	0.133	0.3705	270	1.48	4.13	2.01	0.090	
2,6-Dinitrotoluene	0.0767	0.1952	200			1.72	0.070	
2,4,6-Trinitrotoluene (TNT)	0.00107	0.0038	210	0.925	3.29			
1-Nitronaphthalene	0.702 0.0312	0.072	9.82	0.057	0.132	3.19	3.50	
2-Nitronaphthalene			9.24	0.053	0.183			
4-Nitrobiphenyl			1.231	6.18×10^{-3}	0.045	3.78		
5-Nitro-acenaphthene			0.91	4.57×10^{-3}	0.026			

(Continued)

TABLE 16.2.2 (Continued)

Compound	Selected properties						Henry's law constant	
	Vapor pressure		Solubility				H/(Pa·m³/mol)	
	P ^s /Pa	P _l /Pa	S/(g/m³)	C ^s /(mol/m³)	C _l /(mol/m³)	log K _{OW}	calcd P/C	exptl
Amides: RCONH2								
Acetamide (ethanamide)	2.44	8.3562	408000	6907.1	23650	−1.26	3.53 × 10 ^{−4}	
Acrylamide	0.415	1.5900	2050000	2884	11050	−0.9	1.44 × 10 ^{−4}	
Benzamide	0.00522	0.0544	14000	1692	17630	0.64	4.52 × 10 ^{−5}	
Urea: (NH2)2C=O								
Urea	0.0016	0.0186	1000000	16650	1.93x10 ⁵	−2.11	9.61 × 10 ^{−8}	
Nitrosoamines:								
N-Nitrosodimethylamine			miscible			−0.57		3.343
Di- <i>n</i> -propyl nitrosamine	27		9900	76.04		1.31	0.355	
Diphenyl nitrosamine	13.33	34.27	35.10	0.116	0.299	3.13	114.6	
Heterocyclic compounds:								
1 <i>H</i> -Pyrrole	1100	1100	45000	670.7	670.7	0.75	1.640	
1-Methylpyrrole	3312							
Indazole			827	7.00	100.43			
Indole	2.24	4.187	1874	16.00	29.90	2	0.140	
Indoline			10800	90.63				
Pyridine	2775	2775	miscible			0.65		0.895
2-Methylpyridine	1496	1496	miscible			1.11		1.01
3-Picoline	1333	1333	miscible			1.2–1.24		0.788
4-Picoline	757	757	miscible			1.22		0.601
2,3-Dimethylpyridine	426		104000	970.6				0.725
2,4-Dimethylpyridine	456	456	miscible					0.678
2,6-Dimethylpyridine	746	746	miscible					1.06
2,4,6-Trimethylpyridine	5170	5170	35700	294.6	294.6		17.549	
Quinolines:								
Quinoline	1.21	1.21	6110	47.31	47.31	2.06	0.026	
Isoquinoline	670	693	4521	35.00	36.20	2.08	19.141	
2,7-Dimethylquinoline			1795	11.42	24.77			
Benzo[<i>f</i>]quinoline		0.0067	76.1	0.42	2.02	3.20	0.0096	
Benzo[<i>h</i>]quinoline	0.03	0.0555						
9 <i>H</i> -Carbazole	0.0933	14.976	1.03	0.006	0.989	3.80	15.146	
7 <i>H</i> -Dibenzo[<i>c,g</i>]carbazole	1.3 × 10 ^{−7}	2.5 × 10 ^{−6}	0.063	0.236	4.532	5.75		

Acridine	0.0065	0.0451	38.5	0.215	1.492	3.4	0.030	
Benz[<i>a</i>]acridine						4.45		
Sulfur compounds:								
Carbon disulfide	48210	48210	2100	27.584	27.584		1747.75	
Dimethyl sulfate	128	128						
Diethyl sulfate	49.1	49.1						
Dimethyl sulfoxide (DMSO)	80.0	80.0	253000	354.8	354.8	−1.35	0.225	
Dimethyl sulfone	5.16	34.17				−1.41	200.83	
Dimethyl sulfide	64650	64650	20000	321.9			7.72	
Dimethyl disulfide	4000	4000	6300	66.88	66.88		59.81	
Diethyl sulfide	7782	7782				1.95		
Diethyl disulfide	689	689						
Thiols:								
Methanethiol	201980	201980						
Ethanethiol	70000		15000				289.94	
Propanethiol	20635	20635				1.81		
1-Butanethiol	6070	6070	597	6.62	6.62	2.28	916.94	
2-Butanethiol	10790	10790						
Benzenethiol	397	397				2.52		
2-Methylbenzenethiol	87.4	87.4						
3-Methylbenzenethiol	76.6	76.60						
4-Methylbenzenethiol	85.2	128.3						
Thiophenes:								
Thioazole	2287							
Thiophene	10620	8000	3015	35.833	35.833	1.81	223.3	224
2-Methylthiophene	3318							
3-Methylthiophene	2953							
Benzo[<i>b</i>]thiophene	26.66	26.7	130	0.969	1.107	3.12	24.1	
Dibenzothiophene	0.267		1.11	0.006		4.38	44.3	
Thiourea			90000	1182	36833	−0.99		
Thioacetamide			163000	2170	15722	−0.26		

TABLE 16.2.3

Suggested half-life classes for nitrogen and sulfur containing compounds in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Acetonitrile	6	5	5	6
Propionitrile	6	5	5	6
Acrylonitrile (2-Propenitrile)	3	4	4	5
Dimethylamine	1	3	4	5
Ethylamine	2	3	4	5
Diethylamine	1	2	2	3
<i>n</i> -Butylamine	2	3	3	4
Ethanolamine	1	3	3	4
Diethanolamine	1	4	4	5
Cyclohexylamine	1	3	3	4
Aniline	1	4	4	6
2-Chloroaniline	3	4	5	6
4-Chloroaniline	1	4	4	5
<i>o</i> -Toluidine	1	3	3	4
<i>N,N'</i> -Dimethylaniline	1	4	5	6
2,6-Xylidine	1	4	5	6
Diphenylamine	1	4	5	6
Benzidine	1	4	4	5
3,3'-Dichlorobenzidine	1	1	5	6
<i>N,N'</i> -Bianiline	1	3	3	4
α -Naphthylamine	1	4	4	6
β -Naphthylamine	1	4	4	6
Nitrobenzene	1	6	6	7
2-Nitrotoluene	2	3	6	7
4-Nitrotoluene	2	3	6	7
2,4-Dinitrotoluene (DNT)	2	3	6	7
2,4,6-Trinitrotoluene (TNT)	1	2	6	7
Acetamide	2	4	4	5
Benzamide	2	4	4	5
<i>n</i> -Nitrosodimethylamine	1	2	6	7
<i>n</i> -Nitrosodiethylamine	1	2	6	7
Di- <i>n</i> -propyl nitrosoamine	1	2	6	7
Diphenyl nitrosoamine	1	2	6	7
Pyridine	5	5	6	7
3-Methylpyridine	5	5	6	7
4-Methylpyridine	5	5	6	7
Quinoline	3	4	5	6
Dimethyl sulfate	4	2	2	3
Diethyl sulfate	2	2	3	4
Thiophene	3	3	6	7
Benzo[<i>b</i>]thiophene	4	5	6	7
Thiourea	1	4	4	5
Thioacetamide	2	4	4	5

TABLE 16.2.3 (*Continued*)

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

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17 Herbicides

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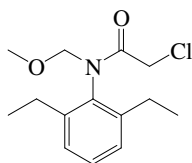
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	Amides:	
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	Diphenamid	3547
	Metolachlor	3591
	Napropamide	3606
	Pronamide	3634
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	Barban	3480
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	Dinitroanilines:	
	Benefin	3482
	Butralin	3495
	Dinitramine	3542
	Fluchloralin	3564
	Isopropalin	3575
	Nitralin	3610
	Oryzalin	3616
	Pendimethalin	3620
	Profluralin	3626
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	Diphenylethers:	
	Bifenox	3484
	Fluorodifen	3568
	Nitrofen	3612
	Phenols:	
	Dinoseb	3544
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	Phenoxyalkanoic acids:	
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	Dichlorprop	3537
	Fenoprop	3560
	MCPA	3584
	MCPB	3587
	Mecoprop	3589
	2,4,5-T	3653
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Propazine	3642
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Terbacil	3657
Ureas:	
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Chlorsulfuron	3507
Chlorotoluron	3510
Diuron	3551
Fenuron	3562
Fluometuron	3566
Isoproturon	3577
Linuron	3580
Monolinuron	3600
Monuron	3602
Neburon	3608
Miscellaneous:	
Amitrole (Triazole)	3469
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Diquat (Bipyridyl)	3549
Ethalfuralin (trifluoroorg-nitro compound)	3558
Fluridone (Fluoro-phenyl pyridinone)	3569
Glyphosate (Phosphate)	3572
Norflurazon	3614
Pyrazon (Pyridazinone)	3647
Triclopyr (pyridine, organochlorine)	3668

17.1 LIST OF CHEMICALS AND DATA COMPILATIONS (By Functional Group)

17.1.1 HERBICIDES

17.1.1.1 Alachlor



Common Name: Alachlor

Synonym: alachlore, alochlor, Alanex, Bronco, Bullet, Cannon, Lasso, Lazo, metachlor, Pillarzo

Chemical Name: 2-chloro-2,6-diethyl-*N*-methoxymethylacetanilide; 2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl)acetamide

Uses: pre-emergence, early post-emergence or soil-incorporated herbicide to control most annual grasses and many annual broadleaf weeds in beans, corn, cotton, milo, peanuts, peas, soybeans, sunflower, and certain woody ornamentals.

CAS Registry No: 15972-60-8

Molecular Formula: $C_{14}H_{20}ClNO_2$

Molecular Weight: 269.768

Melting Point ($^{\circ}C$):

40 (Lide 2003)

Boiling Point ($^{\circ}C$):

100 (at 0.02 mmHg, Ashton & Crafts 1981; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

135 (at 0.30 mmHg, Herbicide Handbook 1989; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.133 ($25^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

240.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

29.288 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.713 (mp at $40^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

242 ($20^{\circ}C$, Weber 1972; Weber et al. 1980)

200 (Bailey & White 1965)

242 (Herbicide Handbook 1974, 1978, 1983, 1989; Martin & Worthing 1977)

240 (Hartley & Graham-Bryce 1980; Beste & Humburg 1983)

148 (Khan 1980)

242 (Ashton & Crafts 1981; Worthing & Walker 1987, Worthing & Hance 1991)

242 (Hartley & Kidd 1983, 1987; Tomlin 1994)

130 ($20^{\circ}C$, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)

148, 242 (literature data variability, Heller et al. 1989)

140 ($23^{\circ}C$, Budavari 1989)

240 (Wauchope 1989)

240 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

23.5 (calculated-group contribution fragmentation method, Kühne et al. 1995)

140 ($23^{\circ}C$, Milne 1995)

512 (predicted-AQUAFAC, Lee et al. 1996)

532, 785 (supercooled liquid S_L : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated):

0.00293	(20°C, Weber 1972; Worthing & Walker 1987, Worthing & Hance 1991)
0.00293	(Herbicide Handbook 1974, 1983, 1989)
0.00293	(20–25°C, Weber et al. 1980)
0.00293	(Ashton & Crafts 1981; Schnoor & McAvoy 1981; Schnoor 1992)
0.00290	(Beste & Humburg 1983)
0.00290	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.00300	(20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
0.00187	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.00413	(Montgomery 1993)
0.0064. 0.0044	(supercooled liquid P_L : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6.20×10^{-3}	(20°C, calculated-P/C, Suntio et al. 1988)
8.43×10^{-4}	(wetted-wall-GC/ECD, Fendinger & Glotfelty 1988)
3.26×10^{-3}	(calculated-P/C, Taylor & Glotfelty 1988)
1.12×10^{-3}	(fog chamber-GC/ECD, Fendinger et al. 1989)
8.38×10^{-4}	(23°C, known LWAPC of Fendinger et al. 1989, Meylan & Howard 1991)
1.21×10^{-5}	(bond-estimated LWAPC, Meylan & Howard 1991)
3.26×10^{-3}	(20°C, calculated-P/C, Muir 1991)
6.20×10^{-3}	(calculated-P/C, Montgomery 1993)
3.22×10^{-3}	(Gish et al. 1995)
7.24×10^{-3} *	(Gas stripping-GC/MS, measured range 10–25°C, Gautier et al. 2003)
$\ln [H'/(M \text{ atm}^{-1})] = -20.946 + 9200/(T/K)$; temp range 2830298 K (gas stripping-GC/MS, Gautier et al. 2003)	
0.00101. 1.49	(literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log K_{OW} :

2.92	(Leo et al. 1971)
2.30	(Kenaga 1980)
2.64	(Rao & Davidson 1980)
3.087	(shake flask, Dubelman & Bremer 1983)
3.52	(shake flask, Log P Database, Hansch & Leo 1987)
3.27	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.52	(recommended, Sangster 1993)
3.52	(recommended, Hansch et al. 1995)
3.27	(RP-HPLC-RT correlation, Finizio et al. 1997)
3.09	(literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} :

9.31	(final adjust value FAV, Muir et al. 2004)
------	--

Bioconcentration Factor, log BCF:

1.45	(calculated-solubility, Kenaga 1980)
0.954	(calculated- K_{OC} , Kenaga 1980)
1.88	(Schnoor & McAvoy 1981, Schnoor 1992)
0.778	(freshwater fish, Call et al. 1984)
1.70	(Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

2.28	(soil, Beestman & Demming 1976)
2.32	(soil, calculated, Kenaga & Goring 1980)
2.30	(soil, Kenaga 1980)
1.70	(sediment/water, Schnoor & McAvoy 1981)

- 1.91 (soil, average for soils 2–7, Weber & Peter 1982)
 2.08 (soil, screening model calculations, Jury et al. 1987b)
 2.28 (Carsel 1989)
 2.18, 2.23, 2.28, 2.53 (soil, lit. values, Bottoni & Funari 1992)
 2.23 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 1.63–2.28 (quoted values, Montgomery 1993)
 2.21 (selected, Wienhold & Gish 1994)
 2.28 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.28; 2.53 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)
 2.22, 2.22, 2.20 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, $0.1 \leq \text{OC} < 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization: $k(\text{measured}) = 9000 \text{ d}^{-1}$ and $k(\text{estimated}) = 49000 \text{ d}^{-1}$ (Glottfelty et al. 1989);
 estimated $t_{1/2} = 2444 \text{ d}$ from 1-m depth of water at 20°C (Muir 1991)
 Volatilization rate $k = 4.4 \times 10^{-4} \text{ d}^{-1}$, $2.8 \times 10^{-3} \text{ d}^{-1}$, $4.3 \times 10^{-3} \text{ d}^{-1}$ at 15, 25, 35°C, respectively, for commercial formulation; $k = 5.8 \times 10^{-5} \text{ d}^{-1}$, $8.7 \times 10^{-3} \text{ d}^{-1}$, $1.4 \times 10^{-2} \text{ d}^{-1}$ at 15, 25, 35°C, respectively, for starch encapsulated formulation after application (Weinhold et al. 1993)
 Photolysis: $t_{1/2} = 2.25 \text{ h}$ in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991); 640 ppb contaminated water in the presence of TiO_2 and H_2O_2 photodegraded to 3.5 ppb by 15 h solar irradiation with complete degradation after 75 h (Muszkat et al. 1992).
 Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k(\text{aq.}) = (3.8 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2–6.0 and 21°C, with a half-life of 2.4 h at pH 7 (Yao & Haag 1991).
 $k(\text{calc}) = 7 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in aqueous solutions at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992) $k_{\text{OH}} = 2.3 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime about 0.5 d at 298 K assuming an average OH concn of $1 \times 10^6 \text{ molecule/cm}^3$ (Gautier et al. 2003)
 Hydrolysis: alkaline chemical hydrolysis $t_{1/2} > 365 \text{ d}$ (Schnoor & McAvoy 1981; quoted, Schnoor 1992).
 Biodegradation: $t_{1/2} < 6$ months for 0.07 $\mu\text{g/mL}$ to biodegrade in ground water, $t_{1/2} > 15$ months for 10.0 $\mu\text{g/mL}$ to biodegrade in groundwater both at 25°C and $t_{1/2} < 12 \text{ wk}$ for 3.2 $\mu\text{g/mL}$ to biodegrade in soil-water suspension at 35°C (Weidner 1974; quoted, Muir 1991);
 $t_{1/2} = 23 \text{ d}$ for 0.244 $\mu\text{g/mL}$ to biodegrade in river water at 23°C with biodegradation rate $k = 0.030 \text{ d}^{-1}$ (Schnoor et al. 1982; quoted, Muir 1991);
 $t_{1/2} = 18 \text{ d}$ from screening model calculations (Jury et al. 1987b);
 $t_{1/2} > 6 \text{ wk}$ for 0.01–1.0 $\mu\text{g/mL}$ to biodegrade in sewage effluent lake water at 28°C (Novick & Alexander 1985; quoted, Muir 1991);
 overall degradation rate constant $k = 0.0403 \text{ h}^{-1}$ with $t_{1/2} = 17.2 \text{ h}$ in sewage sludge and rate constant $k = 0.1601 \text{ d}^{-1}$ with $t_{1/2} = 4.3 \text{ d}$ in garden soil (Müller & Buser 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

- Air: tropospheric lifetime of 0.5 d for gas phase reaction with OH radicals; wet deposition lifetime estimated to be 2.8 d in the atmosphere by rainfall (Gautier et al. 2003)
 Surface water: $t_{1/2} = 23 \text{ d}$ for 0.244 $\mu\text{g/mL}$ to biodegrade in river water at 23°C with biodegradation rate $k = 0.030 \text{ d}^{-1}$ (Schnoor et al. 1982; quoted, Muir 1991);
 $t_{1/2} > 6 \text{ wk}$ for 0.01–1.0 $\mu\text{g/mL}$ to biodegrade in sewage effluent lake water at 28°C (Novick & Alexander 1985; quoted, Muir 1991);
 $k(\text{measured}) = (3.8 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2–6 and 21°C, with $t_{1/2} = 2.4 \text{ h}$ at pH 7 (Yao & Haag 1991).
 Ground water: $t_{1/2} < 6$ months for 0.07 $\mu\text{g/mL}$ to biodegrade in groundwater, and $t_{1/2} > 15$ months for 10.0 $\mu\text{g/mL}$ to biodegrade in groundwater both at 25°C (Weidner 1974; quoted, Muir 1991) reported $t_{1/2} = 7, 4\text{--}21$ and 38 d (Bottoni & Funari 1992)
 Sediment:

Soil: dissipation $t_{1/2} = 7.8$ d in soil (Beestman & Demming 1974); measured dissipation rate $k = 0.077$ d⁻¹ (Zimdahl & Clark 1982);

$t_{1/2} = 23$ and 5.7 d in soil containing 6 and 15% moisture, respectively (Walker & Brown 1985);

$t_{1/2} = 18$ d from screening model calculations (Jury et al. 1987b);

estimated dissipation rate $k = 0.020$ and 0.036 d⁻¹ (Nash 1988);

field $t_{1/2} < 1.5$ wk by using field lysimeters (Bowman 1990);

degradation rate constant $k = (4.52 \pm 0.192) \times 10^{-2}$ d⁻¹ with $t_{1/2} = 15.3$ d in control soil and $k = (7.27 \pm 0.772 \times 10^{-2}$ d⁻¹ with $t_{1/2} = 9.53$ d in pretreated soil in the field; $k = (2.77 \pm 0.226) \times 10^{-2}$ d⁻¹ with $t_{1/2} = 25$ d in control soil and $k = (14.1 \pm 1.75) \times 10^{-2}$ d⁻¹ with $t_{1/2} = 4.93$ d in pretreated soil once only in the laboratory (Walker & Welch 1991);

selected field $t_{1/2} = 15$ d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Richards & Baker 1993);

soil $t_{1/2} = 30$ d (quoted, Pait et al. 1992);

reported $t_{1/2} = 7, 4\text{--}21$ and 38 d (Bottoni & Funari 1992);

soil $t_{1/2} = 14\text{--}28$ d (Di Guardo et al. 1994);

dissipation $t_{1/2} = 42$ d from soil surface (Gish et al. 1995);

degradation $t_{1/2} = 4.3$ d in garden soil (Müller & Buser 1995);

$t_{1/2} = 15$ d (selected, Halfon et al. 1996);

dissipation $t_{1/2}(\text{calc}) = 5$ and 5.3 d in soil in model ecosystem, $t_{1/2} = 3.3$ and 3.4 d in water in model ecosystem (Ramesh & Maheswari 2004).

Biota: biochemical $t_{1/2} = 18$ d from screening model calculations (Jury et al. 1987b).

TABLE 17.1.1.1.1

Reported Henry's law constants of alachlor at various temperatures

Gautier et al. 2003

gas stripping-GC/MS

$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$	$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
10	$1.097 \times 10^{+3}$	23	$3.46 \times 10^{+3}$
10	$1.26 \times 10^{+3}$	25	$6.33 \times 10^{+3}$
10	$1.30 \times 10^{+3}$	25	$8.44 \times 10^{+3}$
11	$9.76 \times 10^{+4}$	25.0	$7.24 \times 10^{+3}$
12	$2.115 \times 10^{+3}$		
15	$1.68 \times 10^{+3}$	Arrhenius expression:	
17	$2.58 \times 10^{+3}$	$\ln H'/(M \text{ atm}^{+1}) = -A + B/(T/K)$	
18	$3.13 \times 10^{+3}$	A	20.946
20	$4.24 \times 10^{+3}$	B	9200
23	$3.07 \times 10^{+3}$		

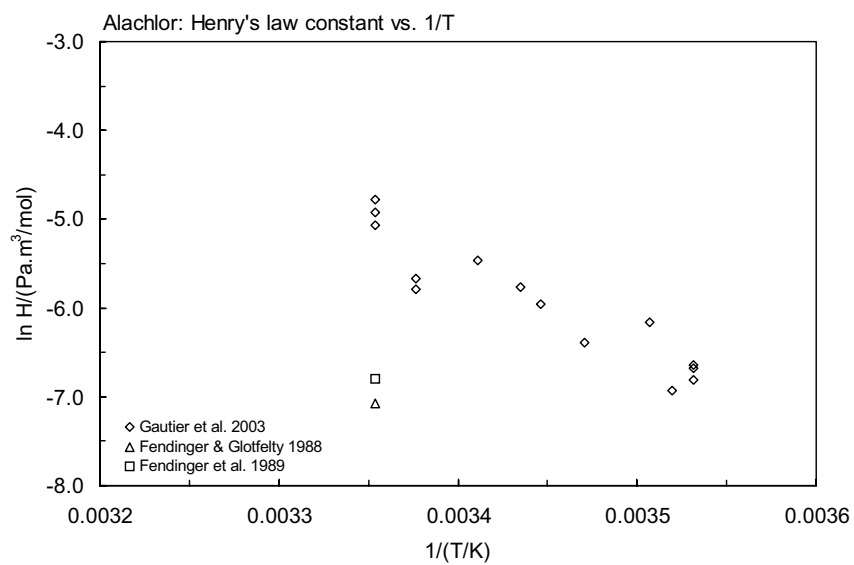
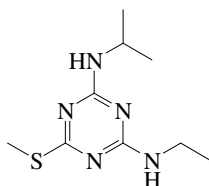


FIGURE 17.1.1.1.1 Logarithm of Henry's law constant versus reciprocal temperature for alachlor.

17.1.1.2 Ametryn



Common Name: Ametryn

Synonym: Amephyt, Ametrex, Evik, Gesapax

Chemical Name: 6-methylthio-2-(ethylamino)-4-(isopropylamino)-1,3,5-triazine; N-ethyl-N'-(1-methylethyl)-6-(methyl-thio)-1,3,5-triazine-2,4-diamine

Uses: herbicide to control broadleaf and grass weeds in corn, sugarcane, some citrus fruits, and in noncropland; also used as pre-harvest and post-harvest dessicant in potatoes to control crop and weeds.

CAS Registry No: 834-12-8

Molecular Formula: $C_9H_{17}N_5S$

Molecular Weight: 227.330

Melting Point ($^{\circ}C$):

88 (Lide 2003)

Boiling Point ($^{\circ}C$): 328.78 (Rordorf 1989)

Density (g/cm^3 at $20^{\circ}C$):

1.19 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

277.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

4.00 (pK_a , Weber 1970; quoted, Bintein & Devillers 1994)

4.10 (pK_a , Worthing & Hance 1991; Montgomery 1993)

10.07 (pK_b , Wauchope et al. 1992; Hornsby et al. 1996)

9.90 (pK_b , Tomlin 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.96 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.8 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

55 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.241 (mp at $88^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

700 (Woodford & Evans 1963)

405, 195, 192 ($26^{\circ}C$, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

185 (Martin & Worthing 1977; Herbicide Handbook 1978)

185 ($20^{\circ}C$, Khan 1980; Ashton & Crafts 1981; Verschueren 1983)

194 (Weber et al. 1980)

185 ($20^{\circ}C$, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

185 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

200 (Tomlin 1994)

134 (calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.12×10^{-4} ($20^{\circ}C$, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50 – $130^{\circ}C$, Friedrich & Stambach 1964) (See figure at the end of this section.)

$\log(P/mmHg) = 11.911 - 4933/(T/K)$, temp range 50 – $130^{\circ}C$ (gas saturation-GC, data presented in Antoine eq., Friedrich & Stambach 1964) (See figure at the end of this section.)

- 1.12×10^{-4} (20°C, Khan 1980; Ashton & Crafts 1981; Verschueren 1983)
- 1.12×10^{-4} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
- $\log(P_g/kPa) = 11.036 - 5270/(T/K)$, temp range 323–403 K, (solid, Antoine eq., Stephenson & Malanowski 1987)
- 1.00×10^{-4} (20°C, selected, Suntio et al. 1988)
- 1.12×10^{-4} , 4.40×10^{-4} (20°C, 30°C, Herbicide Handbook 1989)
- 3.74×10^{-4} , 1.40×10^{-2} , 0.30, 4.40, 46 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
- $\log(P_g/Pa) = 16.85 - 6048.6/(T/K)$; measured range 49.5–85°C (gas saturation-GC, Rordorf 1989)
- $\log(P_L/Pa) = 13.396 - 4803.6/(T/K)$; measured range 49.5–140°C (gas saturation-GC, Rordorf 1989)
- 3.65×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.65×10^{-4} (Tomlin 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 1.20×10^{-4} (20°C, calculated, Suntio et al. 1988)
- 1.38×10^{-4} (calculated-P/C, Montgomery 1993)
- 1.23×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.69 (Kenaga & Goring 1980)
- 2.58 (Gerstl & Helling 1987)
- 2.98 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.82 (Worthing & Hance 1991)
- 2.98 (shake flask, Biagi et al. 1991)
- 3.07 (RP-HPLC-RT correlation, Finizio et al. 1991)
- 2.88 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.98 (recommended, Sangster 1993)
- 2.63 (Tomlin 1994)
- 2.61 (shake flask-UV, Liu & Qian 1995)
- 2.58 (calculated-RP-HPLC- k' correlation, Liu & Qian 1995)
- 2.83 (Milne 1995)
- 2.98 (recommended, Hansch et al. 1995)
- 2.88 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log BCF$:

- 1.52 (calculated-S, Kenaga 1980)
- 1.32 (calculated- K_{oc} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

- 2.59 (soil, Hamaker & Thompson 1972;)
- 2.40 (soil, calculated, Kenaga & Goring 1980)
- 2.59 (soil, Kenaga & Goring 1980)
- 2.59 (Rao & Davidson 1980)
- 2.59, 2.86 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
- 2.59, 2.51 (reported as $\log K_{OM}$, estimated as $\log K_{OM}$, Magee 1991)
- 2.40–2.59, 2.58 (soil, quoted values, Bottoni & Funari 1992)
- 2.48 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.23–2.44 (Montgomery 1993)
- 2.48 (Tomlin 1994)
- 2.42 (calculated- K_{ow} , Liu & Qian 1995)
- 2.59 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 2.70, 2.59 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.52, 2.63, 2.60, 2.35 (soils with organic carbon $OC \geq 0.5\%$ at: pH 4.5–9.0, pH 4.5–5.4, pH 5.5–6.0, pH 6.1, average, Delle Site 2001)
- 1.84, 2.23 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 10$ h for $10 \mu\text{g mL}^{-1}$ to degrade in distilled water under > 290 nm light and $t_{1/2} = 3.3$ h in 1% acetone solution (Burkhard & Guth 1976; quoted, Cessna & Muir 1991);

$t_{1/2} = 2.25$ h for 17% of $33 \mu\text{g mL}^{-1}$ to degrade in 0.2% aqueous solutions of the surfactant Triton X-100 and for 8% of $33 \mu\text{g/mL}$ to degrade in distilled water both under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: $t_{1/2} = 32$ d at pH 1 and $t_{1/2} > 200$ d at pH 13 (Montgomery 1993).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater: reported half-lives or persistence, $t_{1/2} = 7$ –120 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 6.0$ months at 15°C and $t_{1/2} = 4.5$ months at 30°C in soils (Freed & Haque 1973);

$t_{1/2} = 70$ –120 d (Bottoni & Funari 1992);

selected $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 70$ –129 d in soil (Tomlin 1994).

Biota:

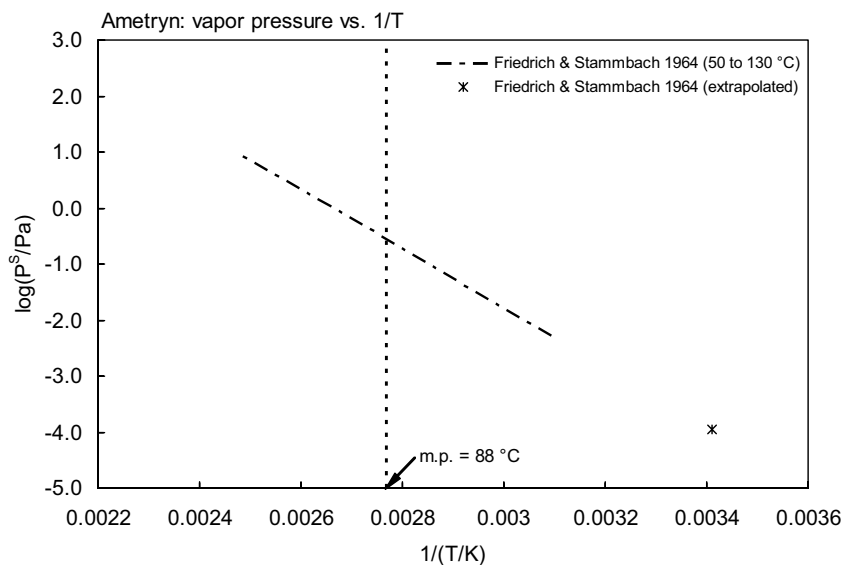
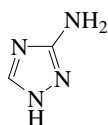


FIGURE 17.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ametryn.

17.1.1.3 Amitrole



Common Name: Amitrole

Synonym: Amazole, Amitrol, Amizole, aminotriazole, Azolan, Azole, cytrol, Diurol

Chemical Name: 3-amino-1,2,4-triazole; 3-amino-*s*-triazole; 1H-1,2,4-triazol-3-amine

Uses: nonselective, foliage-applied herbicide in uncropped land and orchards to control perennial weeds in certain grasses.

CAS Registry No: 61-82-5

Molecular Formula: $C_2H_4N_4$

Molecular Weight: 84.080

Melting Point ($^{\circ}C$):

159 (Khan 1980; Herbicide Handbook 1989; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.138 (Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

85.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

9.83 (pK_b , Wauchope et al. 1992; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.69 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.0484 (mp at $159^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

252000 (Freed & Burschel 1957)

280000 (Martin 1961; Spencer 1981)

280000 (Bailey & White 1965; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Willis & McDowell 1982)

soluble (Wauchope 1978)

280000 (Worthing 1983, Worthing & Hance 1991)

280000 (Hartley & Kidd 1987; Herbicide Handbook 1989; Reinert 1989)

360000 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

280000 ($20^{\circ}C$ at pH 7, quoted, Montgomery 1993)

280000 ($23^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

< 0.001 (Agrochemicals Handbook 1983; quoted, Howard 1991)

< 0.001 (Hartley & Kidd 1987)

5.50×10^{-8} ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

5.87×10^{-5} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

5.51×10^{-7} ($20^{\circ}C$, quoted, Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

$< 3.04 \times 10^{-7}$ (calculated-P/C, Howard 1991)

1.650×10^{-10} ($20^{\circ}C$, calculated-P/C, Montgomery 1993)

1.650×10^{-10} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 0.85 (shake flask, pH 7, Lichtner 1983)
- 0.52 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 0.15 (Reinert 1989; quoted, Howard 1991; Montgomery 1993)
- 0.87, -0.84 (pH 7) (Hansch et al. 1995)
- 0.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, $\log BCF$:

- 0.301 (estimated-S, Lyman et al. 1982; quoted, Howard 1991)
- 0.347 (estimated- $\log K_{ow}$, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{oc}$:

- 2.04 (soil, estimated-molecular topology & QSAR, Sabljic 1984)
- 0.23 (calculated-MCI χ , Gerstl & Helling 1987)
- 1.26 (Reinert 1989)
- 2.00 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.73–2.31 (quoted, Montgomery 1993)
- 2.00 (estimated-chemical structure, Lohninger 1994)
- 1.25 (soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 3.2\text{--}32$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4032$ h, based on reported half-lives in soil and water (Freed & Haque 1973; Reinert & Rogers 1987; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}16128$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 3.8$ d, based on a theoretical calculation for the vapor-phase reaction with hydroxyl radicals in the atmosphere at 25°C (GEMS 1986; quoted, Howard 1989);

$t_{1/2} = 3.2\text{--}32$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 1344\text{--}8640$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).^c

Sediment:

Soil: $t_{1/2} = 1.4, 1.6, 1.3, 92, 36,$ and 56 d with disappearance rates: $k = 0.495, 0.433, 0.533, 0.0075, 0.0193,$ and 0.124 d⁻¹ at pH 6.0, 7.0, 8.0, 5.3, 6.5, and 7.5 (Hamaker 1972; quoted, Nash 1988);

$t_{1/2} = 1.5$ month at 15°C and $t_{1/2} = 1.0$ month at 30°C in soils (Freed & Haque 1973);

persistence of one month in soil (Wauchope 1978);

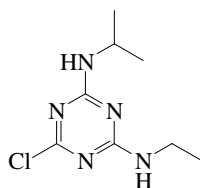
persistence in soil for ca. 2–4 wk (Herbicide Handbook 1989; Tomlin 1994);

$t_{1/2} = 672\text{--}4320$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

selected field $t_{1/2} = 14$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

17.1.1.4 Atrazine



Common Name: Atrazine

Synonym: Aatrex, Akikon, Aktikon, Aktinit, Atratol, Atred, Atrex, Candex, Fenamine, Gesaprim, Hungazin, Inakor, Primatol, Primaze, Radazine, Strazine, Triazine A, Vectal, Weedex A, Wonuk, Zeazine

Chemical Name: 2-chloro-4-(ethylamino)-6-(isopropylamino)-1,3,5-triazine; 6-chloro-*N*-ethyl-*N'*-(1-methylethyl)-1,3,5-triazine-diamine

Uses: pre-emergence and post-emergence herbicide to control some annual grasses and broadleaf weeds in corn, fallow land, rangeland, sorghum, noncropland, certain tropical plantations, evergreen nurseries, fruit crops, and lawns.

CAS Registry No: 1912-24-9

Molecular Formula: $C_8H_{14}ClN_5$

Molecular Weight: 215.684

Melting Point ($^{\circ}C$):

173 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.187 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

250.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

1.68 (pK_a , Weber 1970; Somasundaram et al. 1991; Bintein & Devillers 1994)

1.70 (pK_a , Weber et al. 1980; Willis & McDowell 1982; Worthing & Hance 1991; Francioso et al. 1992; Montgomery 1993; Tomlin 1994)

1.60 (pK_a , Yao & Haag 1991; Haag & Yao 1992)

12.32 (pK_b , Wauchope et al. 1992; Hornsby et al. 1996)

1.62 (pK_a , $20^{\circ}C$, Montgomery 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

40.585 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $20^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$),

F: 0.0353 (mp at $173^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

70.0 ($26^{\circ}C$, Bailey & White 1965)

50.0 (Günther et al. 1968)

31.1, 34.9, 36.8 ($26^{\circ}C$, shake flask-UV at pH 3.0, 7.0. 10.0, Ward & Weber 1968)

98.0 ($50^{\circ}C$, Getzen & Ward 1971)

33.0 (shake flask-GC, Hörmann & Eberle 1972)

29.9 (shake flask-UV, Hurle & Freed 1972)

30.0 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987; Worthing & Hance 1991; Burkhard & Guth 1981)

33.0 ($27^{\circ}C$, Ashton & Crafts 1973, 1981; Khan 1980; Herbicide Handbook 1989; Pait et al. 1992)

32.0 (Freed 1976; Beste & Humburg 1983; Jury et al. 1983)

31.5 (Spencer 1976)

33.0 (Wauchope 1978; Kenaga 1980; Kenaga & Goring 1980)

35.0 (Weber et al. 1980)

30.0 (shake flask-HPLC, Ellgehausen et al. 1981)

24.0 (Thomas 1982)

70.0 (Windholz 1983)

- 28.0 (20°C, Hartley & Kidd 1987)
 29.9, 33, 70 (literature data variability, Heller et al. 1989)
 33.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 28.0, 33.0 (20°C, 27°C, Montgomery 1993)
 33.0 (20°C, Tomlin 1994)
 28.0 (Milne 1995)
 4012, 4012 (supercooled liquid S_L : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 44.0×10^{-5} * (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stambach 1964)
 $\log(P/\text{mmHg}) = 13.766 - 5945/(T/K)$, temp range 50–130°C (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stambach 1964)
 4.00×10^{-5} (20°C, Weber 1972; Worthing 1979; Worthing & Walker 1987, Worthing & Hance 1991; quoted, Khan 1980; Dobbs et al. 1984; Muir 1991)
 3.99×10^{-5} (20°C, gas saturation, extrapolated from Friedrich & Stambach 1964, Spencer 1976)
 4.00×10^{-5} (20°C, Hartley & Graham-Bryce 1980; Beste & Humburg 1983)
 4.00×10^{-5} (20–25°C, Weber et al. 1980)
 4.00×10^{-5} (20°C, Ashton & Crafts 1981)
 1.33×10^{-4} (selected, Schnoor & McAvoy 1981)
 3.70×10^{-5} * (20°C, extrapolated from gas saturation measurement, Grayson & Fosbracey 1982)
 $\ln(P/\text{Pa}) = 36.8 - 13778/(T/K)$, for temp range 51–81.5°C, (Antoine eq., gas saturation, Grayson & Fosbracey 1982)
 1.13×10^{-4} (Thomas 1982)
 4.00×10^{-5} (20°C, Hartley & Kidd 1987)
 $\log(P_s/\text{kPa}) = 12.8909 - 5945/(T/K)$, temp range 323–403 K, (solid, Antoine eq., Stephenson & Malanowski 1987)
 8.70×10^{-5} (selected, Nash 1989)
 3.99×10^{-5} , 18.6×10^{-5} (20°C, 30°C, Herbicide Handbook 1989)
 3.90×10^{-5} * (gas saturation-GC, measured range 40.5–125°C, Rordorf 1989)
 $\log(P_s/\text{Pa}) = 13.27071 - 6558.5/(T/K)$; measured range 40.5–125°C (gas saturation-GC, Rordorf 1989)
 $\log(P_L/\text{Pa}) = 13.396 - 4803.6/(T/K)$; measured range not specified (gas saturation-GC, Rordorf 1989)
 4.05×10^{-5} (Riederer 1990)
 3.85×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 4.00×10^{-5} (20°C, Montgomery 1993)
 2.00×10^{-5} (selected, Sieber et al. 1994)
 3.90×10^{-5} (Tomlin 1994; quoted, Halfon et al. 1996)
 6.70×10^{-4} * (40°C, Knudsen effusion method, measured range 40–80°C, Goodman 1997)
 $\log(P/\text{Pa}) = 16.08 - 6040/(T/K)$; temp range 40–80°C, Goodman 1997)
 0.0096, 0.0096 (supercooled liquid P_L : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 6.20×10^{-4} (calculated-P/C, Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989)
 2.90×10^{-4} (20°C, calculated-P/C, Suntio et al. 1988)
 6.19×10^{-4} (calculated-P/C, Taylor & Glotfelty 1988)
 5.70×10^{-4} (calculated-P/C, Nash 1989)
 3.04×10^{-4} (Riederer 1990)
 2.66×10^{-4} (calculated-P/C, Howard 1991)
 2.89×10^{-4} (20°C, calculated-P/C, Muir 1991)
 3.08×10^{-4} (20°C, calculated-P/C, Montgomery 1993)
 1.00×10^{-3} (calculated-P/C, Sieber et al. 1994)
 6.20×10^{-4} (Gish et al. 1995)
 2.88×10^{-4} (calculated-P/C, this work)
 0.518 (final adjust value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, log K_{ow} :

- 2.75 (shake flask-GC, Erkel & Walum 1979)
- 2.63 (HPLC-RT correlation, Veith et al. 1979, 1980; Veith & Kosian 1982)
- 2.35 (Rao & Davidson 1980)
- 2.71 (shake flask-both phases analyzed by GC and UV spec., Brown & Flagg 1981)
- 2.40, 2.21 (HPLC-k' correlation, McDuffie 1981)
- 2.75 (shake flask, Ellgehausen et al. 1981)
- 2.80 (Elgar 1983)
- 2.05 (RP-HPLC-k' correlation, Braumann et al. 1983)
- 2.64 (shake flask-GC, Geyer et al. 1984)
- 2.75 (Hansch & Leo 1985)
- 2.64 (OECD method 1981, Kerler & Schönherr 1988)
- 2.68 (Lopez-Avila et al. 1989)
- 2.61, 2.61 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
- 2.34 (Worthing & Hance 1991; Milne 1995)
- 2.10 (shake flask, pH 7, Baker et al. 1992)
- 2.33–2.80 (quoted values, Montgomery 1993)
- 2.75 (recommended, Sangster 1993)
- 2.42 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.50 (Tomlin 1994)
- 2.27 (shake flask-UV, Liu & Qian 1995)
- 2.61 (selected, Hansch et al. 1995)
- 2.43 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 2.00 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
- 2.63 ± 0.07, 2.47 ± 0.15, 2.46 ± 0.09 (shake flask, isocratic RP-HPLC-k' correlation, gradient RP-HPLC-k' correlation, Paschke et al. 2004)
- 2.40 (literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} :

- 9.08 (final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:

- 2.00 (vegetation, correlated- K_{ow} , Beynon et al. 1972; quoted, Travis & Arms 1988)
- 1.04 (Metcalf & Sanborn 1975; quoted, Kenaga & Goring 1980; Isensee 1991)
- 1.00 (Isensee 1976)
- 0.50 (whitefish, Burkhard & Guth 1976)
- 0.90 (fathead minnow, Veith et al. 1979)
- 0.30 (catfish, Ellgehausen et al. 1980; quoted, Howard 1991)
- 0.26 (*Daphnia magna*, wet wt. basis, Ellgehausen et al. 1980)
- 0.48 (*Corygonus fera*. at 12°C, Gunkel & Streit 1980)
- 1.93, 0.845 (calculated-S, K_{OC} , Kenaga 1980)
- < 0.90 (Veith et al. 1980)
- 1.90 (selected, Schnoor & McAvoy 1981)
- 1.93, 1.77 (estimated-S, estimated- K_{ow} , Bysshe 1982)
- 0.90 (fathead minnow, Veith & Kosian 1982)
- 2.00 (mottled sculpin, Lynch et al. 1982)
- 1.60 (activated sludge, Freitag et al. 1984)
- 1.00 (golden ide, Freitag et al. 1985)
- 0.477, 0.954, 0.845, 0.778 (zebrafish: egg, embryo, yolk sac fry, juvenile; Görg & Nagel 1990)
- 0.78 (*Brachydanio rerio*, Görg & Nagel 1990)
- 0.983 (*Hydrilla*, Hinman & Klaine 1992)
- 1.98, 0.748, 0.230 (algae *Scenedesmus acutus*, catfish *Ictalurus melas*, *Daphnia magna*, wet wt basis, Wang et al. 1996)

Bioaccumulation Factor, log BAF:

- 1.710 (algae, Ellgehausen et al. 1980;)
- 0.329 (catfish, Ellgehausen et al. 1980)
- 0.261 (daphnids, Ellgehausen et al. 1980)
- 1.72, 0.477, 1.60 (algae, fish, sludge, Klein et al. 1984)
- 1.70, < 1.00, 1.60 (algae, fish, sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 2.17 (soil, Hamaker & Thompson 1972)
- 2.09 (average of 4 soils, Rao & Davidson 1979; Davidson et al. 1980)
- 2.81 (calculated, Kenaga & Goring 1980; Kenaga 1980)
- 2.20 (average of soils/sediments, Rao & Davidson 1980)
- 2.21 (average of 56 soils from lit. review, Rao & Davidson 1980)
- 2.33 (a Georgia pond sediment, sorption isotherms by shake flask-GC/ECD, Brown & Flagg 1981)
- 1.59 (a Swiss soil, Burkhard & Guth 1981)
- 3.11, 2.31; 1.94, 2.42 (estimated-S, calculated-S and mp; estimated- K_{OW} , Karickhoff 1981)
- 0.7–1.48 (selected, sediment/water, Schnoor & McAvoy 1981)
- 2.18 (soil, Thomas 1982)
- 2.29–3.18 (Wolf & Jackson 1982)
- 3.23–4.13 (Means & Wijayaratne 1982)
- 2.21 (soil average, Jury et al. 1983)
- 1.63–3.29 (Wauchope & Myers 1985; 1991)
- 2.46 (calculated-MCI χ , Gerstl & Helling 1987)
- 2.20 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 1.92 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)
- 2.21 (estimated as log K_{OM} , Magee 1991)
- 2.0, 2.18, 2.17–2.81, 2.26 (soil, literature values, Bottoni & Funari 1992)
- 2.27, 2.41, 2.59, 2.16 (soils, no. 1, 2, 3, 4; Francioso et al. 1992)
- 1.81 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
- 2.00 (soil, 20–25°C, selected, Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Wienhold & Gish 1994; Hornsby et al. 1996)
- 1.95–2.71 (quoted values, Montgomery 1993)
- 2.60 (soil with 9.23% organic carbon, Donati et al. 1994)
- 2.04 (agricultural soil, Dousset et al. 1994)
- 2.40 (estimated-chemical structure, Lohninger 1994)
- 2.05 (soil with low organic carbon 0.18%, Roy & Krapac 1994)
- 1.95–2.19 (Tomlin 1994)
- 2.23 (calculated- K_{OW} , Liu & Qian 1995)
- 2.24 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 1.81; 2.36 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 1.00 (sediment/water, Chung et al. 1996)
- 2.64 (Levy wetland soil, sorption equilibrium technique, 24°C, Mersie & Seybold 1996)
- 2.14–2.21; 2.03–2.12 (Teufelsweiher pond sediment: field measurement; exptl laboratory data, Gao et al. 1997)
- 2.19 (sediment from Teufelsweiher pond, batch equilibrium isotherm, Gao et al. 1998)
- 1.93, 1.80–1.85, 1.81 (soil, liquid sewage sludge amended soil, sludge, pH 7.2, batch equilibrium-sorption isotherm, Celis et al. 1998)
- 1.93, 1.83, 1.79 (soil + $CaCl_2$ at pH 7.2, soil + liquid sewage sludge and dissolved organic matter at pH 7.5, soil + liquid sewage sludge at pH 7.2, batch equilibrium-sorption isotherm, Celis et al. 1998)
- 2.566, 1.72, 1.75, 1.505, 2.40 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.24, 2.45; 2.82., 1.81, 2.81, 1.98, 1.99 (quoted lit., calculated- K_{OW} ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 2.154, 1.97, 1.77, 1.61, 2.496 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)

- 1.69 (sandy loam soil, column equilibrium method, 20°C, Xu et al. 1999)
- 2.154, 1.969, 1.769, 1.610, 2.486 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)
- 2.24; 2.27, 2.47 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.59, 2.16 (average values for sediments, soils, Delle Site 2001)
- 2.31, 2.17, 2.56 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH 3.2–8.2, average, Delle Site 2001)
- 2.34, 2.24, 2.06, 2.59 (soils with organic carbon $OC \geq 0.5\%$ at: pH 3.2–5.0, pH 5.1–5.9, pH-6.0, pH 4.4–7.7, average, Delle Site 2001)
- 1.77, 2.10 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization: initial rate constant $k = 6.4 \times 10^{-4} \text{ h}^{-1}$ and predicted rate constant $k = 4.2 \times 10^{-4} \text{ h}^{-1}$ from soil with $t_{1/2} = 1650 \text{ h}$ (Thomas 1982);
- $t_{1/2} = 97 \text{ d}$ (Jury et al. 1983; quoted, Grover 1991);
- rate constants $k(\text{measured}) = 1100 \text{ d}^{-1}$ and $k(\text{est.}) = 6000 \text{ d}^{-1}$ (Glottfelty et al. 1989);
- Half-lives from soil surfaces: $t_{1/2} = 655$ to $> 1000 \text{ d}$ in peat soil and $t_{1/2} = 143\text{--}939 \text{ d}$ in sandy soil; half-lives from plant surfaces: $t_{1/2} = 25.6 \text{ d}$ in bean, $t_{1/2} = 24.3 \text{ d}$ in turnips and $t_{1/2} = 14.6 \text{ d}$ in oats at $20 \pm 1^\circ\text{C}$ (Dörfler et al. 1991)
- Volatilization rate $k = 1.4 \times 10^{-4} \text{ d}^{-1}$, $2.6 \times 10^{-3} \text{ d}^{-1}$, $4.4 \times 10^{-3} \text{ d}^{-1}$ at 15, 25, 35°C, respectively, for commercial formulation; $k = 1.2 \times 10^{-5} \text{ d}^{-1}$, $4.8 \times 10^{-4} \text{ d}^{-1}$, $8.1 \times 10^{-4} \text{ d}^{-1}$ at 15, 25, 35°C, respectively, for starch-encapsulated formulation after application (Weinhold et al. 1993)
- Photolysis: $t_{1/2} = (19 \pm 9) \text{ h}$ under summer sunlight of 9.1 h d^{-1} exposure and $t_{1/2} = 61 \pm 29 \text{ h}$ under spring sunlight of 3.7 h d^{-1} exposure in 10 ppm aqueous solutions: (Burkhard et al. 1975);
- $t_{1/2} = 4.9 \text{ h}$ for 10 $\mu\text{g/mL}$ to degrade in 1% acetone solution and $t_{1/2} = 25 \text{ h}$ for 10 $\mu\text{g/mL}$ to degrade in distilled water both under $> 290 \text{ nm}$ light (Burkhard & Guth 1976);
- nearsurface direct sunlight photolysis rate constant $k = 9 \times 10^{-6} \text{ d}^{-1}$ with $t_{1/2} = 81,000 \text{ d}$ (Schnoor & McAvoy 1981; quoted, Schnoor 1992);
- $t_{1/2} = 2.25 \text{ h}$ for 17–27% of 100 $\mu\text{g/mL}$ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
- rate of photolytic degradation was slightly higher in water ($t_{1/2} = 3\text{--}12 \text{ d}$) than in sediments ($t_{1/2} = 1\text{--}4 \text{ wk}$) (Jones et al. 1982; quoted, Montgomery 1993);
- 40 ppb contaminated water in presence of TiO_2 and H_2O_2 degraded to 4 ppb after 15 h by solar irradiation with complete degradation after 75 h (Muszkat et al. 1992)
- $t_{1/2}(\text{aq.}) = 335 \text{ d}$ at pH 7 under natural light; $t_{1/2} = 17.5 \text{ h}$ at pH 7 using mercury lamp in aqueous solution; soil photolysis $t_{1/2} = 12 \text{ d}$ under natural light, $t_{1/2} = 5 \text{ d}$ using mercury lamp and $t_{1/2} = 45 \text{ d}$ using xenon lamp (Solomon et al. 1996);
- Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
- $k_{\text{OH}} = 147.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with n half-life of 2.6 h at 25°C for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- $k(\text{aq.}) = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to acetophenone) with OH radical in aqueous solutions at pH 3.6 and $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
- $k(\text{aq.}) = (24 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone at pH 4 and 26°C; $k = (13 \pm 1) \text{ M}^{-1} \text{ s}^{-1}$ at pH 4.2 and 21°C and $k = (24 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$ at pH 4.1 and 19°C in water, with a half-life of 1.5 h at pH 7 (Yao & Haag 1991)
- $k(\text{aq.}) = (2.6 \pm 0.4) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.6 and $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992)
- $k(\text{aq.}) = 0.82 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with hydroxyl radical in irradiated field water (Mabury & Crosby 1996)

Hydrolysis: $t_{1/2} \sim 70$ d at pH 3.1 of citrate buffer; $t_{1/2} \sim 75$ d at pH 11.1 of carbonate buffer and $t_{1/2} \sim 2$ d at 3.9 of phosphate buffer + sterile lake sediment in aqueous solutions at 25°C (Armstrong et al. 1967; quoted, Muir 1991)

Over all rate constant $k = 7.6 \times 10^{-5} \text{ s}^{-1}$ with $t_{1/2} = 2.5$ h at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 3.3, 14, 58, 240, 100, 12.5$, and 1.5 d at pH 1, 2, 3, 4, 11, 12, and 13, respectively, in aqueous buffered solutions in soil at 25°C (Armstrong et al. 1967; quoted, Montgomery 1993);

$t_{1/2} = 244$ d without humic materials, $t_{1/2} = 1.37$ d with the presence of 2% humic acid at pH 4 and 25°C (Li & Felbeck 1972; quoted, Howard 1991; Montgomery 1993)

$k = 3.9 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ and $k = 7.6 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 66$ and 81 d in aqueous solutions of pH 3.1 and 11.1, respectively (Wolfe et al. 1976; quoted, Muir 1991)

$k(\text{aq.}) = 19.9 \text{ d}^{-1}$ at pH 2.9, $k = 3.99 \text{ d}^{-1}$ at pH 4.5, $k = 1.74 \text{ d}^{-1}$ at pH 6.0, and $k = 0.934 \text{ d}^{-1}$ at pH 7.0 with corresponding $t_{1/2} = 34.8, 174, 398$, and 742 d all at 25°C in 0.5 mg mL^{-1} concn. of aqueous fulvic acid (Khan 1978; quoted, Howard 1991; Montgomery 1993)

$k(\text{aq.}) = 28.4 \text{ d}^{-1}$ at pH 2.8, $k = 12.6 \text{ d}^{-1}$ at pH 4.5, $k = 3.16 \text{ d}^{-1}$ at pH 6.0, and $k = 1.23 \text{ d}^{-1}$ at pH 7.0 with corresponding $t_{1/2} = 24.4, 55.0, 219$, and 563 d all at 25°C in 1.0 mg mL^{-1} concn. of aqueous fulvic acid (Khan 1978)

$k(\text{aq.}) = 151 \text{ d}^{-1}$ at pH 2.4, $k = 43.7 \text{ d}^{-1}$ at pH 4.5, $k = 13.2 \text{ d}^{-1}$ at pH 6.0, and $k = 7.93 \text{ d}^{-1}$ at pH 7.0 with corresponding $t_{1/2} = 4.60, 15.9, 52.5$ and 87.3 d all at 25°C in 5.0 mg mL^{-1} concn. of aqueous fulvic acid (Khan 1978)

$k(\text{aq.}) = 9.30 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 86$ d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981; quoted, Muir 1991)

$t_{1/2} > 3$ months (in sterile buffer solution at pH 7.2) and $t_{1/2} > 14$ d (in sterile mineral salt solution at pH 7.2) for $20 \text{ } \mu\text{g mL}^{-1}$ to hydrolyze at 23°C (Geller 1980; quoted, Muir 1991)

$k(\text{alkaline}) = 1 \times 10^{-16} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 742$ d (Schnoor & McAvoy 1981; quoted, Schnoor 1992)

$t_{1/2} = 1771$ yr at pH 7 and 25°C (Montgomery 1993)

Biodegradation:

$t_{1/2} = 64$ d in soil (Armstrong et al. 1967; Dao et al. 1979; quoted, Means et al. 1983)

$t_{1/2} = 3.21$ d in aqueous solution from river die-away tests (Furmidge & Osgerby 1967; quoted, Scow 1982)

$t_{1/2}(\text{aerobic}) > 90$ d for $10\text{--}20 \text{ } \mu\text{g mL}^{-1}$ to degrade in soil-water suspension (Goswami & Green 1971; quoted, Muir 1991)

$k(\text{aq.}) = 0.019 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2}(\text{aerobic}) > 35$ d for $0.1\text{--}1.0 \text{ } \mu\text{g mL}^{-1}$ to slowly biodegrade in sediment/water at 25°C (Wolf & Jackson 1982; quoted, Muir 1991)

$t_{1/2} = 36$ and 110 d in soil (Jones et al. 1982; quoted, Means et al. 1983)

$t_{1/2} = 71$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989; quoted, Grover 1991)

$k = 0.22 \text{ d}^{-1}$ of aerobic degradation rate observed in incubations of river water samples (Lyman et al. 1990; quoted, Hemond & Fechner 1994)

$t_{1/2} = 201$ d with 12 mM methanol, for aqueous atrazine using first-order decay rate, $t_{1/2} = 289$ d with 6 mM sodium acetate, $t_{1/2} = 164$ d with 6 mM acetic acid and $t_{1/2} = 200$ d with 2 mM glucose; however $t_{1/2} = 224$ d in the sample reactors without any organic amendments (Chung et al. 1996)

degradation $t_{1/2} = 39$ h and 43 h by soil micro *Rhodococcus*. sp. NI86/21 with atrazine concn $4 \text{ } \mu\text{g/mL}$ and $8 \text{ } \mu\text{g/mL}$ respectively (Van Zwieten & Kennedy 1995)

first order removal of atrazine from sediment organic carbon: $k = -0.0054 \text{ d}^{-1}$ with $t_{1/2} = 128$ d in surface sediment 0–6 cm depth, $k = -0.0016 \text{ d}^{-1}$ with $t_{1/2} = 433$ d in sub-surface sediment 24–34 cm depth from Blue Heron Pond; $k = -0.007 \text{ d}^{-1}$ with $t_{1/2} = 99$ d in surface sediment 0–6 cm depth, $k = -0.0022 \text{ d}^{-1}$ with $t_{1/2} = 630$ d in sub-surface sediment 24–34 cm depth from Oyster Rake Pond; $k = -0.0142 \text{ d}^{-1}$ with $t_{1/2} = 49$ d in surface sediment 0–6 cm depth, $k = -0.0009 \text{ d}^{-1}$ with $t_{1/2} = 770$ d in sub-surface sediment 24–34 cm depth from Trumpet Creeper East Pond, and $k = -0.0149 \text{ d}^{-1}$ with $t_{1/2} = 47$ d in surface sediment 0–6 cm depth, $k = -0.0000 \text{ d}^{-1}$ with $t_{1/2} = 70$ d in sub-surface sediment 24–34 cm depth from Trumpet Creeper North, Kiawah island (Smalling & Aelion 2004)

50–60% degradation in 35–100 d by anaerobic mixed culture microorganisms with atrazine as sole carbon source (Ghosh & Philip 2004)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.0248, 1.26 \text{ h}^{-1}$ (algae, daphnids, Ellgehausen et al. 1980)
 $k_2 = 27.2 \text{ d}^{-1}$ (catfish, Ellgehausen et al. 1980)
 $k_1 = 2.4, 30, 19.0 \text{ h}^{-1}$ (zebrafish: egg, yolk sac fry, juvenile; Görges & Nagel 1990)
 $k_1 = 227.0 \text{ h}^{-1}; k_2 = 2.354 \text{ h}^{-1}$ (algae *Scenedesmus acutus*, Wang et al. 1996)
 $k_1 = 0.412 \text{ h}^{-1}; k_2 = 0.073 \text{ h}^{-1}$ (catfish *Ictalurus melas*, Wang et al. 1996)
 $k_1 = 2.027 \text{ h}^{-1}; k_2 = 1.161 \text{ h}^{-1}$ (water flea *Daphnia magna*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 2.6 \text{ h}$, based on estimated rate constant $k = 147.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard 1991).

Surface water: estimated $t_{1/2} \sim 3.21 \text{ d}$ in aqueous solution from river die-away tests (Furmidge & Osgerby 1967; quoted, Scow 1982);

$t_{1/2} = 1\text{--}4 \text{ wk}$ in estuarine systems (Jones et al. 1982; quoted, Meakins et al. 1994);
 under laboratory conditions in distilled water and river water was completely degraded after 21.3 and 7.3 h, respectively (Mansour et al. 1989; quoted, Montgomery 1993);

$t_{1/2} = 3.2 \text{ d}$ to 7–8 months in aquatic environments (Eisler 1985; quoted, Day 1991);
 measured rate constant $k = (24 \pm 4) \text{ M}^{-1} \text{ s}^{-1}$ at pH 4.0, $k = (13 \pm 1) \text{ M}^{-1} \text{ s}^{-1}$ at pH 4.2, for direct reaction with ozone in water at 26 and 21°C , respectively, with $t_{1/2} = 1.5 \text{ h}$ at pH 7 (Yao & Haag 1991);

$t_{1/2} = 35.6\text{--}168 \text{ h}$ in surface water system of a small stream in Iowa by water quality analyses (Kolpin & Kalkhoff 1993);

$t_{1/2} = 235 \text{ d}$ at 6°C , $t_{1/2} = 164 \text{ d}$ at 22°C in darkness, $t_{1/2} = 59 \text{ d}$ under sunlight conditions for river water at pH 7.3; $t_{1/2} = 130 \text{ d}$ at 22°C in darkness for filtered river water at pH 7.3 and $t_{1/2} = 200 \text{ d}$ at 22°C in darkness, $t_{1/2} = 169 \text{ d}$ under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995)

Groundwater: $t_{1/2} = 6\text{--}15 \text{ months}$ for $0.72\text{--}10 \mu\text{g mL}^{-1}$ to biodegrade slowly at 25°C (Weidener 1974; quoted, Muir 1991)

reported half-lives or persistence, $t_{1/2} = 60\text{--}150, 71, 74$, and 130 d (Bottoni & Funari 1992)

Sediment: $t_{1/2} = 145 \text{ d}$ in a Wisconsin Lake sediment (Armstrong et al. 1967; quoted, Jones et al. 1982; Means et al. 1983) and $t_{1/2} \sim 30 \text{ d}$ for Chesapeake Bay sediment (Ballantine et al. 1978; quoted, Jones et al. 1982);
 $t_{1/2} = 7\text{--}28 \text{ d}$ for $0.1 \mu\text{g mL}^{-1}$ to rapid degrade in both aerobic and low oxygen systems in estuarine sediment/water at $12\text{--}35^\circ\text{C}$ (Jones et al. 1982, quoted, Muir 1991);

$t_{1/2}(\text{aerobic}) > 35 \text{ d}$ for $0.1\text{--}1.0 \mu\text{g mL}^{-1}$ to slowly biodegrade in sediment/water at 25°C (Wolf & Jackson 1982; quoted, Muir 1991)

$t_{1/2} = 60\text{--}120 \text{ d}$ in surface sediment, $t_{1/2} = 60\text{--}223 \text{ d}$ in subsurface sediment

biodegradation $t_{1/2} = 47\text{--}128 \text{ d}$ in the surface and $t_{1/2} = 70\text{--}770$ in subsurface sediment (Smalling & Aelion 2004)

Soil: half-lives in aqueous buffered solutions in soil at 25°C and pH 1, 2, 3, 4, 11, 12, and 13 were reported to be 3.3, 14, 58, 240, 100, 12.5, and 1.5 d , respectively (Armstrong et al. 1967; quoted, Montgomery 1993);

$t_{1/2} = 3\text{--}5 \text{ yr}$ in agricultural soils (Armstrong et al. 1967; quoted, Jones et al. 1982);

estimated persistence of 10 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987a);

$t_{1/2} = 1.73$, and 244 d at 25°C and pH 4 with and without fulvic acid (2%) (Li & Felbeck 1972; quoted, Montgomery 1993);

persistence of 10 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2} = 6.0 \text{ months}$ at 15°C and $t_{1/2} = 2.0 \text{ months}$ at 30°C in soils (Freed & Haque 1973);

persistence of 12 months (Wauchope 1978);

correlated $t_{1/2} = 37 \text{ d}$ at pH 5.1–7.0, and $t_{1/2} = 28 \text{ d}$ at pH 7.7–8.2 (Boddington Barn soil, Hance 1979),

$t_{1/2} \sim 30 \text{ d}$ at pH 4.6–5.3 and $t_{1/2} = 40 \text{ d}$ at pH 6.3–8.0 (Triangle soil, Hance 1979);

$t_{1/2} = 37 \text{ d}$ in agricultural soils (Dao et al. 1979; quoted, Jones et al. 1982);

estimated first-order $t_{1/2} = 36.5 \text{ d}$ from biodegradation rate constant $k = 0.019 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 53$ and 113 d at pH 6.5 at 22°C in a Hatzenbühl soil at pH 4.8 and Neuhofen soil, respectively (Burkhard & Guth 1981; quoted, Montgomery 1993);

$t_{1/2} = 1\text{--}6 \text{ months}$ (Jones et al. 1982; quoted, Meakins et al. 1994);

moderately persistent in soils with $t_{1/2} = 20\text{--}100 \text{ d}$ (Willis & McDowell 1982);

biodegradation $t_{1/2} = 71 \text{ d}$ from screening model calculations (Jury et al. 1984; 1987a,b; Jury & Ghodrati 1989);

$t_{1/2} \sim 6\text{--}10$ wk (Hartley & Kidd 1987; quoted, Montgomery 1993);

field $t_{1/2} = 4$ wk by using lysimeters (Bowman 1990);

half-lives from soil surfaces: $t_{1/2} = 655$ to > 1000 d in peat soil and $t_{1/2} = 143\text{--}939$ d in sandy soil at $20 \pm 1^\circ\text{C}$ (Dörfler et al. 1991);

degradation rate constant $k = (1.20 \pm 0.097) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 57.8$ d in control soil and $k = (1.01 \pm 0.034) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 68.6$ d in pretreated soil once only in the laboratory (Walker & Welch 1991);

$t_{1/2} \sim 21$ d based on extractable residues in microcosm studies, compared to $t_{1/2} = 14$ d in surface field soil (Winkelmann & Klaine 1991);

selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Hornsby et al. 1996);

soil $t_{1/2} = 130$ d (quoted, Pait et al. 1992);

field $t_{1/2} = 35\text{--}50$ d in soil and water but may be longer under cold or dry conditions; $t_{1/2} = 105$ to > 200 d under groundwater conditions, depending on test system (Wood et al. 1991; quoted, Tomlin 1994);

reported $t_{1/2} = 60\text{--}150$ d, 71 d, 74 d and 130 d (Bottoni & Funari 1992);

first-order $k = -0.017$ to -0.003 d^{-1} with corresponding $t_{1/2} = 41$ d in the 0- to 30-cm soil to $t_{1/2} = 231$ d in the 90 to 120-cm soil in Ames, Iowa (Kruger et al. 1993);

dissipation $t_{1/2} = 71$ d from soil surface (Gish et al. 1995);

$t_{1/2} = 60$ d (selected, Halfon et al. 1996).

$t_{1/2} = 60$ d (Gao et al. 1997)

Biota: $t_{1/2} = 0.03$ h in algae, $t_{1/2} = 1.52$ d in catfish and $t_{1/2} = 9.5$ h in daphnids (Ellgehausen et al. 1980);

biochemical $t_{1/2} = 64$ d from screening model calculations (Jury et al. 1987b);

$t_{1/2} = 25.6$ d in bean, $t_{1/2} = 24.3$ d in turnips and $t_{1/2} = 14.6$ d in oats at $20 \pm 1^\circ\text{C}$ from plant surfaces (Dörfler et al. 1991).

TABLE 17.1.1.4.1

Reported vapor pressures of atrazine at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Friedrich & Stambach 1964		Grayson & Fosbracey 1982		Rordorf 1989		Goodman 1997	
gas saturation-GC		gas saturation-GC		gas saturation-GC		Knudsen effusion method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	4.0 × 10 ⁻⁵	51.0	0.0040	25	3.9 × 10 ⁻⁵	40	6.7 × 10 ⁻⁴
	extrapolated	55.5	0.0048	50	1.9 × 10 ⁻³	50	2.2 × 10 ⁻³
measured range 50–130°C		63.0	0.0095	75	0.056	60	9.5 × 10 ⁻³
Antoine eq.		66.0	0.0337	100	1.0	70	0.030
eq. 1	P/mmHg	66.7	0.023	125	13.0	80	0.098
A	13.766	76.5	0.0713				
B	5945	81.5	0.117	eq. 1	P _g /Pa	eq. 1	P/Pa
		20	3.7 × 10 ⁻⁵	A	17.583	A	16.08
				B	6558.5	B	6040
		eq. 1a	P/Pa	for temp range 40–125°C			
		A	36.80				
		B	13.778				
					liquid		
				eq. 1	P _L /Pa		
				A	13.2701		
				B	4626.79		

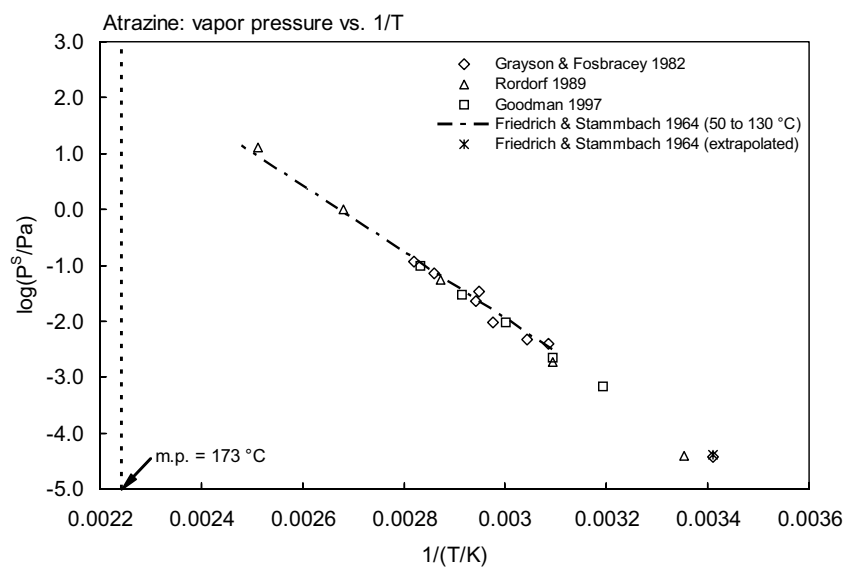
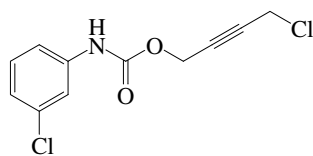


FIGURE 17.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for atrazine.

17.1.1.5 Barban



Common Name: Barban

Synonym: Barbamate, Barbane, Carbine, Carbyne, CBN, Chlorinat

Chemical Name: carbamic acid, (3-chlorophenyl)-, 4-chloro-2-butynyl ester; 4-chlorobut-2-ynyl 3-chloro-carbanilate; 4-chloro-2-butynyl 3-chlorophenylcarbamate

Uses: herbicide for post-emergence control of wild oats in wheat, barley, broad beans, field beans, soybeans, peas, sugar beet, flax, lucerne, lentils, mustard, oilseed rape, sunflowers, etc.

CAS Registry No: 101-27-9

Molecular Formula: $C_{11}H_9Cl_2NO_2$

Molecular Weight: 258.101

Melting Point ($^{\circ}C$):

75 (Khan 1980; Herbicide Handbook 1989; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.403 ($25^{\circ}C$, Hartley & Kidd 1987)

Molar Volume (cm^3/mol):

262.8 (calculated-Le Bas method at normal boiling point, this work)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

109.1 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

26.8 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.323 (mp at $75^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

15.0 (Swezey & Nex 1961)

11.0 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

11.0 (Martin & Worthing 1977; Ashton & Crafts 1981; Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989, Budavari 1989; Milne 1995)

11.0 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.33×10^{-3} ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

5.00×10^{-5} (Hartley & Kidd 1987)

1.60×10^{-4} (Worthing & Walker 1987)

5.05×10^{-5} (Herbicide Handbook 1989)

3.50×10^{-5} , 1.0×10^{-3} , 0.019, 0.240, 2.20 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 14.669 - 5703.8/(T/K)$; measured range 72 – $150^{\circ}C$ (gas saturation-GC, Rordorf 1989)

5.07×10^{-5} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.00117 ($20^{\circ}C$, calculated-P/C, Muir 1991)

1.17 (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)

0.00117 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.68 (selected, Gerstl & Helling 1987)

Bioconcentration Factor, $\log BCF$:

2.20 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$ at 25°C or as indicated:

3.06 (soil, calculated-S, Kenaga 1980)

2.66 (calculated-MCI χ , Gerstl & Helling 1987)

3.00 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 6690$ d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: $t_{1/2} = 2.25$ h for 22–99% of 10 $\mu\text{g/ml}$ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

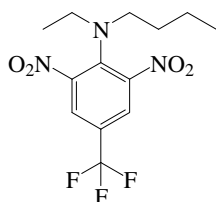
Soil: estimated persistence of 2 months (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 2 weeks in soil (Edwards 1973; quoted, Morrill et al. 1982);

persistence of about 3 weeks in soil (Herbicide Handbook 1989);

selected field $t_{1/2} = 5$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.6 Benefin



Common Name: Benefin

Synonym: Balan, Bonalan, benfluralin

Chemical Name: *N*-butyl-*N*-ethyl- α,α,α -trifluoro-2,6-dinitro-*p*-toluidine

Uses: as pre-emergence herbicide for the control of annual grasses and broadleaf weeds in chicory, cucumbers, endive, groundnuts, lettuce, lucerne, and other foliage crops.

CAS Registry No: 1861-40-1

Molecular Formula: $C_{13}H_{16}F_3N_3O_4$

Molecular Weight: 335.279

Melting Point ($^{\circ}C$):

66 (Lide 2003)

Boiling Point ($^{\circ}C$):

121–122 (0.5 mmHg), 148–149 at 7 mmHg (Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.28 (tech., Tomlin 1994)

Molar Volume (cm^3/mol):

295.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

38.70 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.396 (mp at $66^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

< 1.0 (Ashton & Crafts 1973)

0.50 (Weber et al. 1980)

1.0 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.10 (Herbicide Handbook 1983; Tomlin 1994)

0.10 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.00519 ($30^{\circ}C$, Ashton & Crafts 1973)

0.0104 (Herbicide Handbook 1983)

0.0040 ($20^{\circ}C$, estimated, Suntio et al. 1988)

0.0087 (Tomlin 1994)

0.0088 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

1.34 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{ow} :

5.34 (selected, Magee 1991)

5.29 ($20^{\circ}C$, pH 7, Tomlin 1994)

5.29 (pH 7, selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

3.36 (calculated-S per Kenaga 1980, this work)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.03 (quoted exptl., Sabljic 1987)
- 4.03, 3.75 (quoted, estimated; Magee 1991)
- 3.95 (soil, Hornsby et al. 1996)
- 2.96 (2.59–3.33) (soil: organic carbon OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric and aqueous photolysis half-lives were estimated to be 288–864 h (Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} \sim 0.782$ –7.82 h based on reaction with OH radicals in air (Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aerobic $t_{1/2} \sim 504$ –2880 h in soil, and anaerobic soil $t_{1/2} = 144$ –480 h (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.782$ –7.82 h based on estimated reaction with OH radicals in the gas-phase (Howard et al. 1991).

Surface water: $t_{1/2} = 288$ –864 h based on observed photolysis by sunlight (Howard et al. 1991).

Groundwater: $t_{1/2} = 144$ –5760 h based on unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

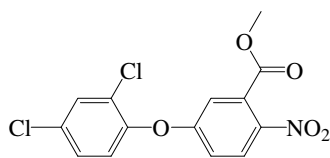
Sediment:

Soil: $t_{1/2} = 504$ –2880 h based on aerobic solid die-away test data (Howard et al. 1991);

field $t_{1/2} = 40$ d (Hornsby et al. 1996).

Biota:

17.1.1.7 Bifenox



Common Name: Bifenox

Synonym: MC-4379, Modown

Chemical Name: benzoic acid, 5-(2,4-dichlorophenoxy)-2-nitro-, methyl ester; methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate

Uses: selective pre-emergence and post-emergence herbicide to effectively control a wide variety of broadleaf weeds in corn, grain, sorghum, maize, rice, and soybeans.

CAS Registry No: 42576-02-3

Molecular Formula: $C_{14}H_9Cl_2NO_5$

Molecular Weight: 342.131

Melting Point ($^{\circ}C$):

85 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.155 (Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

305.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

90.5 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

26.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

74.0 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.258 (mp at $85^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.35 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

0.35 (Martin & Worthing 1977; Herbicide Handbook 1978)

0.35 (Ashton & Crafts 1981; Herbicide Handbook 1989; Budavari 1989)

0.35 ($30^{\circ}C$, Worthing & Walker 1987)

0.35 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

0.398 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00032 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

0.00032 ($30^{\circ}C$, Ashton & Crafts 1981; Worthing & Hance 1991; Tomlin 1994)

0.00032 ($30^{\circ}C$, Hartley & Kidd 1987; Budavari 1989; Montgomery 1993)

5.40×10^{-6} , 2.0×10^{-4} , 4.40×10^{-3} , 0.064, 0.67 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log (P_s/Pa) = 14.996 - 6040.4/(T/K)$; measured range 36.9 – $85.5^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/Pa) = 13.815 - 5582.5/(T/K)$; measured range 90.5 – $175^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

0.00032 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.321 ($20^{\circ}C$, calculated-P/C, Muir 1991)

0.011 (calculated-P/C, Montgomery 1993)

0.313 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

- 5.63 (selected, Dao et al. 1983)
- 4.50 (Worthing & Hance 1991)
- 4.48 (Montgomery 1993; Tomlin 1994)
- 4.48 (selected, Hansch et al. 1995)
- 5.24 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 2.30 (static water, Metcalf & Sanborn 1975; quoted, Kenaga & Goring 1980; Isensee 1991)
- 3.05 (calculated-S, Kenaga 1980; quoted, Isensee 1991)

Sorption Partition Coefficient, log K_{oc} :

- 3.89 (soil, calculated per Kenaga & Goring, Kenaga 1980)
- 4.0 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.24–4.39 (Montgomery 1993)
- 4.0 (estimated-chemical structure, Lohninger 1994)
- 2.70–4.36 (Tomlin 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 29.8$ d from 1 m depth of water at 30°C (Muir 1991).

Photolysis: with < 5% degradation by UV light of 290–400 nm in 48 h (Worthing & Hance 1991).

Oxidation:

Hydrolysis: stable in aqueous solution at pH 5.0–7.3 but rapidly hydrolyzed at pH 9.0 both at 22°C (Worthing & Hance 1991).

Biodegradation: $t_{1/2} = 2$ –5 d for 10 µg/mL to biodegrade in flooded soil at 30°C (Ohyama & Kuwatsuka 1978; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} = 2$ –5 d for 10 µg/mL to biodegrade in flooded soil at 30°C (Ohyama & Kuwatsuka 1978; quoted, Muir 1991);

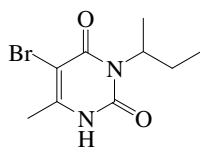
average $t_{1/2} = 7$ –14 d in soils (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);

selected field $t_{1/2} = 7.0$ d (Wauchope et al. 1992; Hornsby et al. 1996);

average $t_{1/2} = 7$ –14 d (Herbicide Handbook 1989);

$t_{1/2} \sim 5$ –7 d in soil (Tomlin 1994).

17.1.1.8 Bromacil



Common Name: Bromacil

Synonym: Borea, Bromax, Bromazil, Cynogan, Hyvar, Hyvarex, Krovar I or II, Nalkil, Uragan, Urox B, Uron HX, Weed Blast

Chemical Name: 5-bromo-3-*sec*-butyl-6-methyluracil; 5-bromo-6-methyl-3-(1-methylpropyl)-2,4-(1*H*,3*H*)pyrimidinedione

Uses: Herbicide applied to soil to control annual and perennial grasses, broadleaf weeds, and general vegetation on uncropped land; also used for selective weed control in apple, asparagus, cane fruit, hops, and citrus crops.

CAS Registry No: 314-40-9

Molecular Formula: C₉H₁₃BrN₂O₂

Molecular Weight: 261.115

Melting Point (°C):

158 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.55 (25°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993)

1.59 (23°C, Tomlin 1994)

1.55 (Milne 1995)

Molar Volume (cm³/mol):

193.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

9.10 (Wauchope et al. 1992; Hornsby et al. 1996)

< 7.0 (Montgomery 1993)

9.27 (Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0496 (mp at 158°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

815 (Bailey & White 1965; Khan 1980; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

815 (Melnikov 1971; Spencer 1973; Herbicide Handbook 1978; Herbicide Handbook 1989)

815 (20°C, Weber 1972; Worthing & Walker 1987, Worthing & Hance 1991)

820 (Beste & Humburg 1983; Jury et al. 1983)

1064 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984; Gerstl & Helling 1987)

626, 775, 1043 (4, 25, 40°C, shake flask-LSS, Madhun et al. 1986)

700 (20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

700, 807, 1287 (at pH 7, 5, 9, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

5 × 10⁻⁵ (20°C, Weber 1972; Worthing & Walker 1987)

3 × 10⁻⁵ (estimated, USEPA 1975)

0.107 (100°C, Khan 1980)

2.9 × 10⁻⁵ (Jury et al. 1983)

0.00033 (Hartley & Kidd 1987; Worthing & Hance 1991)

4 × 10⁻⁵ (20–25°C, selected, Wauchope et al. 1992)

3.3 × 10⁻⁵ (Montgomery 1993)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C at 25°C or as indicated):

- 9.17×10^{-6} (Beste & Humburg 1983; Jury et al. 1983)
- 9.17×10^{-5} (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
- 0.0019 (20°C , selected, Suntio et al. 1988)
- 1.06×10^{-5} (20°C , calculated-P/C, Muir 1991)
- 1.06×10^{-5} (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.02 (Rao & Davidson 1980)
- 1.33 (selected, Dao et al. 1983)
- 1.84 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
- 1.84, 1.87, 1.90 (4, 25, 40°C , shake flask-LSS, Madhun et al. 1986)
- 1.85 (selected, Gerstl & Helling 1987)
- 2.11 selected, Magee 1991; Devillers et al. 1996)
- 1.84–2.04 (Montgomery 1993)
- 2.11 (selected, Sangster 1993)
- 1.87, 1.88, 1.63 (at pH 7, 5, 9, Tomlin 1994)
- 2.11 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.505 (measured, Kenaga 1980)
- 2.27 (calculated-S, Kenaga 1980)
- 0.477 (calculated- K_{OC} , Kenaga 1980)
- 0.51 (*Pimephales promelas*, Call et al. 1987)

Sorption Partition Coefficient, $\log K_{\text{OC}}$ at 25°C or as indicated:

- 1.86 (soil, Hamaker & Thompson 1972)
- 3.13 (soil, calculated as per Kenaga & Goring 1980, Kenaga 1980)
- 1.86 (Rao & Davidson 1980)
- 2.33, 1.34, 1.63 (estimated-S, calculated-S and mp, calculated- K_{OW} , Karickhoff 1981)
- 1.61 (sediments average-Freundlich adsorption, Corwin & Farmer 1984)
- 1.41–2.46 (California lake sediments, Corwin & Farmer 1984)
- 1.98, 1.88 (4, 25°C , Semiahmoo soil, in $\mu\text{mol}/\text{kg}$ OC, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.11, 1.88 (4, 25°C , Adkins soil, in $\mu\text{mol}/\text{kg}$ OC, Madhun et al. 1986)
- 1.90, 1.66, 1.75; 1.86, 1.89, 1.34 (estimated- K_{OW} ; S, Madhun et al. 1986)
- 1.53, 2.73 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
- 1.86 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989; Carsel 1989)
- 2.56 (calculated-MCI χ , Bahnick & Doucette 1988)
- 1.86, 1.80 (reported, estimated as $\log K_{\text{OM}}$, Magee 1991)
- 1.53, 1.86, 3.13 (soil, quoted values, Bottoni & Funari 1992)
- 1.51 (soil, 20 – 25°C , selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.51 (Montgomery 1993)
- 2.09 (estimated-chemical structure, Lohninger 1994)
- 1.60 (quoted or calculated-QSAR MCI χ , Sabljic et al. 1995)
- 1.43, 1.72 (average values for sediments, soils, Delle Site 2001)
- 1.48, 1.46, 1.53 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, $0.1 \leq \text{OC} < 0.5\%$, and pH 6.3–7.9, average, Delle Site 2001)
- 1.80, 1.72 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, and pH ≤ 7.3 undissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: estimated $t_{1/2} \sim 10,000$ d from 1 m depth of water at 20°C (Muir 1991).
- Photolysis: 115 ppb contaminated water in the presence of TiO_2 and H_2O_2 photodegraded to 6 ppb by 15 h solar irradiation with complete degradation after 75 h (Muszkat et al. 1992).
- Oxidation:
- Hydrolysis:

Biodegradation: $t_{1/2} = 350$ d for 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported $t_{1/2} = 150$ –158 and 350 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 7.0$ months at 15°C and $t_{1/2} = 4.5$ months at 30°C in soils (Freed & Haque 1973);

rate constant $k = 0.0038 \text{ d}^{-1}$ with biodegradation $t_{1/2} = 350$ d under field conditions (Rao & Davidson 1980; quoted, Jury et al. 1984);

$t_{1/2} = 350$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

$t_{1/2} > 100$ d (Willis & McDowell 1982)

$t_{1/2} \sim 5429$ –46200 d in loamy sand and peat at 25–35°C as follows (Madhum & Freed 1987):

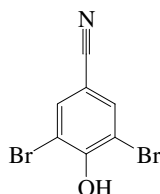
$t_{1/2} = 46200$, 12391, and 5856 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg, while $t_{1/2} = 18851$, 9925, and 7588 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives in peat. $t_{1/2} = 5429$, 6789, and 8044 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while $t_{1/2} = 6293$, 5986, and 6784 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahoo mucky peat (Madhun & Freed 1987)

selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 150$ –180d and 350 d (Bottoni & Funari 1992).

Biota: biochemical $t_{1/2} = 350$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

17.1.1.9 Bromoxynil



Common Name: Bromoxynil

Synonym: Brittox, Brominal, Brominex, Brominil, Broxynil, Bucril, Chipco crab-kleen, ENT 20852, Nu-lawn weeder, Oxytril M, Partner

Chemical Name: 3,5-dibromo-4-hydroxybenzonitrile; 4-cyano-2,6-dibromophenol

Uses: herbicide for post-emergence control of annual broadleaf weeds and it is often used in combination with other herbicides to extend the spectrum of control.

CAS Registry No: 1689-84-5

Molecular Formula: $C_7H_3Br_2NO$

Molecular Weight: 276.913

Melting Point ($^{\circ}C$):

190 (Khan 1980; Herbicide Handbook 1989; Montgomery 1993; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

176.7 (calculated-Le Bas method at normal boiling point, this work)

Dissociation Constant pK_a :

4.20 (radiometer/pH meter, Cessna & Grover 1978)

4.06 (Herbicide Handbook 1989; Montgomery 1993)

4.06 (Budavari 1989; Worthing & Hance 1991)

3.86 (Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

31.80 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0241 (mp at $190^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

130 ($20-25^{\circ}C$, Spencer 1973)

131 (Kenaga 1980)

< 200 (Khan 1980)

130 ($20-25^{\circ}C$, Ashton & Crafts 1981)

130 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

130 (Worthing & Walker 1987, Worthing & Hance 1991)

130 ($20-25^{\circ}C$, Herbicide Handbook 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

< 0.0010 ($20^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

0.00064 (Herbicide Handbook 1989)

0.00064 (Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.14180 ($20-25^{\circ}C$, calculated-P/C, Montgomery 1993)

1.36×10^{-3} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.60 (selected, Dao et al. 1983)

< 2.00 (Herbicide Handbook 1989)

< 2.00 (Montgomery 1993)

Bioconcentration Factor, log BCF:

1.60 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

2.48 (soil, quoted from Kenaga 1980, Bottoni & Funari 1992)

2.48 (calculated, Montgomery 1993)

2.86, 3.06 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant of degradation in water, $k = 1.04 \times 10^{-3} \text{ s}^{-1}$ at pH 8.3 and $k = 1.08 \times 10^{-3} \text{ s}^{-1}$ at pH 11.6 (Kochany 1992).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} \sim 24 \text{ h}$ for $0.03 \text{ }\mu\text{g/mL}$ to biodegrade in runoff water at $20\text{--}25^\circ\text{C}$ (Brown et al. 1984; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

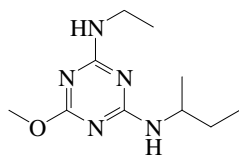
Surface water: $t_{1/2} \sim 24 \text{ h}$ for $0.03 \text{ }\mu\text{g mL}^{-1}$ to biodegrade in runoff water at $20\text{--}25^\circ\text{C}$ (Brown et al. 1984; quoted, Muir 1991).

Ground water: reported $t_{1/2} = 10 \text{ d}$ (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} \sim 10 \text{ d}$ in soil (Hartley & Kidd 1987; Worthing & Hance 1991; quoted, Bottoni & Funari 1992; Montgomery 1993; Tomlin 1994);.

Biota:

17.1.1.10 *sec*-Bumeton

Common Name: *sec*-Bumeton

Synonym: etazine, GS14254, secbumeton

Chemical Name: *N*-ethyl-6-methoxy-*N'*-(1-methylpropyl)-1,3,5-triazine-2,4-diamine

CAS Registry No: 26259-45-0

Uses: herbicide

Molecular Formula: C₁₀H₁₉N₃O

Molecular Weight: 225.291

Melting Point (°C):

87 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.105 (Hartley & Kidd 1987; Worthing & Walker 1987)

Molar Volume (cm³/mol):

Dissociation Constant pK_a:

4.4 (Worthing 1987)

4.4, 4.36 (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.246 (mp at 87°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

620 (quoted, Kenaga & Goring 1980)

620 (Ashton & Crafts 1981)

600 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987)

600 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

9.7 × 10⁻⁴ (20°C, Ashton & Crafts 1981; Worthing & Walker 1987)

9.71 × 10⁻⁴ (20°C, Hartley & Kidd 1987)

9.7 × 10⁻⁴ (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:

3.20 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

1.20 (fish, Kenaga 1980b)

Sorption Partition Coefficient, log K_{OC}:

2.54 (soil, calculated, Kenaga & Goring 1980)

2.11 (soil, calculated, Kenaga 1980b)

2.18 (soil, pH 7, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

2.78; 2.29 (soil: quoted, calculated-MCI χ, Meylan et al. 1992)

2.78 (soil, calculated-MCI χ, Sabljic et al. 1995)

2.78; 2.78, 2.55 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: on hydrolysis at 20°C, $t_{1/2} \sim 30$ d at pH 1, $t_{1/2} = 75$ d at pH 13 (Worthing & Walker 1987).

Half-Lives in the Environment:

Air:

Surface water: on hydrolysis at 20°C, $t_{1/2} \sim 30$ d at pH 1, $t_{1/2} = 75$ d at pH 13 (Worthing & Walker 1987).

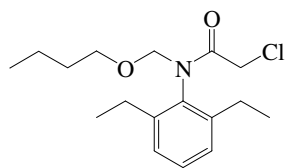
Ground water:

Sediment:

Soil: field $t_{1/2} \sim 60$ d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

17.1.1.11 Butachlor



Common Name: Butachlor

Synonym: Butanex, Butanox, CP 53619, Lambast, Machete, Pillarsete

Chemical Name: N-butoxymethyl-2-chloro-2'-diethylacetanilide; N-(butoxymethyl)-2-chloro-N-(2,6-diethylphenyl)-acetamide

Uses: herbicide for pre-emergence control of most annual grasses, some broadleaf weeds, and many aquatic weeds in both seeded and transplanted rice.

CAS Registry No: 23184-66-9

Molecular Formula: $C_{17}H_{26}ClNO_2$

Molecular Weight: 311.847

Melting Point ($^{\circ}C$):

< -5.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

156 (at 0.5 mmHg, Ashton & Crafts 1981; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.07 ($25^{\circ}C$, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

387.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

23 ($20^{\circ}C$, Weber 1972; Worthing 1987)
 20 (Martin & Worthing 1977)
 23 ($24^{\circ}C$, Ashton & Crafts 1981; Herbicide Handbook 1989)
 20 ($20^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
 23 ($24^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991)
 23 ($20-25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0007 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)
 0.0006 (Ashton & Crafts 1981; Herbicide Handbook 1989)
 0.0006 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
 0.0006 ($20-25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.00817 ($20^{\circ}C$, calculated-P/C, Muir 1991)
 0.00814 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.50 (quoted and recommended, Hansch et al. 1995; quoted, Sabljic et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.06 (calculated-S, Kenaga 1980)
 1.03, 0.756 (18, 9 $\mu g/L$ concn in water; carp, 3-5 d exposure, Wang et al. 1992)

0.38, 0.845 (10, 1 $\mu\text{g/L}$ concn in water; tilapia, 3–5 d exposure, Wang et al. 1992)
0.447, 0.845 (10, 1 $\mu\text{g/L}$ concn in water; loach, 3–5 d exposure, Wang et al. 1992)
1.76, 2.02 (2.5, 1.25 $\mu\text{g/L}$ concn in water; grass carp, 3–5 d exposure, Wang et al. 1992)
1.71, 1.90 (5, 2.5 $\mu\text{g/L}$ concn in water; eel, 3–5 d exposure, Wang et al. 1992)
1.99, 2.34 (2.4, 0.4 $\mu\text{g/L}$ concn in water; black silver carp, 3–5 d exposure, Wang et al. 1992)
0.041, 0.778 (100, 10 $\mu\text{g/L}$ concn in water; freshwater clam, 3–5 d exposure, Wang et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

2.92 (calculated-solubility, Kenaga 1980)
2.85 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
2.86 (soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 1049$ d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: $t_{1/2} = 0.8\text{--}5.4$ h in distilled water (Chen et al. 1982; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: $t_{1/2} > 2.5$ months for 2 $\mu\text{g/mL}$ to hydrolyze in phosphate buffer at pH 6 and borate buffer at pH 9 both at 25°C (Chen & Chen 1979; quoted, Muir 1991).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

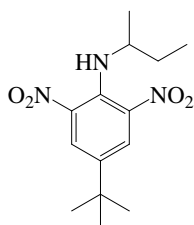
Soil: persists for 6–10 wk in soil (Hartley & Kidd 1987; Tomlin 1994);

$t_{1/2} = 4$ to 8 d depending upon soil type (Herbicide Handbook 1989);

persists in soil 42–70 d (Worthing & Hance 1991);

selected field $t_{1/2} = 12$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.12 Butralin



Common Name: Butralin

Synonym: Amex, Butalin, Rutralin, Sector, Tamex

Chemical Name: N-*sec*-butyl-4-*tert*-butyl-2,6-dinitroaniline; 4-(1,1-dimethylethyl)-N-(1-methylpropyl)-2,6-dinitrobenzenamine

Uses: herbicide for pre-emergence control of annual broadleaf weeds and grasses in cotton, beans, barley, rice, soybeans, alliums, vines, ornamentals and orchards of fruit and nut trees; also to control suckers on tobacco.

CAS Registry No: 33629-47-9e

Molecular Formula: $C_{14}H_{21}N_3O_4$

Molecular Weight: 295.335

Melting Point ($^{\circ}C$):

60 (Lide 2003)

Boiling Point ($^{\circ}C$):

134–136 (at 0.5 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

313.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.454 (mp at $60^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.0 (Herbicide Handbook 1978)
 1.0 (Khan 1980)
 10 ($24^{\circ}C$, Ashton & Crafts 1981)
 1.0 ($24^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
 1.0 (24 – $26^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991)
 1.0 (Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$):

0.002 (Ashton & Crafts 1981)
 0.0017 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
 0.0017 (Budavari 1989)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.502 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.54 (selected, Dao et al. 1983)
 5.16 (quoted LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.79 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 2.80 (calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

- 3.64 (calculated, Kenaga & Goring 1980; quoted, Kenaga 1980)
- 3.91 (soil, Kenaga & Goring 1980; quoted, Sabljic 1987; Bahnick & Doucette 1988)
- 3.75 (calculated-MCI χ , Bahnick & Doucette 1988)
- 3.98 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.98; 3.38 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 8$ h for 25% of 2000 $\mu\text{g/mL}$ to degrade in methanol under sunlight (Plimmer & Klingebiel 1974; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} = 24$ d for 0.5 $\mu\text{g/mL}$ to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991).

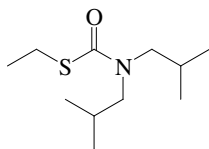
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} = 24$ d for 0.5 $\mu\text{g/mL}$ to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991).

17.1.1.13 Butylate



Common Name: Butylate

Synonym: Butilate, diisocarb, Genate, R 1910, Sutan

Chemical Name: *S*-ethyl-diisobutylthiocarbamate; *S*-ethyl-bis(2-methylpropylcarbamothioate

Uses: herbicide to control annual grass weeds in maize, by pre-plant soil incorporation; also to control some broadleaf weeds.

CAS Registry No: 2008-41-5

Molecular Formula: $C_{11}H_{23}NO_S$

Molecular Weight: 217.372

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

137.5–138 (at 21 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

71.0 (at 10 mmHg, Herbicide Handbook 1989)

Density (g/cm^3 at $20^{\circ}C$):

0.9402 ($25^{\circ}C$, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994)

0.9417 (Milne 1995)

Molar Volume (cm^3/mol):

280.9 (calculated-Le Bas method at normal boiling point, Suntio et al. 1988)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

45.0 (Kenaga 1980; Weber et al. 1980)

45.0 ($22^{\circ}C$, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)

46.0 ($20^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991)

44.0 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

36.0 ($20^{\circ}C$, Tomlin 1994)

45.0 ($22^{\circ}C$, Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.73 (Ashton & Crafts 1973)

0.096 ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

1.733 (Herbicide Handbook 1983, 1989)

0.287 ($20^{\circ}C$, GC-RT correlation, Kim 1985)

0.10 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.17 (Worthing & Hance 1991)

1.733 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.73 (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.560 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.15 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)

4.15 (recommended, Hansch et al. 1995)

4.17, 4.01, 3.45 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.86 (calculated-S, Kenaga 1980)
- 3.06 (calculated- K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC} :

- 2.73 (soil, Kenaga 1980)
- 2.73, 4.09 (quoted values, Bottoni & Funari 1992)
- 2.60 (soil, 20–25°C, selected, Wauchope et al. 1992)
- 2.60 (estimated-chemical structure, Lohninger 1994)
- 2.11 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 2.39, 2.13 (soil, estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported half-lives or persistence, $t_{1/2}$ = 11–21 d (Bottoni & Funari 1992)

Sediment:

Soil: measured dissipation rate k = 3.6 d⁻¹ (Nash 1983; quoted, Nash 1988);

estimated dissipation rate k = 23 and 0.61 d⁻¹ (Nash 1988);

$t_{1/2}$ = 1.5–3.0 wk in several soils under crop growing conditions (Herbicide Handbook 1989);

selected field $t_{1/2}$ = 13 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)

reported $t_{1/2}$ = 11–21 d (Bottoni & Funari 1992);

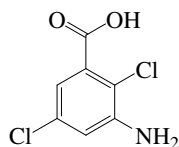
soil $t_{1/2}$ = 12 d (quoted, Pait et al. 1992);

$t_{1/2}$ = 1.5–10 wk in soil and water (Tomlin 1994);

soil $t_{1/2}$ = 13 d (selected, Halfon et al. 1996).

Biota: disappear from the stems and leaves of corn plants 7 to 14 d after application (Herbicide Handbook 1989).

17.1.1.14 Chloramben



Common Name: Chloramben

Synonym: ACP-M-728, Amiben, Amoben, Chlorambed, Chlorambene, M-728, NCI-C00055, Ornamental weeder, Vegaben, Vegiben

Chemical Name: 3-amino-2,5-dichlorobenzoic acid

Uses: pre-emergence or pre-plant herbicide used in many vegetable and field crops to control annual broadleaf weeds and grasses.

CAS Registry No: 133-90-4

Molecular Formula: $C_7H_5Cl_2NO_2$

Molecular Weight: 206.027

Melting Point (C):

200 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

190.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

3.40 (Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

38.91 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0192 (mp at 200°C)

Water Solubility (g/m³ or mg/L at 25°C):

700 (Spencer 1973; Ashton & Crafts 1981)

700 (Martin & Worthing 1977; Herbicide Handbook 1978; 1989)

700 (Hartley & Kidd 1987; Budavari 1989; Montgomery 1993; Milne 1995)

700 (Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):

0.933 (100°C, Segal & Sutherland 1967; Spencer 1976)

0.93 (100°C, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

52.7 (Worthing & Walker 1987)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.274 (calculated-P/C as per Worthing 1987)

Octanol/Water Partition Coefficient, log K_{ow} :

1.11 (quoted, Rao & Davidson 1980)

1.46 (selected, Dao et al. 1983)

-2.64 (selected, Gerstl & Helling 1987)

1.11 (Magee 1991)

1.11 (Montgomery 1993)

1.11 (Log P database of Hansch & Leo 1987, Sangster 1993)

1.90 (CLOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

1.18 (calculated-S, Kenaga 1980)

-0.097 (calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.32 (soil, Harris & Warren 1964; Farmer 1976)
- 2.08 (soil, calculated as per Kenaga & Goring 1980, Kenaga 1980)
- 1.78 (calculated-MCI χ , Gerstl & Helling 1987)
- 1.32 (reported as $\log K_{OM}$, Magee 1991)
- 2.28 (Montgomery 1993)
- 1.56 (selected, Lohninger 1994)
- 1.48 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 6$ h for 206 $\mu\text{g/mL}$ to degrade in distilled water under sunlight (Sheets 1963; quoted, Cessna & Muir 1991);

$t_{1/2} < 2$ d for 16 $\mu\text{g/mL}$ to degrade in distilled water under sunlight (Hahn et al. 1969; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} > 70$ d for 50 $\mu\text{g/mL}$ to degrade in incubated soil with nutrient medium of 3 g/L (Schliebe et al. 1965; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

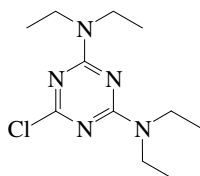
Half-Lives in the Environment:

Soil: estimated persistence of 3 months (Kearney et al. 1969; quoted, Jury et al. 1987);

$t_{1/2} = 36, 38, 41$, and 20 d with disappearance rates: $k = 0.0193, 0.0182, 0.0169$ and 0.0347 d^{-1} at pH 4.3, 5.3, 6.5 and 7.5 (Hamaker 1972; quoted, Nash 1988);

persistence in soil is of 6–8 wk (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993).

17.1.1.15 Chlorazine



Common Name: Chlorazine

Synonym:

Chemical Name: 6-chloro-*N,N,N',N'*-tetraethyl-1,3,5-triazine-2,4-diamine

Uses: herbicide

CAS Registry No: 580-48-3

Molecular Formula: $C_{11}H_{20}ClN_5$

Molecular Weight: 257.764

Melting Point ($^{\circ}C$):

27 (Howard 1991; Lide 2003)

Boiling Point ($^{\circ}C$):

154–156/4.0 mmHg (Howard 1991)

Density (g/cm^3):

Acid Dissociation Constants, pK_a :

1.74 (pK_a of conjugate acid, Howard 1991)

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.956 (mp at $27^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

23.7, 22.2, 21.4 ($26^{\circ}C$, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.236 (estimated, Howard 1991)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.033 (estimated-S, Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

2.90 (calculated-S, Howard 1991)

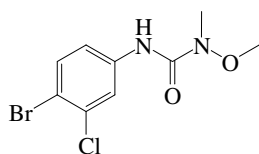
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Hydrolysis: may be more important at low pH (Howard 1991).

Half-Lives in the Environment:

Air: $t_{1/2} = 2.5$ h for the vapor phase reaction with OH radicals (estimated, Howard 1991).

17.1.1.16 Chlorbromuron



Common Name: Chlorbromuron

Synonym: Maloran

Chemical Name: 3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea

Uses: herbicide

CAS Registry No: 13360-45-7

Molecular Formula: $C_9H_{10}BrClN_2O_2$

Molecular Weight: 293.544

Melting Point ($^{\circ}C$):

96 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3): 1.69 (Tomlin 1994)

Acid Dissociation Constants, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, (assuming $\Delta S_{fus} = 56\ J/mol\ K$) F: 0.201 (mp at $96^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

50 (Kenaga & Goring 1980, Kenaga 1980a; Ashton & Crafts 1981)

35 ($20^{\circ}C$, Spencer 1982; Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)

35; 27.4 (quoted; calculated-MCI χ , Patil 1994)

35 (selected, 20 – $25^{\circ}C$, Augustijn-Beckers 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

5.33×10^{-5} ($20^{\circ}C$, Ashton & Crafts 1981)

5.3×10^{-5} (Spencer 1982; Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)

5.33×10^{-5} (selected, 20 – $25^{\circ}C$, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.06 (quoted, Rao & Davidson 1980)

3.09 (shake flask, Brigg 1981)

3.09; 3.26 (quoted lit.; calculated-MCI χ , Patil 1994)

3.09 (recommended, Hansch et al. 1995)

2.86, 2.99, 3.45 (RP-HPLC-RT correlation, CLOGP, HPLC- k' correlation, Finizio et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.83, 1.40 (quoted, calculated, Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{OC}$:

2.66 (soil, Kenaga & Goring 1980)

2.66, 2.71 (quoted, calculated- K_{ow} , Kenaga 1980b)

3.00 (mean value of 5 soils, Rao & Davidson 1980)

2.34, 2.94 (quoted, calculated-MCI χ , Gerstl & Helling 1987)

2.19–3.61 (range of reported data, Augustijn-Beckers et al. 1994)

- 2.70 (estimated and recommended, soil, Augustjin-Beckers et al. 1994; Hornsby et al. 1996)
2.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.70, 2.97 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
2.54, 2.55 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Hydrolysis: slowly hydrolyzed in neutral, slightly acidic, and slightly alkaline media (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

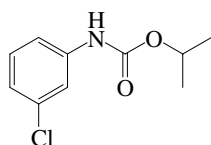
Soil: persists in soil > 56 d (Worthing 1983);

$t_{1/2}$ = 45 d (Hartley & Kidd 1987);

$t_{1/2}$ = 45–120 d (Tomlin 1994);

$t_{1/2}$ = 21–45 d and 40 d (range of reported values and recommended field half-life, Augustjin-Beckers et al. 1994; Hornsby et al. 1996)

17.1.1.17 Chlorpropham



Common Name: Chlorpropham

Synonym: Beet-Kleen, Bud-nip, Chlor-IFC, Chloro-IPC, CIPC, Ebanil, ENT 18060, Fasco Wy-hoe, Furloe, Nexoval, Prevenol, Preweed, Sprout-nip, Taterpex

Chemical Name: isopropyl N-(3-chlorophenyl) carbamate; isopropyl 3-chlorocarbamate

Uses: pre-emergent and post-emergent herbicide used to regulate plant growth and control weeds in carrot, onion, garlic, and other crops.

CAS Registry No: 101-21-3

Molecular Formula: $C_{10}H_{12}ClNO_2$

Molecular Weight: 213.661

Melting Point ($^{\circ}C$):

41 (Lide 2003)

Boiling Point ($^{\circ}C$):

149 (at 2 mmHg, Budavari 1989)

Density (g/cm^3 at $20^{\circ}C$):

1.180 ($30^{\circ}C$, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

1.5388 (Budavari 1989)

Molar Volume (cm^3/mol):

232.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.67 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.50 (DSC method, Plato & Glasgow 1969)

16 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.697 (mp at $41^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.470 (Brust 1966)

102.3 (shake flask-GC, Freed et al. 1967)

108 ($20^{\circ}C$, Günther et al. 1968)

89 ($20^{\circ}C$, Weber 1972; Martin & Worthing 1977; Worthing & Walker 1987)

2.0 (Spencer 1973; quoted, Shiu et al. 1990)

88 (Martin & Worthing 1977; Herbicide Handbook 1978, 1989)

0.70 ($19^{\circ}C$, shake flask-GC, Bowman & Sans 1979)

0.73 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a,b)

88 (Khan 1980; Ashton & Crafts 1981)

80–102 (Weber et al. 1980)

89 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

89 (selected, Gerstl & Helling 1987; Montgomery 1993; Lohninger 1994)

2.0 ($20^{\circ}C$, Worthing & Walker 1987)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00050 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

0.00133 (extrapolated, Spencer 1976)

0.00133 (Khan 1980)

0.00133 (Ashton & Crafts 1981; Herbicide Handbook 1989)

0.00100 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.012, 0.30, 5.0, 56, 470 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log (P_s/Pa) = 16.402 - 5467.7/(T/K)$; measured range 44.9–140°C (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/Pa) = 13.753 - 4631.9/(T/K)$; measured range 44.9–140°C (liquid, gas saturation-GC, Rordorf 1989)

0.00130 (selected, Taylor & Spencer 1990)

0.00107 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.00133 (estimated, Montgomery 1993)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

0.0021 (20°C, calculated-P/C, Suntio et al. 1988)

0.0032 (20°C, calculated-P/C, Muir 1991)

0.0021 (20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.06 (Rao & Davidson 1980; Karickhoff 1981)

3.42 (selected, Dao et al. 1983; Gerstl & Helling 1987)

3.51 (shake flask, Mitsutake et al. 1986)

3.10 (selected, Suntio et al. 1988)

3.51 (recommended, Sangster 1993)

3.09 (calculated, Patil 1994)

3.51 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.70 (calculated-S, Kenaga 1980)

1.52 (calculated- K_{oc} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

2.77 (soil, Hamaker & Thompson 1972)

2.57 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)

2.85, 2.80 (estimated-S, Karickhoff 1981)

3.17, 3.08 (estimated-S and mp, Karickhoff 1981)

2.67 (estimated- K_{ow} , Karickhoff 1981)

2.31 (calculated-MCI χ , Gerstl & Helling 1987)

2.32 (calculated-MCI χ and fragment contribution method, Meylan et al. 1992)

2.60 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

2.77, 2.91 (Montgomery 1993)

2.60 (estimated-chemical structure, Lohninger 1994)

2.53 (soil, calculated-MCI χ , Sabljic et al. 1995)

2.40, 2.05 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

2.62 (2.37–2.87) (soil: organic carbon OC \geq 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 2220$ d from 1-m depth of water at 20°C (estimated, Muir 1991).

Photolysis: $t_{1/2} = 130$ h for 4 $\mu\text{g/mL}$ to degrade in distilled water under > 280 nm light (Guzik 1978; quoted, Cessna & Muir 1991)

direct photolysis $t_{1/2} = 121$ d in distilled water pH 5–7 for a mid-summer day at latitude of 40° (Wolfe et al. 1978)

$t_{1/2} = 2.25$ h for 21–76% of 80 $\mu\text{g/mL}$ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: $t_{1/2} > 4$ months for 4274 $\mu\text{g/mL}$ to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

$k(\text{alkaline}) = 2.0 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C, $1.9 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ at 50°C, $6.4 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ at 70°C; with $t_{1/2} > 1 \times 10^4$ d at pH 5, 7 and 9 (Wolfe et al. 1978)

$t_{1/2} > 1$ wk for 2.10 $\mu\text{g/mL}$ to hydrolyze in natural waters at 67°C (Schnoor et al. 1982; quoted, Muir 1991).

Biodegradation:

$t_{1/2}(\text{aerobic}) = 10\text{--}75$ d for 0.1–5.4 $\mu\text{g/mL}$ to biodegrade in activated sludge (Schwartz 1967; quoted, Muir 1991)

$k = (3.6\text{--}6.7) \times 10^{-10}$ $\text{mL cell}^{-1} \text{d}^{-1}$ of different river water samples (Paris et al. 1978; quoted, Scow 1982)

$t_{1/2} = 120$ d by fungi *Aspergillus fumigatus* and $t_{1/2} = 2.9$ d by bacteria at 28°C (Wolfe et al. 1978)

$k = 2.5 \times 10^{-4}$ $\text{L (mg M)}^{-1} \text{h}^{-1}$ with $t_{1/2} = 120$ d for 2–25 $\mu\text{g/mL}$ fungus *Aspergillus fumigatus*; $k = 0.1$ $\text{L (mg M)}^{-1} \text{h}^{-1}$ with $t_{1/2} = 2.9$ d for bacteria *Pseudomonas striata* to biodegrade in stream water at pH 7 and 28°C (Wolfe et al. 1978; quoted, Muir 1991)

$k = (1.6\text{--}1.8) \times 10^{-8}$ $\text{mL cell}^{-1} \text{d}^{-1}$ of different river water samples (Steen et al. 1979; quoted, Scow 1982)

$k = (2.6 \pm 0.72) \times 10^{-14}$ $\text{L cell}^{-1} \text{h}^{-1}$ in North American waters (Paris et al. 1981; quoted, Battersby 1990)

$k = (1.3\text{--}4.9) \times 10^{-4}$ $\text{L org}^{-1} \text{h}^{-1}$ with $t_{1/2}(\text{aerobic}) = 190$ h for 0.1–1.0 $\mu\text{g/mL}$ to biodegrade in lake water at 22°C (Schnoor et al. 1982; quoted, Muir 1991)

$k = (1.4\text{--}4.2) \times 10^{-13}$ $\text{L org}^{-1} \text{h}^{-1}$ for 75 $\mu\text{g/mL}$ to biodegrade at 28°C in natural and sediment waters (Steen et al. 1982; quoted, Muir 1991);

$t_{1/2}(\text{aerobic}) > 4$ months for 6–7 $\mu\text{g/mL}$ to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: rate constant $k = 3.6\text{--}6.7 \times 10^{-10}$ $\text{mL cell}^{-1} \text{d}^{-1}$ from measurements of different river water samples (Paris et al. 1978; quoted, Scow 1982);

hydrolysis $t_{1/2} > 1 \times 10^4$ d based on neutral and alkaline hydrolysis assuming pseudo-first order kinetics; direct photolysis $t_{1/2} = 121$ d assuming a quantum efficiency of 1 and for a mid-summer day at altitude 40°, and biolysis $t_{1/2} = 120$ d for 1mg/L of fungus and $t_{1/2} = 2.9$ d for bacteria at 28°C (Wolfe et al. 1978);

$k = (1.6\text{--}1.8) \times 10^{-8}$ $\text{mL cell}^{-1} \text{d}^{-1}$ from measurements of different river water samples (Steen et al. 1979; quoted, Scow 1982);

aerobic $t_{1/2} = 190$ h for 0.1–1.0 $\mu\text{g/mL}$ to biodegrade in lake water with biodegradation rate of $(1.3\text{--}4.9) \times 10^{-4}$ $\text{L org}^{-1} \text{h}^{-1}$ at 22°C (Schnoor et al. 1982; quoted, Muir 1991);

aerobic $t_{1/2} > 4$ months for 6–7 $\mu\text{g mL}^{-1}$ to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

Ground water:

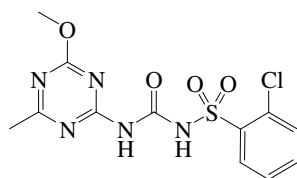
Sediment: aerobic half-life of 10–75 d for 0.1–5.4 $\mu\text{g/mL}$ to biodegrade in activated sludge (Schwartz 1967; quoted, Muir 1991).

Soil: $t_{1/2} = 65$ and 30 d soil at 15 and 29°C, respectively (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993; Tomlin 1994);

selected field $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

17.1.1.18 Chlorsulfuron



Common Name: Chlorsulfuron

Synonym: DPX 4189, Finesse, Glean, Telar

Chemical Name: 2-chloro-*N*-(((4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino)-carbonyl)-benzenesulfonamide;
1-(*o*-chlorophenyl)-3-(4-methoxy-6-methyl-*s*-triazin-2-yl)urea

Uses: herbicide to control broadleaf weeds and some grass weeds.

CAS Registry No: 64902-72-3

Molecular Formula: C₁₂H₁₂ClN₅O₄S

Molecular Weight: 357.773

Melting Point (°C):

176 (Lide 2003)

Boiling Point (°C):

192 (dec., Herbicide Handbook 1989; Montgomery 1993)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

Dissociation Constant pK_a:

3.6 (Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0330 (mp at 176°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

300 (at pH 5, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
27900 (at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
28000 (at pH 7 with ionic strength 0.05, Herbicide Handbook 1989)
7000 (20–25°C, at pH 7, selected, Wauchope et al. 1992; quoted, Majewski & Capel 1995)
7000 (20–25°C, at pH 7, selected, Hornsby et al. 1996)
60, 7000 (at pH 5, pH 7, Montgomery 1993)
32000 (selected, Armbrust 2000)

Vapor Pressure (Pa at 25°C or as indicated):

6.10 × 10⁻⁴ (Hartley & Kidd 1987)
6.13 × 10⁻⁴ (Herbicide Handbook 1989)
3.00 × 10⁻⁹ (Worthing & Hance 1991; Tomlin 1994)
1.98 × 10⁻² (20–25°C, Wauchope et al. 1992)
3.11 × 10⁻⁹ (Montgomery 1993)
6.13 × 10⁻⁴ (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

3.60 × 10⁻¹¹ (calculated-P/C, Montgomery 1993)
1.98 × 10⁻⁵ (20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
6.79 × 10⁻⁶ (selected, Armbrust 2000)

Octanol/Water Partition Coefficient, log K_{ow}:

-0.84, 0.17, 1.09 (pH 8.4, pH 7.1, pH 4.5, UV, Ribo 1988)
-0.88, 1.05 (pH 8.4, pH 4.5, HPLC, Ribo 1988)
-1.34, 0.74 (pH 7, pH 4.5, Hay 1990)

2.20 (Grayson & Kleier 1990)
 -1.0 (Montgomery 1993)
 -0.88, 1.05, -1.34, 0.74, 2.20 (reported values, Sangster 1993)
 -1.00 (at pH 7, Tomlin 1994)
 0.74, -1.34 (lit. values, Hansch et al. 1995)
 2.14 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

0.622 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC} :

1.02 (Flanagan silt loam, Montgomery 1993)
 1.60 (Tomlin 1994)
 2.19 (calculated-MCI $^1\chi$, Sabljic et al. 1995)
 1.60 (at pH 7, selected, Hornsby et al. 1996)
 1.56 (selected, Armbrust 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: assuming first-order kinetics, calculated $t_{1/2} \sim 186$ h for 33 $\mu\text{g/mL}$ to degrade in distilled water, $t_{1/2} = 31$ h for creek water, $t_{1/2} = 136$ h for silica gel and $t_{1/2} = 115$ h for montmorillonit under sunlight (Herrmann et al. 1985; quoted, Cessna & Muir 1991);
 under indoor conditions $t_{1/2} = 92$ h in methanol, $t_{1/2} = 78$ h in distilled water but $t_{1/2} = 18$ h in natural creek water (Herrmann et al. 1985);
 reported $t_{1/2} = 18$ h in distilled water at > 290 nm (Montgomery 1993)
 aqueous photolysis rate constant, $k = 5.0 \times 10^{-4} \text{ h}^{-1}$ (Armbrust 2000).

Oxidation:

Hydrolysis: $t_{1/2} = 4\text{--}8$ wk at 20°C and pH 5.7–7.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994);

stable aqueous hydrolysis rates at pH 7, 9; measured hydroxy radical rate constant for chlorsulfuron $6.9 \times 10^{12} \text{ M}^{-1}/\text{h}$ (Armbrust 2000).

Biodegradation: aerobic rate constant, $k = 1.44 \times 10^{-3} \text{ h}^{-1}$ (Armbrust 2000).

Biotransformation:

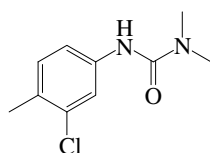
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: hydrolysis rates will be increased by warm soil temperatures at low pH and in the presence of moisture with an average $t_{1/2} = 4\text{--}6$ wk under growing conditions (Hartley & Kidd 1987; Herbicide Handbook 1989)
 $t_{1/2} = 4\text{--}6$ wk for degradation in soil via hydrolysis followed by microbial degradation (Hartley & Kidd 1987; quoted, Montgomery 1993; Tomlin 1994);
 degradation rate constants: $k = 0.033 \text{ d}^{-1}$ at depth 0–20 cm with $t_{1/2} = 21$ d, $k = 0.0315 \text{ d}^{-1}$ at depth 20–40 cm with $t_{1/2} = 22$ d and for depth 40–60 cm with $t_{1/2} > 150$ d (Soakwaters soil, Walker et al. 1989);
 degradation $k = 0.0116 \text{ d}^{-1}$ at depth 0–20 cm with $t_{1/2} = 60$ d, $k = 0.0120 \text{ d}^{-1}$ at depth 20–40 cm with $t_{1/2} = 58$ d, and $k = 0.0076 \text{ d}^{-1}$ at depth 40–60 cm with $t_{1/2} = 91$ d (Wharf ground soil, Walker et al. 1989);
 degradation $k = 0.0126 \text{ d}^{-1}$ at depth 0–20 cm with $t_{1/2} = 55$ d, $k = 0.0073 \text{ d}^{-1}$ at depth 20–40 cm with $t_{1/2} = 95$ d, and $k = 0.0056 \text{ d}^{-1}$ at depth 40–60 cm with $t_{1/2} = 124$ d (Cottage Field soil, Walker et al. 1989);
 degradation $k = 0.0147 \text{ d}^{-1}$ at depth 0–20 cm with $t_{1/2} = 47$ d, 0.0116 d^{-1} at depth 20–40 cm with $t_{1/2} = 60$ d, and $k = 0.0047 \text{ d}^{-1}$ at depth 40–60 cm with $t_{1/2} = 147$ d (Hunts Mill soil, Walker et al. 1989);
 degradation 0.0094 d^{-1} (depth 0–20 cm with $t_{1/2} = 74$ d), 0.0096 d^{-1} (depth 20–40 cm with $t_{1/2} = 72$ d) and 0.0082 d^{-1} (depth 40–60 cm with $t_{1/2} = 85$ d) (Bottom Barn soil, Walker et al. 1989);
 degradation $k = 0.0141 \text{ d}^{-1}$ at depth 0–20 cm with $t_{1/2} = 49$ d, $k = 0.0126 \text{ d}^{-1}$ at depth 20–40 cm with $t_{1/2} = 55$ d, and $k = 0.0089 \text{ d}^{-1}$ at depth 40–60 cm with $t_{1/2} = 78$ d (Long Ashton soil, Walker et al. 1989);
 degradation $k = 0.0144 \text{ d}^{-1}$ at depth 0–20 cm with $t_{1/2} = 48$ d, $k = 0.0126 \text{ d}^{-1}$ at depth 20–40 cm with $t_{1/2} = 55$ d, and $k = 0.0124 \text{ d}^{-1}$ at depth 40–60 cm with $t_{1/2} = 56$ d (Norfolk Agricultural Station soil, Walker et al. 1989)

degradation $k = 0.0248 \text{ d}^{-1}$ at depth 0–20 cm with $t_{1/2} = 28 \text{ d}$, $k = 0.0289 \text{ d}^{-1}$ at depth 20–40 cm with $t_{1/2} = 24 \text{ d}$, and $k = 0.0347 \text{ d}^{-1}$ at depth 40–60 cm with $t_{1/2} = 20 \text{ d}$ (Norfolk Agricultural Station soil, Walker et al. 1989); selected field $t_{1/2} = 40 \text{ d}$ (Hornsby et al. 1996).

17.1.1.19 Chlorotoluron



Common Name: Chlorotoluron

Synonym: C 2242, Clortokem, Deltarol, Dicuran, Highuron, Higaluron, Tolurex

Chemical Name: 3-(3-chloro-*p*-tolyl)-1,1-dimethylurea; *N'*-(3-chloro-4-methylphenyl)-N,N-dimethylurea

Uses: herbicide to control pre- and post-emergent annual grasses and broadleaf weeds in winter cereals, particularly wheat and barley.

CAS Registry No: 15545-48-9

Molecular Formula: C₁₀H₁₃ClN₂O

Molecular Weight: 212.675

Melting Point (°C):

147 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.40 (Tomlin 1994)

Molar Volume (cm³/mol):

192 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0635 (mp at 147°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

10.0 (20°C, Spencer 1973)

70.0 (Martin & Worthing 1977)

10.0 (20°C, Khan 1980)

70.0 (20°C, Ashton & Crafts 1981)

56.4, 80.6, 99.1 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)

70.0 (20°C, Hartley & Kidd 1987; Worthing & Walker 1991)

90.0 (Spurlock 1992; Spurlock & Biggar 1994)

10660 (calculated, Patil 1994)

74.0 (Tomlin 1994)

49.3 (predicted-AQUAFAC, Lee et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

4.8 × 10⁻⁶ (20°C, Khan 1980)

1.7 × 10⁻⁵ (20°C, Ashton & Crafts 1981)

1.7 × 10⁻⁵ (20°C, Hartley & Kidd 1987)

1.7 × 10⁻⁵ (Tomlin 1994; selected, Halfon et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

5.17 × 10⁻⁵ (20°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow}:

2.41 (shake flask-UV, Briggs 1981)

2.54 (Dao et al. 1983; Spurlock 1992; Spurlock & Biggar 1994)

2.33, 2.34, 2.32 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)

2.41 (shake flask, Mitsutake et al. 1986)

2.0 (shake flask, pH 7, Baker et al. 1992)

- 2.241 (calculated, Evelyne et al. 1992)
- 2.41 (recommended, Sangster 1993)
- 2.25 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 0.26 (calculated, Patil 1994)
- 2.50 (Tomlin 1994)
- 2.41 (recommended, Hansch et al. 1995)
- 2.38, 2.44 (shake flask-UV, calculated-RP-HPLC-k' correlation, Liu & Qian 1995)
- 2.25, 2.49, 2.42 (RP-HPLC-RT correlation, CIOGP, calculated-S, Finizio et al. 1997)
- 2.0 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 1.75 (calculated-S, Kenaga 1980)
- 2.09, 2.16 (cuticle/water 24 h: tomato, pepper, Chaumat et al. 1991)
- 2.01, 2.15 (cuticle/water 24 h: box tree, pear, Chaumat et al. 1991)
- 1.30 (cuticle/water 24 h: vanilla, Chaumat et al. 1991)
- 2.09, 2.16 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Sorption Partition Coefficient, log K_{OC}:

- 2.62 (soil, calculated-S, Kenaga 1980)
- 1.78 (reported as log K_{OM}, Briggs 1981)
- 2.75, 2.62 (4°C, 25°C, Semiahmoo soil, in µmol/kg OC, batch equilibrium-sorption isotherm-liquid scintillation spectrometer LSS, Madhun et al. 1986)
- 2.57, 2.43 (4°C, 25°C, Adkins soil, in µmol/kg OC, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.48, 2.18; 2.54, 2.50 (estimated-K_{OW}; solubility, Madhun et al. 1986)
- 2.81, 2.58 (exptl., calculated-K_{OW}, Liu & Qian 1995)
- 2.02 (soil, calculated-MCI ¹χ, Sabljic et al. 1995)
- 2.02; 2.05, 2.15 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.00, 2.00 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
- 2.14, 2.36 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: calculated t_{1/2} > 200 d at pH 5, 7, 9 and 30°C (Tomlin 1994).

Biodegradation: Biological degradation rate followed a first order kinetics with t_{1/2} = 21.6 d by raw water microflora from River Nile, t_{1/2} = 13.8 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Biotransformation: 4% of the selected 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted 50% of chlorotoluron (100 mg/L) in 5-d experiment. (Vroumsia et al. 1996)

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: Biological degradation t_{1/2} = 21.6 d by raw water microflora from River Nile, t_{1/2} = 13.8 d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Ground water:

Sediment:

Soil: t_{1/2} = 4 wk in the moist silty loam at (25 ± 1)°C (Smith & Briggs 1978);

t_{1/2} ~ 200–4000 d in loamy sand and peat for 25–35°C as follows (Madhum & Freed 1987):

t_{1/2} = 4340, 904, and 381 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg, while t_{1/2} = 1335, 524, and 266 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives in peat. t_{1/2} = 2306, 1245, and 618 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while t_{1/2} = 1949, 1024, and 582 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahmoo mucky peat (Madhum & Freed 1987)

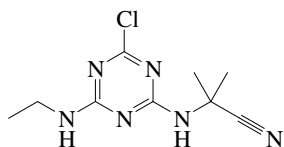
degradation by microorganism in biometer systems, $t_{1/2} = 93$ d in silty sand standard metabolism experiments, $t_{1/2} = 140$ d corrected standard conditions, $t_{1/2} = 110$ d in simulated outdoor conditions; $t_{1/2} = 40$ d in silty loam standard conditions, $t_{1/2} = 60$ d corrected standard conditions, $t_{1/2} = 31$ d in simulated outdoor conditions; at constant soil moisture and 20°C. Degradation by microorganism in small lysimeter systems: $t_{1/2} = 52$ d outdoor fallow, $t_{1/2} = 14$ d outdoor barley in silty sand, and $t_{1/2} = 49$ d outdoor fallow, $t_{1/2} = 38$ d outdoor barley in silty loam (Rüdel et al. 1993)

$t_{1/2} = 30\text{--}40$ d in soil (Tomlin 1994);

$t_{1/2} = 135$ d (selected, Halfon et al. 1996).

Biota:

17.1.1.20 Cyanazine



Common Name: Cyanazine

Synonym: Bladex, 90DF, DW 3418, Fortrok, Fortrol, Payze, SD 15418, WL 19805

Chemical Name: 2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methyl-propionitrile

Uses: herbicide to control annual grasses and broadleaf weeds in cereals, cotton, maize, onions, peanuts, peas, potatoes, soybeans, sugar cane, and wheat fallow.

CAS Registry No: 21725-46-2

Molecular Formula: $C_9H_{13}ClN_6$

Molecular Weight: 240.692

Melting Point ($^{\circ}C$):

168 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant:

1.00 (pK_a , Weber et al. 1980; Willis & McDowell 1982)

12.9 (pK_b , Wauchope et al. 1992; Hornsby et al. 1996)

0.63, 1.1 (pK_a , Montgomery 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0395 (mp at $168^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

171 (Melnikov 1971; Wauchope 1978; Weber et al. 1980; Ashton & Crafts 1981)

171 (Martin & Worthing 1977; Herbicide Handbook 1978; Worthing & Walker 1987, Worthing & Hance 1991; Majewski & Capel 1995)

150 (selected, Schnoor & McAvoy 1981; Schnoor 1992)

171 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

160 ($23^{\circ}C$, Herbicide Handbook 1989)

171 (Budavari 1989; Milne 1995)

170 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

6046 (calculated, Patil 1994)

45 (calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2.13×10^{-7} ($20^{\circ}C$, Ashton & Crafts 1973; 1981; Spencer 1982; Herbicide Handbook 1989)

2.67×10^{-7} (20 – $25^{\circ}C$, Weber et al. 1980)

5.33×10^{-7} (selected, Schnoor & McAvoy 1981; Schnoor 1992)

1.00×10^{-5} ($20^{\circ}C$, extrapolated from gas saturation measurement, Grayson & Fosbracey 1982)

$\ln(P/Pa) = 25.7 - 10913/(T/K)$, temp range 65.7 – $92^{\circ}C$, (Antoine eq., gas saturation, Grayson & Fosbracey 1982)

2.00×10^{-7} ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Majewski & Capel 1995)

5.21×10^{-6} (Worthing & Walker 1987)

1.33×10^{-6} ($30^{\circ}C$, Herbicide Handbook 1989)

2.13×10^{-7} ($20^{\circ}C$, Budavari 1989)

2.13×10^{-7} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

2.13×10^{-7} ($20^{\circ}C$, Montgomery 1993)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 2816 (20– 25°C , calculated-P/C, Montgomery 1993)
- 2.87×10^{-7} (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
- 3.00×10^{-7} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.18 (Kenaga & Goring 1980)
- 2.24 (shake flask-GC, Brown & Flagg 1981)
- 1.80, 1.66 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
- 2.22 (selected, Magee 1991)
- 1.80, 2.24 (Montgomery 1993)
- 2.22 (recommended, Sangster 1993)
- 0.79 (calculated, Patil 1994)
- 2.10 (Tomlin 1994)
- 2.22 (recommended, Hansch et al. 1995)
- 2.04 (shake flask-UV, Liu & Qian 1995)
- 1.64, 1.29, 3.02 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
- 1.70 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.53 (calculated-S, Kenaga 1980)
- 1.00 (calculated- K_{OC} , Kenaga 1980)
- 1.48 (selected, Schnoor & McAvoy 1981; Schnoor 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.30 (Kenaga 1980; Kenaga & Goring 1980; Karickhoff 1981; Sabljic 1987; Bahnick & Doucette 1988)
- 2.41 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.26 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
- 2.71, 1.75, 1.85 (estimated-S, calculated-S and mp, calculated- K_{OW} , Karickhoff 1981)
- 0.48–1.48 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
- 2.57, 2.26 (soil, quoted, Madhun et al. 1986)
- 2.36, 2.09; 2.33, 1.75 (estimated-reported K_{OW} s; estimated-reported solubilities, Madhun et al. 1986)
- 2.23 (soil, screening model calculations, Jury et al. 1987b)
- 2.35 (calculated-MCI χ , Bahnick & Doucette 1988)
- 2.30, 2.16 (reported, estimated as $\log K_{\text{OM}}$, Magee 1991)
- 2.23, 2.26, 2.30 (soil, quoted values, Bottoni & Funari 1992)
- 2.28 (soil, 20– 25°C , selected, Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)
- 1.58–2.63 (Montgomery 1993)
- 2.54 (selected, Lohninger 1994)
- 2.05, 2.11 (exptl., calculated- K_{OW} , Liu & Qian 1995)
- 2.28 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 2.28; 2.33, 2.25 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.14, 2.19 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, pH 5.6–8.0, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: alkaline chemical hydrolysis $t_{1/2} > 365$ d (Schnoor & McAvoy 1981; quoted, Schnoor 1992).

Biodegradation: aerobic $t_{1/2} = 14$ d for $0.06 \mu\text{g/mL}$ to degrade in pond water and $t_{1/2} > 28$ d in pond sediment both at $10\text{--}20^\circ\text{C}$ (Roberts 1974; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: aerobic $t_{1/2} = 14$ d for 0.06 $\mu\text{g/mL}$ to degrade in pond water at 10–20°C (Roberts 1974; quoted, Muir 1991).

Ground water: reported half-lives or persistence, $t_{1/2} = 10$ –29, 14 and 108 d (Bottoni & Funari 1992)

Sediment: aerobic $t_{1/2} > 28$ d for 0.06 $\mu\text{g/mL}$ to slowly degrade in pond sediment at 10–20°C (Roberts 1974; quoted, Muir 1991).

Soil: $t_{1/2} \sim 2$ wk in soil (Beynon et al. 1972; quoted, Tomlin 1994);

persistence of 12 months in soil (Wauchope 1978);

$t_{1/2} = 13.5$ d from screening model calculations (Jury et al. 1987b);

$t_{1/2} = 12$ –15 d in sandy loam soils and $t_{1/2} = 20$ –25 d in silt and clay loam soils (Herbicide Handbook 1989; quoted, Montgomery 1993);

disappearance $t_{1/2} = 181$ d from the upper 15 cm on a clay loam Ontario soil in 1987 and $t_{1/2} = 90$ d in 1988 with $t_{1/2}(\text{calc}) = 27$ and 12 d, respectively (Frank et al. 1991);

reported $t_{1/2} = 10$ –29 d, 13 d and 108 d (Bottoni & Funari 1992);

selected field $t_{1/2} = 14$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996)

soil $t_{1/2} = 19$ d (Pait et al. 1992).

Biota: biochemical $t_{1/2} = 13.5$ d from screening model calculations (Jury et al. 1987b).

TABLE 17.1.1.20.1
Reported vapor pressures of cyanazine at various temperatures

Grayson & Fosbracey 1982

gas saturation-GC	
$t/^{\circ}\text{C}$	P/Pa
65.7	0.0016
70.0	0.0025
77.5	0.0040
85.8	0.0101
87.8	0.0096
92.0	0.0181
20	$1. \times 10^{-5}$
$\ln P = A - B/(T/K)$	
	P/Pa
A	25.7
B	10913

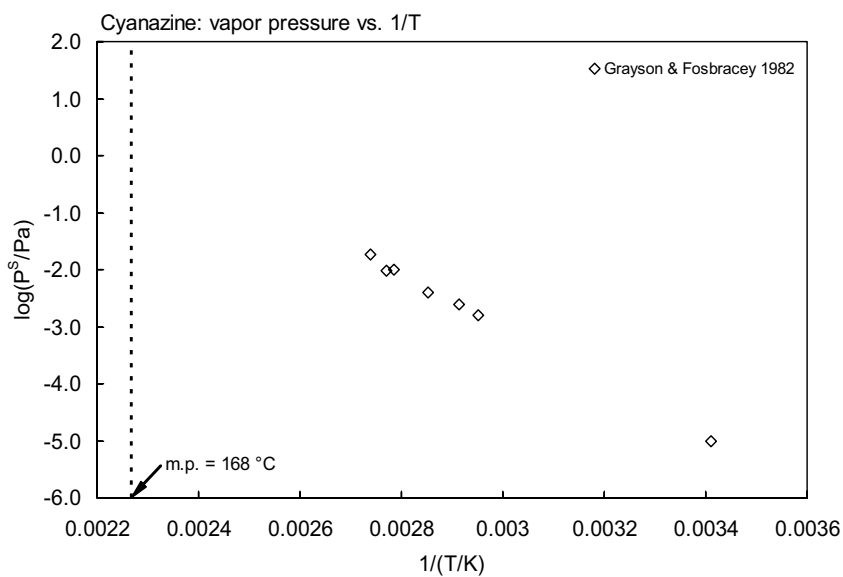
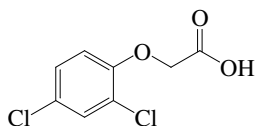


FIGURE 17.1.1.20.1 Logarithm of vapor pressure versus reciprocal temperature for cyanazine.

17.1.1.21 2,4-D

(See also [Chapter 13](#), Carboxylic Acids)



Common Name: 2,4-D

Synonym: 2,4-Dichlorophenoxyacetic acid

Chemical Name: 2,4-dichlorophenoxyacetic acid

Uses: post-emergence control of annual and perennial broadleaf weeds in cereals, maize, sorghum, grassland, established turf, grass seed crops, orchards, cranberries, asparagus, sugar cane, rice, forestry, and on noncropland, etc.

CAS Registry No: 94-75-7

Molecular Formula: $C_8H_6Cl_2O_3$, $Cl_2C_6H_3OCH_2COOH$

Molecular Weight: 221.038

Melting Point ($^{\circ}C$):

140.5 (Hartley & Kidd 1987; Howard 1991; Tomlin 1994; Lide 2003)

Boiling Point ($^{\circ}C$):

160 (at 0.4 mmHg, Dean 1985)

215 (Neely & Blau 1985)

Density (g/cm^3 at $25^{\circ}C$):

1.565 ($30^{\circ}C$, Neely & Blau 1985; Tomlin 1994)

1.416 (Montgomery 1993)

Molar Volume (cm^3/mol):

209.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.73 (potentiometric method, Nelson & Faust 1969)

2.87 (spectrophotometric method, Cessna & Grover 1978)

2.80 (Reinert & Rogers 1984; selected, Wauchope et al. 1992)

2.64 (Dean 1985; Haag & Yao 1992; Lee et al. 1993)

2.61–3.31 (Howard 1991)

2.97 (Sangster 1993)

3.10 (Kollig 1993)

2.64–3.31 (Montgomery 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

93.89 (Rordorf 1989)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

38.074 (DSC method, Plato & Glasgow 1969)

39.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0736 (mp at $140.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

890 (Hodgman 1952; Hamaker 1975; Verschueren 1983; Montgomery 1993)

522 (shake flask-UV, Leopold et al. 1960)

725 (Bailey & White et al. 1965)

725, 400, 900, 550 (Gunther et al. 1968)

900 (Herbicide Handbook 1974; Wauchope 1978; Kenaga 1980a,b; Kenaga & Goring 1980)

600 ($20^{\circ}C$, Khan 1980)

620–900 (Weber et al. 1980)

470 (20 – $25^{\circ}C$, pH 5.6, Geyer et al. 1981)

633, 812 (15, $25^{\circ}C$, shake flask method, average values of 5 laboratories, OECD 1981)

620 ($20^{\circ}C$, Hartley & Kidd 1983, 1987)

620	(Worthing & Walker 1983)
609	(Gerstl & Helling 1987)
400	(20°C, selected, Suntio et al. 1988)
703	(Gustafson 1989)
682	(Yalkowsky et al. 1987)
540–890	(Nyholm et al. 1992)
900, 600, 890, 703, 1072	(Wauchope et al. 1992)
890	(20–25°C, selected, Wauchope et al. 1992)
311	(pH 1, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

8.0×10^{-5}	(Hamaker 1975)
0.180–1.69	(transpiration method, Spencer 1976)
53.0	(160°C, Hartley & Kidd 1983, 1987)
8.0×10^{-5}	(recommended, Neely & Blau 1985; Lyman 1985)
1.0	(20°C, selected, Suntio et al. 1988)
6.0×10^{-6}	(selected, Nash 1989)
4.10×10^{-5} , 2.0×10^{-3} , 0.058, 1.10, 13.0	(25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
$\log (P_s/\text{Pa}) = 17.56 - 6544.1/(T/K)$; measured range 70.2–135°C (solid, gas saturation-GC, Rordorf 1989)
$\log (P_L/\text{Pa}) = 13.558 - 4904.6/(T/K)$; measured range 140–196°C (liquid, gas saturation-GC, Rordorf 1989)
0.20, 0.0032	(quoted, estimated from Henry's law constant, Howard 1991)
5.6×10^{-5}	(selected, Mackay & Stiver 1991)
1.40, 3.2×10^{-3}	(quoted, estimated from HLC, Howard 1991)
1.33×10^{-5} , 8.0×10^{-5} , 1.07×10^{-3} , 1.07×10^{-3}	(20–25°C, quoted lit; selected, Wauchope et al. 1992)
0.627	(Montgomery 1993)
0.011	(Tomlin 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

1.36×10^{-5}	(calculated-P/C, Jury et al. 1983)
1.39×10^{-5}	(calculated-P/C, Jury et al. 1987a, Jury & Ghodrati 1989)
0.55	(20°C, calculated-P/C, Suntio et al. 1988)
0.0015	(calculated, Nash 1989)
1.03×10^{-3}	(calculated-bond contribution, Howard 1991)
6.80, 0.853	(pH 1, pH 7 at 20°C, wetted wall column-GC, Rice et al. 1997b)
1.82×10^{-7}	(quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.81	(shake flask-UV, Fujita et al. 1964)
2.59	(electrometric titration, Freese et al. 1979)
1.57	(Kenaga & Goring 1980; Kenaga 1980b)
2.74	(selected, Dao et al. 1983)
2.81	(20°C, Verschueren 1983)
1.57, 4.88	(shake flask-OECD 1981 Guidelines, Geyer et al. 1984)
2.65	(shake flask, log P Database, Hansch & Leo 1987)
2.50	(OECD 1981 method, Kerler & Schönherr 1988)
2.649	(liquid/liquid-countercurrent-chromatography, Ilchmann et al. 1993)
2.81	(recommended, Sangster 1993)
1.44–4.18	(quoted lit. range, Montgomery 1993)
2.58–2.83	(pH 1, Tomlin 1994)
2.81	(selected, Hansch et al. 1995)
0.59	(RP-HPLC-RT correlation, CLOGP, Calculated-S, Finizio et al. 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 1.11, -0.097 (calculated-S, K_{OW} , Kenaga 1980a)
- 2.46, 1.30 (beef fat, fish, Kenaga 1980b)
- 0.778, 1.94 (alga *Chlorella*: exptl. 24 h exposure, calculated-S, Geyer et al. 1981)
- 0.778 (algae, Freitag et al. 1982)
- < 1.00 (golden orfe, Freitag et al. 1982)
- 1.23 (activated sludge, Freitag et al. 1982)
- 0.0 (fish, microcosm conditions, Garten & Trabalka 1983;)
- 0.778, 1.23 (algae, calculated- K_{OW} , Geyer et al. 1984)
- 1.23 (algae, Geyer et al. 1984)
- 1.11 (calculated, Isensee 1991)
- 5.00 (bluegill sunfish and channel catfish, Howard 1991)
- 2.70 (frog tadpoles, Howard 1991)
- 3.0, -2.52 (pH 7.8, seaweeds, Howard 1991)
- 0.778, 0.85 (quoted: alga, fish, Howard 1991)
- 0.0, 0.505 (catfish *Ictalurus melas*, water flea *Daphnia magna*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.51 (Hamaker 1975)
- 1.30, 2.0 (quoted, calculated, Kenaga 1980a)
- 1.30, 2.11 (quoted, Kenaga & Goring 1980)
- 1.30 (quoted, Kenaga 1980b)
- 1.76 (quoted, average value of 3 soils, McCall et al. 1980)
- 2.25, 2.04, 2.35 (soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
- 1.29 (soil, Neely & Blau 1985)
- 1.30 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 1.61 (soil, quoted, Sabljic 1987)
- 1.75, 2.00 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
- 2.59 (HPLC- k' correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
- 1.00, 1.23, 2.29 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
- 1.30–1.78, 1.30–2.0, 1.72 (soil, quoted lit. values, Bottoni & Funari 1992)
- 1.30, 1.78, 1.51, 1.26, 1.72, 1.75, 1.76 (soil, quoted values, Wauchope et al. 1992)
- 1.30 (soil, selected, Wauchope et al. 1992)
- 0.68 (calculated- K_{OW} , Kollig 1993)
- 1.68–2.73 (Montgomery 1993)
- 1.66 (calculated-QSAR MCI χ , Sabljic et al. 1995)
- 2.09, 1.04, 1.40, 0.778 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 1.65, 1.36, 1.37, 0.899 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 1.652 (second generation Eurosoil ES-1, HPLC- k' correlation, Gawlik et al. 2000)
- 1.68 (soil, quoted, Armbrust 2000)
- 1.79, 1.77 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, pH 2.8–8.0, average, Delle Site 2001)
- 2.16, 2.13 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, pH 2.8–5.0, average, Delle Site 2001)
- 1.68, 1.68 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, pH > 5.0, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: volatilization from water is negligible, calculated volatilization $t_{1/2} = 660$ d (from 1 cm) and $t_{1/2} = 7.1$ yr (from 10 cm) from soil (Howard 1991).

Photolysis: aqueous photolysis $t_{1/2} = 2\text{--}4$ d when irradiated at 356 nm, $t_{1/2} = 50$ min in water when irradiated at 254 nm and $t_{1/2} = 29\text{--}43$ d when exposed to September sunlight (Howard 1991); aqueous photolysis rate constant, $k = 2.2 \times 10^{-3} \text{ h}^{-1}$ (Armbrust 2000).

Oxidation:

photooxidation $t_{1/2} = 1.8\text{--}18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)

$k(\text{aq.}) = (1.0\text{--}2.3) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.5–2.9 and $21 \pm 1^\circ\text{C}$, with $t_{1/2} = 3.9$ h at pH 7 (Yao & Haag 1991).

$k(\text{calc}) = 5.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ (Haag & Yao 1992)

$k_{\text{OH}}(\text{aq.}) = 1.6 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with hydroxyl radical in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996; quoted, Armbrust 2000);

$k_{\text{OH}}(\text{aq.}) = 8.4 \times 10^{12} \text{ M}^{-1} \text{ h}^{-1}$ at pH 5, 7, 9; measured hydroxyl radical rate constant for 2,4-D, (Armbrust 2000)

Hydrolysis: no hydrolyzable groups and rate constant at neutral pH is zero (Kollig et al. 1987; selected, Howard et al. 1991); generally resistant to hydrolysis, may become important at pH > 8 (Howard 1991).

Biodegradation:

$k = 0.7\text{--}14.0 \text{ d}^{-1}$ and $t_{1/2} = 10$ to > 50 d in clear to murky river water with lag time ranges from 6–12 d (Nesbitt & Watson 1980a);

$t_{1/2} = 4$ d in river with nutrient and suspended sediments and $t_{1/2} = 10$ d with a lag time of 5 d for filtered river water (Nesbitt & Watson 1980b);

degradation kinetics not first-order, time for 50% decomposition in six soils: Commerce 5 d, Catlin 1.5 d, Keith 3.9 d, Cecil 3.0 d, Walla-Walla 2.5 d and Fargo 8.5 d, with an average time of 4 d (McCall et al. 1981)

aerobic degradation $k = 0.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 97.0$ d for control system, $k = 9.5 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 3.1$ d for metabolism, $k = 16.2 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 1.8$ d for co-metabolism; anaerobic degradation $k = 0.24 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 120$ d for control system, $k = 0.21 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 135$ d for metabolism, $k = 0.42 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 69$ d for co-metabolism, by a mixture of microorganisms from activated sludge, soil and sediment in cyclone fermentors (Liu et al. 1981)

$k = (3.6\text{--}28.8) \times 10^{-6} \text{ mL cell}^{-1} \text{ d}^{-1}$ in natural water (Paris et al. 1981; quoted, Klečka 1985)

$k < 0.14\text{--}0.07 \text{ d}^{-1}$ in river water at 25°C (Nesbitt & Watson 1980; quoted, Klečka 1985)

$k = (0.058 \pm 0.006) \text{ d}^{-1}$ in lake water at 29°C (Subba-Rao et al. 1982; quoted, Klečka 1985)

$k = 0.08\text{--}0.46 \text{ d}^{-1}$ in soil at 25°C (McCall et al. 1981; quoted, Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 240\text{--}1200$ h, based on unacclimated aerobic river die-away test data (Nesbitt & Watson 1980; selected, Howard et al. 1991);

$t_{1/2}(\text{anaerobic}) = 672\text{--}4320$ h, based on unacclimated aqueous screening test data (Liu et al. 1981; selected, Howard et al. 1991);

$k = 0.035 \text{ d}^{-1}$ in die-away test, $k = 0.029 \text{ d}^{-1}$ in CO_2 evolution test, in soil and $k = 6.9 \times 10^{-1} \text{ mL (g bacteria)}^{-1} \text{ d}^{-1}$ by activated sludge cultures (Scow 1982);

$t_{1/2} = 18$ to over 50 d in clear river water, and $t_{1/2} = 10$ to 25 d in muddy river water with lag times of 6 to 12 d; degradation with a mixture of microorganisms from activated sludge, soil, and sediments lead to half-lives of 1.8–3.1 d under aerobic conditions and 69–135 d under anaerobic conditions (Howard 1991)

$k(\text{aerobic}) = 5.25 \times 10^{-3} \text{ h}^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.0092 \text{ h}^{-1}$; $k_2 = 0.0092 \text{ h}^{-1}$ (catfish *Ictalurus melas*, Wang et al. 1996)

$k_1 = 0.8560 \text{ h}^{-1}$; $k_2 = 0.2690 \text{ h}^{-1}$ (Water flea *Daphnia magna*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 1.8\text{--}18$ h, based on estimated rate constant for the reaction with OH radical (Howard et al. 1991); photooxidation $t_{1/2} = 23.9$ h for reactions with OH radical in air (Howard 1991).

Surface water: $t_{1/2} = 48\text{--}96$ h, based on reported photolysis half-lives for aqueous solution irradiated at UV wavelength of 356 nm (Baur & Bovey 1974; selected, Howard et al. 1991);

degradation $t_{1/2} = 14$ d in sensitized, filtered and sterilized river water, based on sunlight photolysis test of $1 \mu\text{g mL}^{-1}$ in distilled water (Zepp et al. 1975; quoted, Cessna & Muir 1991);

$t_{1/2} = 1.8$ and 3.1 d for cometabolism and metabolism, respectively, easily degraded under aerobic conditions; $t_{1/2} = 69$ and 135 d under anaerobic conditions (Liu et al. 1981);

typical biodegradation $t_{1/2} = 10$ to < 50 d with longer expected in oligotrophic waters, photolysis $t_{1/2} = 29$ –43 d for water solutions irradiated at sunlight (Howard 1991);

degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2} \sim 6$ to 170 d (Muir 1991);

rate constant $k(\text{exptl}) = (1.0$ – $2.3) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.5–2.9 and 21°C, with $t_{1/2} = 3.9$ h at pH 7 (Yao & Haag 1991);

rate constant $k(\text{calc}) = 5 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in aqueous solution (Haag & Yao 1992);

$t_{1/2} = 2$ –4 d when irradiated at $\lambda = 356$ nm in aqueous solution (Montgomery 1993).

Ground water: $t_{1/2} = 480$ –4320 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

reported $t_{1/2} = 4, 15, 1$ –35, 7–21 d (Bottoni & Funari 1992)

Sediment: $t_{1/2} < 1$ d for degradation in sediments and lake muds (Howard 1991);

degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2} = 6$ to 170 d (Muir 1991).

Soil: degradation $t_{1/2} = 5.0$ and 4.0 d in Quachita Highlands' forest and grassland soil respectively, $t_{1/2} = 4$ d in Gross Timbers Forest soil, average $t_{1/2} = 4$ d in 3 soils (shake flask, Altom & Stritzke 1973);

field $t_{1/2} = 5.2$ d in Arid range (Lane et al. 1977; quoted, Nash 1983);

field $t_{1/2} = 19$ d in Dykland soil (Stewart & Gaul 1977; quoted, Nash 1983);

lab. $t_{1/2} = 5.5$ d in Naff soil (Wilson & Cheng 1978; quoted, Nash 1983);

microagroecosystem $t_{1/2} = 11$ d for granular application to bluegrass turf (Nash & Beall 1980)

non-persistent in soil with $t_{1/2} < 20$ d (Willis & McDowell 1982);

microagroecosystem $t_{1/2} = 3$ d in moist fallow soil (Nash 1983);

$t_{1/2} = 15$ d in soil (Jury et al. 1983, 1987a,b; Jury & Ghodrati 1989);

persistence of one month in soil (Jury et al. 1987);

$t_{1/2} = 240$ –1200 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

biodegradation $t_{1/2} < 1$ d to several weeks, $t_{1/2} = 3.9$ and 11.5 d in 2 moist soils and $t_{1/2} = 9.4$ to 254 d in the same soils under dry conditions (Howard 1991);

degraded relatively slowly when incubated in natural waters or in soil/sediment suspensions, with $t_{1/2} = 6$ to 170 d (Muir 1991);

reported $t_{1/2} = 4, 15, 1$ –35 and 7–21 d (Bottoni & Funari 1992);

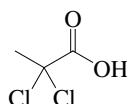
field $t_{1/2} = 2$ –16 d, with a selected value of 10 d (Wauchope et al. 1992);

soil $t_{1/2} = 18$ d (Pait et al. 1992);

rate constants for Amsterdam silt loam at soil depth 0–30 cm: $k = 0.0053 \text{ d}^{-1}$ at 10°C, $k = 0.0046 \text{ d}^{-1}$ at 17°C and $k = 0.0127 \text{ d}^{-1}$ at 24°C with corresponding first-order $t_{1/2} = 7, 7,$ and 2 d; at soil depth 30–60 cm: $k = 0.00012 \text{ d}^{-1}$ at 10°C, $k = 0.0044 \text{ d}^{-1}$ at 17°C and $k = 0.0077 \text{ d}^{-1}$ at 24°C with corresponding first-order $t_{1/2} = 273, 8,$ and 4 d; and at soil depth 60–120 cm: $k = 0.00005 \text{ d}^{-1}$ at 10°C, $k = 0.0013 \text{ d}^{-1}$ at 17°C and $k = 0.0022 \text{ d}^{-1}$ at 24°C with corresponding first-order $t_{1/2} = 593, 25,$ and 12 d (Veeh et al. 1996).

Biota: depuration $t_{1/2} = 13.8$ h in daphnids, $t_{1/2} = 1.32$ d in catfish (Ellgehausen et al. 1980).

17.1.1.22 Dalapon



Common Name: Dalapon

Synonym: Alatex, Basinex P, Crisapon, D-Granulat, Dawpon-Rae, Ded-Weed, Dowpon, DPA, Gramevin, Kenapon, Liropon, Proprop, Radapon

Chemical Name: 2,2-dichloropropanoic acid; 2,2-dichloropropionic acid; α -dichloropropanoic acid; α,α -dichloropropionic acid

Uses: selective systemic herbicide to control perennial and annual grasses on noncropland, fruits, vegetables, and some aquatic weeds.

CAS Registry No: 75-99-0

Molecular Formula: $C_3H_4Cl_2O_2$

Molecular Weight: 1432.969

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

185–190 (Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994)

98–99 (sodium salt at 20 mmHg, Budavari 1989)

Density (g/cm^3 at $20^{\circ}C$):

1.389 (Nelson & Faust 1969; quoted, Kenaga 1974; Montgomery 1993)

1.389 ($22.8^{\circ}C$, Herbicide Handbook 1989)

1.4014 (Budavari 1989; Milne 1995)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

1.84 (potentiometric titration, Nelson & Faust 1969; Freed 1976; Hornsby et al. 1996)

1.74 (Kenaga 1974; quoted, Howard 1991)

1.74–1.84 (Worthing & Hance 1991; Tomlin 1994)

2.06 (Yao & Haag 1991; Haag & Yao 1992)

1.84 (free acid, Montgomery 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

900000 (Woodford & Evans 1963; Bailey & White 1965)

> 800000 (Kenaga 1974)

502000 (Martin & Worthing 1977)

450000 (Weber et al. 1980; Budavari 1989)

501200 (Garten & Trabalka 1983)

431850 (selected, Gerstl & Helling 1987)

900000 (sodium salt, Worthing & Walker 1987, Worthing & Hance 1991)

500000 (Reinert 1989)

450000–900000 (Montgomery 1993)

900000 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

16.0 (calculated from high temp., Foy 1976)

1.0×10^{-5} (Worthing & Hance 1991; Tomlin 1994)

0.0 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.50×10^{-3} (Hine & Mookerjee 1975)

0.608 (calculated, Montgomery 1993)

4.56×10^{-3} (calculated-P/C as per Howard 1991, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.76 (Kenaga 1974)
 0.78 (Kenaga 1980)
 1.34 (selected, Dao et al. 1983)
 -2.76 (selected, Gerstl & Helling 1987)
 1.48 (Reinert 1989)
 0.78 (selected, Hansch et al. 1995)
 1.47 (LOGSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

0.477 (dalapon sodium salt in fish, Kenaga 1974)
 -0.444 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 0.301 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

0.477 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 0.97 (calculated-MCI χ , Gerstl & Helling 1987)
 2.13 (Reinert 1989)
 0.48, 2.13 (soil, quoted values, Bottoni & Funari 1992)
 0.27–2.18 (calculated, Montgomery 1993)
 0.40 (soil, calculated-MCI 1χ , Sabljic et al. 1995)
 0.0 (soil, 20–25°C, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

photooxidation $t_{1/2} = 289\text{--}2893$ h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

$k(aq.) = 4.6 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.4 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 6.4 and 22°C , with a half-life of > 2 yr at pH 7 (Yao & Haag 1991).

$k(aq.) = (7.3 \pm 0.3) \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.4 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 336\text{--}1440$ h, based on unacclimated aerobic soil grab sample data (Corbin & Upchurch 1967; Kaufman & Doyle 1977; quoted, Howard et al. 1991);

rate constant $k = 0.047 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic $t_{1/2} = 1344\text{--}5760$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 289\text{--}2893$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 336\text{--}1440$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured rate constant $k \leq 0.0005 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 6.4 and 22°C, with a $t_{1/2} \geq 2 \text{ yr}$ at pH 7 (Yao & Haag 1991).

Groundwater: $t_{1/2} = 672\text{--}2880 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

reported $t_{1/2} = 30 \text{ d}$ (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 7\text{--}8 \text{ d}$ in soil (Kaufman 1966; quoted, Kaufman 1976);

persistence across 43 soils from $< 2 \text{ wk}$ to $> 8 \text{ wk}$ (Day et al. 1963; quoted, Kaufman 1976);

$t_{1/2} = 336\text{--}1440 \text{ h}$, based on unacclimated aerobic soil grab sample data (Corbin & Upchurch 1967; Kaufman & Doyle 1977; quoted, Howard et al. 1991);

estimated persistence of 8 months (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 8 wk in soil (Edwards 1973; quoted, Morrill et al. 1982);

persistence of about 2 wk in growing season in most agricultural soils (Herbicide Handbook 1974; quoted, Kaufman 1976);

estimated first-order $t_{1/2} = 15 \text{ d}$ from biodegradation rate constant $k = 0.047 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

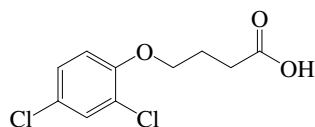
non-persistent in soil with $t_{1/2} < 20 \text{ d}$ (Willis & McDowell 1982);

reported half-life or persistence, 30 d (Verschuren 1983; Bottoni & Funari 1992);

field $t_{1/2} = 30 \text{ d}$ at 20–25°C (selected, Hornsby et al. 1996).

Biota:

17.1.1.23 2,4-DB



Common Name: 2,4-DB

Synonym: Butoxon, Butyrac, Butyrac 118, Embutox, Legumex D

Chemical Name: 4-(2,4-dichlorophenoxy)butanoic acid; 4-(2,4-dichlorophenoxy)butyric acid

Uses: herbicide for post-emergence control of many annual and perennial broadleaf weeds in lucerne, clovers, undersown cereals, grassland, forage legumes, soybeans, and groundnuts.

CAS Registry No: 94-82-6

Molecular Formula: $C_{10}H_{10}Cl_2O_3$

Molecular Weight: 249.090

Melting Point ($^{\circ}C$):

118 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

254.2 (calculate-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

5.95 (Bailey & White 1965; Que Hee et al. 1981)

4.80 (Worthing & Walker 1987; Hornsby et al. 1996)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.29 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

33.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.122 (mp at $118^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

82.3 (Bailey & White 1965)

53 (rm. temp., Melnikov 1971)

46 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)

46 (Weber et al. 1980)

46 (Hartley & Kidd 1987; Budavari 1989; Milne 1995)

46 ($20-25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

negligible (Hartley & Kidd 1987)

1.0×10^{-5} , 5.90×10^{-4} , 0.019, 0.38, 5.20 ($25, 50, 70, 100, 125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_g/Pa) = 17.692 - 6760.5/(T/K)$; measured range $80-120^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 12.682 - 4768.7/(T/K)$; measured range $125-196^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.53 (shake flask-HPLC/UV, Jafvert et al. 1990)

3.53 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.85 (calculated-S, Kenaga 1980)

2.21 (calculated- $\log K_{ow}$ as per Mackay 1982, this work)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.72 (soil, calculated-S, Kenaga 1980)
- 1.3 (organic carbon, Wauchope et al. 1991)
- 2.64 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 6\text{--}60$ h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: stable in distilled water for 40 d (Chau & Thomson 1978; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated soil grab sample data (Smith 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 6\text{--}60$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; Howard et al. 1991).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

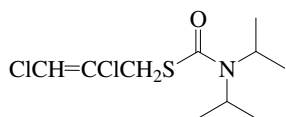
Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
reported $t_{1/2} < 7$ d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on unacclimated soil grab sample data (Smith 1978; quoted, Howard et al. 1991)
selected $t_{1/2} = 10$ d (Wauchope et al. 1991; quoted, Dowd et al. 1993);
 $t_{1/2} < 7$ d (Worthing & Hance 1991; Bottoni & Funari 1992);
field $t_{1/2} = 5$ d (20–25°C, selected, Hornsby et al. 1996).

Biota:

17.1.1.24 Diallate



Common Name: Diallate

Synonym: Avadex, CP 15336, DATC, Pyradex

Chemical Name: *S*-(2,3-dichloroallyl)diisopropyl(thiocarbamate); *S*-(2,3-dichloro-2-propenyl)bis(1-methylethyl)-carbamothioate

Uses: pre-emergent and selective herbicide to control wild oats and blackgrass in barley, corn, flax, lentils, peas, potatoes, soybeans, and sugar beets.

CAS Registry No: 2303-16-4

Molecular Formula: $C_{10}H_{17}Cl_2NOS$

Molecular Weight: 270.219

Melting Point ($^{\circ}C$):

25–30 (Herbicide Handbook 1989; Montgomery 1993)

Boiling Point ($^{\circ}C$):

97 (at 0.15 mmHg, Herbicide Handbook 1989)

108 (at 0.25 mmHg, Herbicide Handbook 1989; Montgomery 1993)

150 (at 9 mmHg, Howard 1991; Milne 1995; Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

1.188 ($25^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993)

Molar Volume (cm^3/mol):

305.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

40.0 (Günther et al. 1968)

14.0 (Ashton & Crafts 1973, 1981)

40.0 (rm. temp., Spencer 1973; Khan 1980)

40.0 (Martin & Worthing 1977; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

14.0 (Herbicide Handbook 1978; Herbicide Handbook 1989; Montgomery 1993)

68.8 ($22^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983a,b)

40.5 (20 – $25^{\circ}C$, shake flask-GC, Kanazawa 1981)

52.5 (Garten & Trabalka 1983)

14.0 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.020 (Ashton & Crafts 1973; Herbicide Handbook 1989)

0.0117 ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

0.0337 ($20^{\circ}C$, GC-RT correlation, Kim 1985)

0.020 (Hartley & Kidd 1987)

0.013 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.020 ($20^{\circ}C$, Montgomery 1993)

0.020 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.250 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

0.385 (calculated-P/C, Howard 1991)

0.253 (20 – $25^{\circ}C$, calculated-P/C, Montgomery 1993)

0.108 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.23 (estimated, USEPA 1988; quoted, Howard 1991)
 3.29 (calculated, Montgomery 1993)
 3.67 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.15 (calculated-S, Kenaga 1980; quoted, Howard 1991; Isensee 1991)
 2.08 (calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{OC}$:

3.28 (soil, Grover 1974)
 2.96, 2.46, 2.59, 2.49, 2.65 (Melfort loam, Weyburn sandy loam, Regina clay, Indian Head sandy loam, Asquith loamy sand, Grover et al. 1979)
 3.28 (soil, measured value, Kenaga 1980; Kenaga & Goring 1980)
 3.00 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 2.77 (calculated-MCI χ , Bahnick & Doucette 1988)
 2.28 (Montgomery 1993)
 3.52 (selected, Lohninger 1994)
 2.70 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 3.28 (soil, calculated-MCI χ , Sabljic et al. 1995)
 3.28; 3.21, 2.66 (soil, *cis*-isomer, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 3.28; 3.21, 2.65 (soil, *trans*-isomer, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 4$ h, < 1% of 135 $\mu\text{g/mL}$ to degrade in distilled water under > 300 nm light (Ruzo & Casida 1985; quoted, Cessna & Muir 1991).

Oxidation: photooxidation $t_{1/2} = 0.58$ –5.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: neutral hydrolysis rate constant $k = (1.2 \pm 0.7) \times 10^{-5} \text{ h}^{-1}$ with a calculated first-order $t_{1/2} = 6.6$ yr at pH 7 (Ellington et al. 1987, 1988);

first-order $t_{1/2} = 6.6$ yr, based on measured first-order base catalyzed hydrolysis rate constant at pH 7 (Ellington et al. 1987; quoted, Howard et al. 1991)

$t_{1/2} = 2400$ d at pH 2, $t_{1/2} = 2500$ d at pH 7 and $t_{1/2} = 32$ d at pH 12 in natural waters (Capel & Larson 1995).

Biodegradation: aqueous aerobic $t_{1/2} = 252$ –2160 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 1008$ –8640 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 11$ d, $t_{1/2}(\text{anaerobic}) = 42$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.58$ –5.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 252$ –2160 h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 11$ d, $t_{1/2}(\text{anaerobic}) = 42$ d, hydrolysis $t_{1/2} = 2400$ d at pH 2, $t_{1/2} = 2500$ d at pH 7 and $t_{1/2} = 32$ d at pH 12 in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 504\text{--}4320$ h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991).

Sediment:

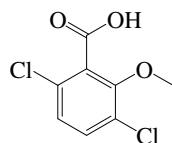
Soil: $t_{1/2} = 252\text{--}2160$ h, based on aerobic soil die-away test data (Anderson & Domsch 1976; Smith 1970; quoted, Howard et al. 1991; Montgomery 1993);

$t_{1/2} = 30$ d (Hartley & Kidd 1987; quoted, Montgomery 1993);

selected field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

17.1.1.25 Dicamba



Common Name: Dicamba

Synonym: Banex, Banvel, Banvel D, Brush buster, Dianat, MDBA, Mediben

Chemical Name: 3,6-dichloro-2-methoxybenzoic acid; 3,6-dichloro-*o*-anisic acid

Uses: systemic pre-emergent and post-emergent herbicide to control both annual and perennial broadleaf weeds.

CAS Registry No: 1918-00-9

Molecular Formula: $C_8H_6Cl_2O_3$

Molecular Weight: 221.038

Melting Point ($^{\circ}C$):

115 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.570 ($25^{\circ}C$, Hartley & Kid 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

207.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

1.94 (Kearney & Kaufman 1975; Spencer 1982; Lee et al. 1993)

1.90 (Cessna & Grover 1978; Weber et al. 1980; Willis & McDowell 1982; Howard 1991; Montgomery 1993; Armbrust 2000)

1.95 (Worthing & Hance 1991; Montgomery 1993; Caux et al. 1993)

1.87 (Tomlin 1994)

1.91 (Hornsby et al. 1996)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.85 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.59 (DSC method, Plato & Glasgow 1969)

19.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.131 (mp at $115^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

7900 (Freed 1966; Verschuere 1983)

4500 (Martin & Worthing 1977; quoted, Kenaga 1980; Kenaga & Goring 1980; Khan 1980; Ashton & Crafts 1981; Weber et al. 1980; Hartley & Graham-Bryce 1980)

6500 (Hartley & Kidd 1987; Herbicide Handbook 1989; Caux et al. 1993)

6500 (Worthing & Walker 1987, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

5600 ($20^{\circ}C$, selected, Suntio et al. 1988)

4410, 221 (quoted, calculated-group contribution fragmentation method, Kühne et al. 1995)

8310 (selected., Armbrust 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00454 (Ashton & Crafts 1973; 1981)

0.00267 (Baur & Bovey 1974; Spencer 1976)

0.49 ($20^{\circ}C$, Hartley & Graham-Bryce 1980; Khan 1980)

< 0.00013 (20 – $25^{\circ}C$, Weber et al. 1980; Willis & McDowell 1982)

0.00453 (Herbicide Handbook 1983, 1989; Worthing & Hance 1991)

0.0045 (Hartley & Kidd 1987; Tomlin 1994)

0.50 ($100^{\circ}C$, Budavari 1989)

2.90×10^{-3} , 6.40×10^{-2} , 0.88, 8.60, 63.0 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log (P_s/Pa) = 14.706 - 5139.1/(T/K)$; measured range 60.1–110°C (solid, gas saturation-GC, Rordorf 1989)
 $\log (P_L/Pa) = 11.911 - 4067.0/(T/K)$; measured range 115–176°C (liquid, gas saturation-GC, Rordorf 1989)
 0.50 (20°C, selected, Taylor & Spencer 1990)
 0.0045 (20°C, Montgomery 1993)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.00012 (20°C, calculated-P/C, Suntio et al. 1988)
 0.0248 (calculated-P/C, Taylor & Glotfelty 1988)
 0.0918 (Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
 2.2×10^{-5} (calculated-P/C, Nash 1989)
 1.22×10^{-4} (20–25°C, calculated-P/C, Montgomery 1993)
 0.00012, 0.000154 (20, 25°C, quoted, Caux et al. 1993)
 4.46×10^{-5} (quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.477 (Rao & Davidson 1980)
 2.41 (selected, Dao et al. 1983)
 2.21 (shake flask, Log P Database, Hansch & Leo 1985, 1987)
 -1.69 (selected, Gerstl & Helling 1987)
 3.01 (selected, Travis & Arms 1988)
 2.46 (Reinert 1989)
 2.49 (shake flask-HPLC/UV, Jafvert et al. 1990)
 2.46 (EPA Environmental Fate one-liner database Version 3.04, Lee et al. 1993)
 2.21 (recommended, Sangster 1993)
 0.48 (Montgomery 1993)
 -0.80 (pH 7, Tomlin 1994)
 2.21 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

0.699 (calculated-S, Kenaga 1980)
 -2.00 (calculated- K_{OC} , Kenaga 1980)
 -4.58 (beef biotransfer factor $\log B_b$, correlated- K_{ow} , Oehler & Ivie 1980)
 -4.60 (milk biotransfer factor $\log B_m$, correlated- K_{ow} , Oehler & Ivie 1980)
 1.450 (estimated- K_{ow} per Hansch & Leo 1985, Lyman et al. 1982)
 0.903 (estimated-S per Suntio et al. 1988, Lyman et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

-0.398 (soil, quoted exptl., Kenaga 1980)
 1.63 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 0.342 (av. soils/sediments, Rao & Davidson 1980)
 -0.40, 2.08 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
 0.34 (soil, screening model calculations, Jury et al. 1987b)
 2.67 ($K_{OC} = 470$ reported, Reinert 1989)
 0.643 (soil, estimated, Shirmohammadi et al. 1989)
 -1.00 (selected, USDA 1989; quoted, Neary et al. 1993)
 0.30 (organic carbon, Wauchope et al. 1991)
 -0.40, 1.62, 0.18, 0.34 (soil, quoted values, Bottoni & Funari 1992)
 1.50; 1.46 (soil, quoted exptl.; calculated-MCI χ and fragment contribution Meylan et al. 1992)
 -0.40, 0.34 (Montgomery 1993)
 0.30 (Tomlin 1994)
 1.50 (quoted or calculated-QSAR MCI χ , Sabljic et al. 1995)
 1.114 (quoted lit., Armbrust 2000)

Sorption Partition Coefficient, $\log K_{OM}$:

2.74 (organo-clay DODMA140-SAz, sorption isotherm, Zhao et al. 1996)

- 2.57 (organo-clay DODMA-SAz, sorption isotherm-HPLC/UV, Zhao et al. 1996)
 2.48 (organo-clay HDTMA-SAz, sorption isotherm-HPLC/UV, Zhao et al. 1996)
 2.59 (organo-clay HDTMA-SWy, sorption isotherm-HPLC/UV, Zhao et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: aqueous photolysis rate constant $k = 7.5 \times 10^{-4} \text{ h}^{-1}$ (Armbrust 2000).

Oxidation: photooxidation $t_{1/2} = 2.4\text{--}6.0 \text{ d}$, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991); measured hydroxy radical reaction rate constant for dicamba $4.8 \times 10^{12} \text{ M}^{-1} / \text{h}$ (Armbrust 2000).

Hydrolysis: $t_{1/2} > 133 \text{ d}$ for $2 \mu\text{g mL}^{-1}$ to hydrolyze in dark sterile pond water at $37\text{--}39^\circ\text{C}$ (Scifres et al. 1973; quoted, Muir 1991);

stable aqueous hydrolysis rates at pH 5, 7, 9 (Armbrust 2000).

Biodegradation: $t_{1/2} = 60 \text{ d}$ to $> 160 \text{ d}$ for $100 \mu\text{g mL}^{-1}$ to degrade in pond sediment/water under lighted conditions at $20\text{--}30^\circ\text{C}$ (Scifres et al. 1973; quoted, Muir 1991); under lab. conditions using nonsterile sandy loam, silty clay, or heavy clay soil, 50% of applied dicamba degraded within 2 weeks; however in sterilized (via heating) soil, over 90% of applied dicamba was recovered after 4 weeks, suggesting that microbes were responsible for the decomposition (Smith 1973; quoted, Howard 1991);

$t_{1/2} > 25 \text{ d}$ for 5.85 mg of labeled dicamba to plants to degrade following washoff from plants and sands in model ecosystem (derived from data of Yu et al. 1975; Muir 1991);

$k = 0.022 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

rate of biodegradation in soil generally increases with temperature and soil moisture (up to 50%) and tends to be faster when the soil is slightly acidic (Herbicide Handbook 1983; quoted, Howard 1991);

aerobic rate constant $k = 1.60 \times 10^{-3} \text{ h}^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} \sim 2.42 \text{ d}$ for reaction with hydroxyl radicals (estimated, Eisenreich et al. 1981; quoted, Caux et al. 1993)
 $t_{1/2} = 2.42\text{--}6.0 \text{ d}$, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Surface water:

Ground water: $t_{1/2} = 23.5 \text{ d}$ determined under batch conditions at 28°C , $t_{1/2} = 38 \text{ d}$ at 20°C , and $t_{1/2} = 151 \text{ d}$ at 12°C and were all higher than $t_{1/2} \sim 13.5 \text{ d}$ from the decrease in column effluent concentrations over time (Comfort et al. 1992);

reported $t_{1/2} = 14\text{--}433, 201$ and 25 d (Bottoni & Funari 1992)

$t_{1/2} < 7 \text{ d}$ in surface water (Caux et al. 1993).

Sediment:

Soil: estimated persistence of 2 months (Kearney et al. 1969; quoted, Jury et al. 1987a);

$t_{1/2} = 59, 19$, and 17 d with disappearance rates: $k = 0.0117, 0.036$ and 0.041 d^{-1} at pH 4.3, 5.3 and 6.5 (Hamaker 1972; quoted, Nash 1988);

persistence of 2 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

degradation $t_{1/2} = 32 \text{ d}$ and 17 d in Quachita Highlands = forest and grassland soil respectively, $t_{1/2} = 26 \text{ d}$ in

Gross Timbers Forest soil, average $t_{1/2} = 25 \text{ d}$ in 3 soils (Altom & Stritzke 1973);

first-order $t_{1/2} \sim 31.5 \text{ d}$ in soil from biodegradation rate constant $k = 0.022 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

nonpersistent in soils with $t_{1/2} < 20 \text{ d}$ (Willis & McDowell 1982);

mean $t_{1/2} = 14 \text{ d}$ under lab. conditions from review of persistence literature, while the mean $t_{1/2} = 8 \text{ d}$ under field conditions (Rao & Davidson 1982; quoted, Howard 1991);

non-persistent with $t_{1/2} < 20 \text{ d}$ in soil (Willis & McDowell 1982);

$t_{1/2} = 14 \text{ d}$ from screening model calculations (Jury et al. 1987b);

$t_{1/2} < 14 \text{ d}$ under conditions amenable to rapid metabolism (Herbicide Handbook 1989);

selected $t_{1/2} = 14 \text{ d}$ (Wauchope et al. 1991; quoted, Dowd et al. 1993);

$t_{1/2} < 14\text{--}25 \text{ d}$ (Worthing & Hance 1991; quoted, Montgomery 1993);

reported $t_{1/2} = 20$ d, 25 d and 14–433 d (Bottoni & Funari 1992);

$t_{1/2} = 4$ –555 d with a mean $t_{1/2} = 24$ d (Caux et al. 1993);

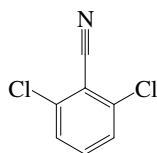
$t_{1/2} < 14$ d (Tomlin 1994).

Biota: biochemical $t_{1/2} = 14$ d from screening model calculations (Jury et al. 1987b);

average $t_{1/2} = 25$ d in the forest (USDA 1989; quoted, Neary et al. 1993);

biological $t_{1/2} = 0.64$ h (Caux et al. 1993).

17.1.1.26 Dichlobenil



Common Name: Dichlobenil

Synonym: Barrier 2G, Barrier 50W, Casoron, DBN, DCB, Decabane, Du-Sprex, Dyclomec, NIA 5996, Niagara 5006, Niagara 5996, Norosac

Chemical Name: 2,6-dichlorobenzonitrile

Uses: soil applied herbicide to control many annual and perennial broadleaf weeds.

CAS Registry No: 1194-65-6

Molecular Formula: $C_7H_3Cl_2N$

Molecular Weight: 172.012

Melting Point ($^{\circ}C$):

144.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

270 (Verloop 1972; Khan 1980; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

> 1.0 (Milne 1995)

Molar Volume (cm^3/mol):

148.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

65.74 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.94 (DSC method, Plato & Glasgow 1969)

34.33 (Verloop 1972)

24.2 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0672 (mp at $144.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

18 ($20^{\circ}C$, Günther et al. 1968; Weber 1972; Verloop 1972; Spencer 1982; Verschueren 1983)

25 (Günther et al. 1968; Montgomery 1993)

18 (Martin & Worthing 1977; Herbicide Handbook 1978)

18 (Wauchope 1978; Khan 1980; Burkhard & Guth 1981)

18 ($20^{\circ}C$, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)

18 ($20^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)

21.2 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

18, 25 ($20^{\circ}C$, $25^{\circ}C$, Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.072 ($20^{\circ}C$, effusion manometer technique, Barnsley & Rosher 1961)

0.0733 ($20^{\circ}C$, Verloop 1972; Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)

0.0667 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

0.0004 ($20^{\circ}C$, Spencer 1976)

0.0666 ($20^{\circ}C$, effusion method, Spencer 1976)

0.0733 (20 – $25^{\circ}C$, Weber et al. 1980)

0.073 ($20^{\circ}C$, Hartley & Kidd 1987)

0.070 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.110, 1.80, 20.0, 160, 970 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 14.787 - 4698.2/(T/K)$; measured range 32.4 – $125^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/P_a) = 11.754 - 3434.1/(T/K)$; measured range 32.4–125°C (liquid, gas saturation-GC, Rordorf 1989)
 0.133 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.0733 (Montgomery 1993)
 0.088 (20°C, gas saturation, Tomlin 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.700 (20°C, volatilization rate, Burkhard & Guth 1981)
 0.669 (20°C, calculated-P/C, Suntio et al. 1988)
 0.637 (20°C, calculated-P/C, Muir 1991)
 0.669 (20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.90 (Rao & Davidson 1980; selected, Suntio et al. 1988, Magee 1991)
 2.57; 2.65 (RP-HPLC-RT correlation; shake flask, Eadsforth & Moser 1983)
 3.06 (shake flask, Geyer et al. 1984)
 2.94 (Hansch & Leo 1985)
 1.63 (Reinert 1989)
 2.98 (selected, Dao et al. 1983, Gerstl & Helling 1987)
 2.90 (shake flask, Log P Database, Hansch & Leo 1987)
 2.90 (recommended, Sangster 1993)
 2.70 (Tomlin 1994)
 2.74 (recommended, Hansch et al. 1995)
 2.95 (RP-HPLC-RT correlation, Nakamura et al. 2001)
 2.98 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$:

1.74 (fish in static water, Kenaga 1975; Kenaga & Goring 1980)
 2.08 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 1.08 (calculated- K_{oc} , Kenaga 1980)
 1.18–1.60 (fish, Freitag et al. 1982)
 1.30 (algae, Freitag et al. 1982)
 1.72 (estimated-S, Lyman et al. 1982; quoted, Howard 1991)
 2.03–2.32 (Montgomery 1993)

Sorption Partition Coefficient, $\log K_{oc}$ at 25°C or as indicated:

2.91 (potting soil with 22% organic content, Massini 1961)
 2.08 (sandy loam with 5% organic content, Massini 1961)
 2.37 (soil, Hamaker & Thompson 1972–1987)
 2.95 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 2.35 (Rao & Davidson 1980)
 2.94 (soil, estimated-S, Lyman et al. 1982; quoted, Howard 1991)
 2.37, 1.45 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
 2.96 (Reinert 1989)
 2.37; 2.31 (reported as $\log K_{OM}$; estimated as $\log K_{OM}$, Magee 1991)
 2.21, 2.57–2.96 (soil, quoted values, Bottoni & Funari 1992)
 2.60 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
 2.60 (estimated-chemical structure, Lohninger 1994)
 2.31 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 7.4$ d, based on Henry's law constant for a model river 1-m deep with a wind velocity of 3 m/s and flowing at 1 m/s (estimated, Lyman et al. 1982; quoted, Howard 1991);
 $t_{1/2} \sim 11$ d from 1 m depth of water at 20°C (estimated, Muir 1991).
 Photolysis: photolytic $t_{1/2} = 15$ d in water (Tomlin 1994).

Oxidation: photooxidation $t_{1/2} = 92$ d in air, based on estimation for the vapor-phase reaction with hydroxyl radicals in atmosphere (Atkinson 1987; quoted, Howard 1991).

Hydrolysis:

Biodegradation: $t_{1/2} \sim 7$ d for 5 $\mu\text{g/mL}$ to biodegrade in sediment suspension at 30°C (Miyazaki et al. 1975; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 92$ d, based on estimation for the vapor-phase reaction with hydroxyl radicals in atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water:

Ground water: reported $t_{1/2} = 44\text{--}360$ d (Bottoni & Funari 1992)

Sediment: $t_{1/2} \sim 7$ d for 5 $\mu\text{g/mL}$ to biodegrade in sediment suspension at 30°C (Miyazaki et al. 1975; quoted, Muir 1991).

Soil: estimated persistence of 4 months (Kearney et al. 1969; quoted, Jury et al. 1987);

$t_{1/2} = 1\text{--}6$ months in soil depending on soil type (Beynon & Wright 1972; Verloop 1972; quoted, Tomlin 1994);

persistence of 4 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

persistence of 4 months (Wauchope 1978);

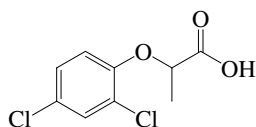
$t_{1/2} = 1.5$ to 12 months depending upon soil type (Herbicide Handbook 1989);

selected $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);

reported $t_{1/2} = 45\text{--}360$ d (Bottoni & Funari 1992).

Biota:

17.1.1.27 Dichlorprop



Common Name: Dichlorprop

Synonym: Cornox RK, dichloroprop, Dikofag DP, 2,4-DP, Hedonal DP, Polymone

Chemical Name: (±)-2-(2,4-dichlorophenoxy) propanoic acid; (±)-2-(2,4-dichlorophenoxy) propionic acid

Uses: herbicide and growth regulator to control annual broadleaf and grass weeds; also to control aquatic weeds and chemical maintenance of embankments and roadside verges.

CAS Registry No: 120-36-5

Molecular Formula: $C_9H_8Cl_2O_3$

Molecular Weight: 235.064

Melting Point ($^{\circ}C$):

117.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.64 ($25^{\circ}C$, Bailey & White 1965)

1.42 (Herbicide Handbook 1989; Tomlin 1994)

Molar Volume (cm^3/mol):

232.0 (calculated-Le Bas method at normal boiling point)

165.6 (calculated-density)

Dissociation Constant pK_a :

2.855 (Cessna & Grover 1978)

2.86 (Wauchope et al. 1992; Hornsby et al. 1996)

3.00 (Tomlin 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

127.9 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

34.31 (DSC method, Plato 1972)

30.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.124 (mp at $117.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

350 ($20^{\circ}C$, Woodford & Evans 1963; Spencer 1973)

350 (Martin & Worthing 1977)

350 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987, 1991)

710 ($28^{\circ}C$, Herbicide Handbook 1989)

50 (ester, 20 – $25^{\circ}C$, estimated, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.50×10^{-4} ($20^{\circ}C$, Hartley & Kidd 1987)

2.90×10^{-7} , 4.10×10^{-5} , 2.8×10^{-3} , 0.11, 2.80 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 21.26 - 8289.2/(T/K)$; measured range 95.7 – $118^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_l/Pa) = 17.174 - 6682.8/(T/K)$; measured range 120 – $150^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

4.00×10^{-4} (20 – $25^{\circ}C$, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

$< 1.0 \times 10^{-5}$ ($20^{\circ}C$, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.69×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.75 (RP-HPLC- k' correlation, Braumann et al. 1983)
- 3.43 (shake flask-GC, Ilchmann et al. 1993)
- 2.06 to -0.22 (pH 4–7, shake flask-LSC, Riise & Salbu 1992)
- 1.77 (Tomlin 1994)
- 3.43 (recommended, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

- 1.36 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

- 2.23 (soil, calculated-S, Kenaga 1980)
- 3.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
- 2.05, 2.07, 1.70, 1.79, 1.73 (5 soils: soil A 30.4% OC and pH 4.4, soil B 14.6% OC pH 4.1, soil C/loam 3.3% OC pH 5.0, soil D/silty clay 1.3% OC pH 5.1, soil E/sand 1.4% OC pH 5.3, batch equilibrium-sorption isotherms, Riise Salbu 1992)
- 1.08–1.60 (Tomlin 1994)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

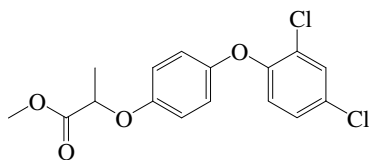
Photolysis: photodegradation $t_{1/2} = 10$ to 19 d on 3 Spanish natural dry soils; $t_{1/2} = 22$ to 59 d on 10% peat-amended dry soils; degradation $t_{1/2} \sim 2$ –6 d on moist soils at field capacity and saturation soils for degradation at 0, 1 and 2 exposures days; and $t_{1/2} = 16$ –37 d on moist soils at field capacity and saturated soils for degradation at 2, 4 and 10 exposure days (Romero et al. 1998)

Half-Lives in the Environment:

Soil: $t_{1/2} = 12$ d and 8 d in Quachita Highlands = forest and grassland soil, respectively, $t_{1/2} = 10$ d in gross timbers forest soil, average $t_{1/2} = 10$ d in 3 soils (Altom & Stritzke 1973); selected field $t_{1/2} = 10$ d (Wauchope et al. 1992; Hornsby et al. 1996); $t_{1/2} \sim 8$ d in soil (Tomlin 1994)

photodegradation $t_{1/2} = 10$ –19 d in 3 Spanish natural dry soils, $t_{1/2} = 22$ –59 d in the 10% peat-amended dry soils; degradation $t_{1/2} \sim 2$ –6 d on moist soils at field capacity and saturation soils for degradation at 0, 1 and 2 exposures days; and $t_{1/2} = 16$ –37 d on moist soils at field capacity and saturated soils for degradation at 2, 4 and 10 exposure days (Romero et al. 1998)

17.1.1.28 Diclofop-methyl



Common Name: Diclofop-methyl

Synonym: Hoelon, dichlordiphenoprop, Hoegrass, Illoxan

Chemical Name: methyl 2-[4-(2',4'-dichlorophenoxy)-phenoxy]propanoate

Uses: herbicide to control post-emergent wild oats, wild millets, and other annual grass weeds in wheat, barley, rye, red fescue, and broadleaf weeds in crops such as soybeans, sugar cane, fodder beet, flax, legumes, oilseed rape, sunflowers, clover, lucerne, groundnuts, brassicas, carrots, celery, beet root, parsnips, lettuce, spinach, potatoes, tomatoes, fennel, alliums, herbs, etc.

CAS Registry No: 51338-27-3

Molecular Formula: $C_{16}H_{14}Cl_2O_4$

Molecular Weight: 341.186

Melting Point ($^{\circ}C$):

40 (Lide 2003)

Boiling Point ($^{\circ}C$):

175–176 (at 0.1 mmHg, Hartley & Kidd 1987; Herbicide Handbook 1989)

Density (g/cm^3):

1.30 (40 $^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989)

1.035 (Herbicide Handbook 1989)

Acid Dissociation Constants, pK_a :

3.1 (Wauchope et al. 1992; Hornsby et al. 1996)

Molar Volume (cm^3/mol):

349.6 (calculated-Le Bas method at normal boiling point)

329.7 (calculated-density)

Dissociation Constant pK_a :

3.1 (Wauchope et al. 1992; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.713 (mp at 40 $^{\circ}C$)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated):

3.0 (22 $^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991)

3.0 (22 $^{\circ}C$, Herbicide Handbook 1989)

0.80 (20–25 $^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.80 (20 $^{\circ}C$, pH 7, Tomlin 1994)

4.23 (Majewski & Capel 1995)

4.06 (calculated-group contribution method, Kühne et al. 1995)

3.0 (Lohninger 1994; Milne 1995)

0.8 (selected, Halfon et al. 1996)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated):

3.44×10^{-5} (20 $^{\circ}C$, Worthing 1983, 1987; Hartley & Kidd 1987)

3.40×10^{-5} (20 $^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991)

3.47×10^{-5} , 1.6×10^{-4} , 3.87×10^{-3} (20 $^{\circ}C$, 30 $^{\circ}C$, 54.3 $^{\circ}C$, Herbicide Handbook 1989)

5.91×10^{-5} (selected, Wauchope et al. 1992; Hornsby et al. 1996)

2.5×10^{-4} , 7.7×10^{-3} (20 $^{\circ}C$, 50 $^{\circ}C$, Tomlin 1994)

4.80×10^{-5} (quoted, Majewski & Capel 1987)

4.7×10^{-4} (selected, Halfon et al. 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 0.00387 (calculated-P/C, Majewski & Capel 1995)
 0.199 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 4.80 (shake flask, Log P Database, Hansch & Leo 1987)
 4.601 (Stevens et al. 1988)
 4.58 (Worthing & Hance 1991)
 4.60 (shake flask, pH 7, Baker et al. 1992)
 4.80 (recommended, Sangster 1993)
 4.5775 (Tomlin 1994)
 4.80 (recommended, Hansch et al. 1995)
 5.52 (Pomona-database, Müller & Kördel 1996)
 4.87 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_B$:

- 2.74 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, $\log K_{oc}$:

- 4.69, 4.20 (Wauchope et al. 1992)
 4.15–4.39 (soil, quoted values, Bottoni & Funari 1992)
 4.20 ($20\text{--}25^\circ\text{C}$, soil, recommended, Wauchope et al. 1992; Hornsby et al. 1996)
 4.25 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995b)
 4.15–4.39 (soil, Tomlin 1994)
 4.20 (estimated-chemical structure, Lohninger 1994)
 4.25; 3.61 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 5.505, 5.334, 4.122, 4.737, 4.182 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 4.002, 3.731, 3.453, 3.257, 3.715 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: first-order rate constants $k = -0.0883, -0.225, -0.266 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.0158, -0.0139, -0.0134 \text{ h}^{-1}$ in sterile sediment by shake-tests at Davis Bayou, $k = -0.0457, -0.103, -0.120 \text{ h}^{-1}$ in nonsterile water and $k = -0.00233, -0.00722, -0.00785 \text{ h}^{-1}$ in sterile water by shake-tests at Davis Bayou (Walker et al. 1988)

$t_{1/2} = 10 \text{ d}$ in sandy soils and $t_{1/2} \sim 30 \text{ d}$ in sandy clay soils under aerobic conditions (Herbicide Handbook 1989)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 363 \text{ d}$ at 25°C and pH 5, $t_{1/2} = 31.7 \text{ d}$ at pH 7 and $t_{1/2} = 0.52 \text{ d}$ at pH 9 (Tomlin 1994).

Ground water: reported $t_{1/2} = 6\text{--}9, 23\text{--}38$ and 150 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 10 \text{ d}$ in sandy soils and $t_{1/2} \sim 30 \text{ d}$ in sandy clay soils while under anaerobic conditions, results were similar except that the very rapid cleavage of the ester bond by hydrolysis within one hour to propionic acid derivatives was experienced and within 2 d, up to 86% of the parent compound was metabolized into various free acid metabolites and up to 3.7% of phenol metabolites (Herbicide Handbook 1989);

$t_{1/2}$ = 6–9 d, 23–38 d and 150 d (Bottoni & Funari 1992);

selected field $t_{1/2}$ = 30 d at pH 7.0 (Wauchope et al. 1992; Hornsby et al. 1996)

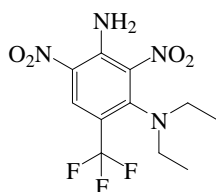
V = 1–57 d and $t_{1/2}$ = 30–281 d for various soils in field trials (Tomlin 1994).

$t_{1/2}$ = 30 d (selected, Halfon et al. 1996).

Biota: $t_{1/2}$ = 3–7 d for wheat (Herbicide Handbook 1989)

$t_{1/2}$ = 3 d in sugar beet (Tomlin 1994).

17.1.1.29 Dinitramine



Common Name: Dinitramine

Synonym: Cobex, Cobexo

Chemical Name: *N,N*-diethyl-2,6-dinitro-4-(trifluoromethyl)-*m*-phenylenediamine

Uses: herbicide for selective pre-plant soil incorporating control of many annual grass and broadleaf weeds in cotton, soybeans, peas, groundnuts, beans, sunflowers, safflowers, carrots, turnips, fennel, chicory, etc. and in transplanted tomatoes, capsicums, aubergines, and brassicas.

CAS Registry No: 29091-05-2

Molecular Formula: $C_{11}H_{13}N_4O_4F_3$

Molecular Weight: 322.241

Melting Point ($^{\circ}C$):

98 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.50 ($25^{\circ}C$, Ashton & Crafts 1981; Hartley & Kidd 1987)

Molar Volume (cm^3/mol):

265.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

4.5 (Haag & Yao 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.192 (mp at $98^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.1 (Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Khan 1980; Isensee 1991)

1.0 (Wauchope 1978; Verschueren 1983)

1.0 ($20^{\circ}C$, Ashton & Crafts 1981; Hartley & Kidd 1987)

1.1 (Worthing & Walker 1987, 1991)

1.1 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

1.0 ($20^{\circ}C$, Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.00048 (Khan 1980; Ashton & Crafts 1981)

0.00048 (Verschueren 1983)

0.000479 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

0.00040 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.00048 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.160 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.31 (selected, Dao et al. 1983)

4.30 (Worthing & Hance 1991; Tomlin 1994)

4.30 (Milne 1995)

4.30 (recommended, Hansch et al. 1995)

3.89 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

- 2.77 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- 2.45 (calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

- 3.60 (soil, Harvey 1974)
- 3.61 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 3.60 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 3.84 (estimated-chemical structure, Lohninger 1994)
- 3.63 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.63; 3.42 (soil, quoted exptl.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} < 1$ h in distilled water, river water and ocean water under sunlight (Newsom & Woods 1973; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} = 22$ d for 0.5 $\mu\text{g/mL}$ to biodegrade in flooded soil with approximately 1 cm of water on top of the soil (Savage 1978; quoted, Muir 1991).

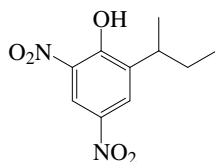
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} = 22$ d for 0.5 $\mu\text{g/mL}$ to biodegrade in flooded soil with approximately 1 cm of water on top of the soil (Savage 1978; quoted, Muir 1991);
 persistence of 3 months in soil (Wauchope 1978);
 selected field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
 $t_{1/2} = 10$ –66 d (Tomlin 1994).

17.1.1.30 Dinoseb



Common Name: Dinoseb

Synonym: Anatox, Aretit, Basanite, Butaphene, Caldon, Chemox, Dibutox, Dinitrall, DNBP, DN-289, DNOSAP, DNOSBP, DNSBP, Dow General, Dyanap, Dytap

Chemical Name: 2-*sec*-butyl-4,6-dinitrophenol

Uses: herbicides/insecticides; pre- or post-emergence control of broadleaf weeds in cereals, maize, lucerne, clover, trefoil, grass leys, potatoes, peas, onions, garlics, peas, leeks, soya beans, orchards, groundnuts, strawberries, vineyards and other crops; for control of strawberry runners and raspberry suckers and overwintering forms of insect pests on fruit trees; also used as a desiccant for leguminous seed crops; destruction of potato haulms; as a pre-harvest hop defoliant, etc.

CAS Registry No: 88-85-7

Molecular Formula: $C_{10}H_{12}N_2O_5$

Molecular Weight: 240.212

Melting Point ($^{\circ}C$):

40 (Lide 2003)

Boiling Point ($^{\circ}C$):

362 (estimated, Grain 1982)

Density (g/cm^3 at $20^{\circ}C$):

1.265 ($45^{\circ}C$, Hartley & Kidd 1987; Herbicide Handbook 1989; Milne 1995)

Molar Volume (cm^3/mol):

218.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

4.62 (radiometer/pH meter, Cessna & Grover 1978; Hornsby et al. 1996)

4.61 (radiometer/pH meter, Cessna & Grover 1978)

4.62 (Worthing & Walker 1987, 1991)

4.50 (Yao & Haag 1991)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.713 (mp at $40^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

50 (Günther 1968; Spencer 1982; Thomas 1982)

52 (Kearney & Kaufman 1975; Khan 1980)

50 (Martin & Worthing 1977; Kenaga 1980)

52 (Ashton & Crafts 1981; Herbicide Handbook 1989)

100 (rm. temp., Worthing & Walker 1983, Worthing & Hance 1991)

52 ($20^{\circ}C$, Hartley & Kidd 1987; Milne 1995)

52 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

130 ($151.5^{\circ}C$, Khan 1980)

133 ($151.1^{\circ}C$, Ashton & Crafts 1981)

0.0008, 0.0067 (supercooled liquid, estimated, Grain 1982)

0.0067 (Thomas 1982)

0.0023 ($30^{\circ}C$, Spencer 1982)

10 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.183 ($60^{\circ}C$, Worthing & Hance 1991)

0.0067 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

51.1 (20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.59 (Hansch & Leo 1979)
 3.69 (calculated, Zitko et al. 1976)
 3.69 (Hansch & Leo 1985)
 4.10 (RP-PHLC-RT correlation, Klein et al. 1988)
 3.14 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 3.0, 3.57 (pH 7, pH 2, shake flask, Brooke et al. 1990)
 3.69 (recommended, Sangster 1993)
 3.56 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

1.83 (calculated-S, Kenaga 1980a; quoted, Howard 1991)
 0.778 (calculated- K_{oc} , Kenaga 1980)
 1.51 (measured, Kenaga 1980; quoted, Isensee 1991)

Sorption Partition Coefficient, $\log K_{oc}$:

2.85 (soil, Thomas 1982)
 2.09 (soil, Kenaga 1980a; Kenaga & Goring 1980)
 2.71 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980a)
 3.82 (HPLC- k' correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
 2.68 (estimated as $\log K_{om}$, Magee 1991)
 1.80, 2.04, 2.08 (soil, literature values, Bottoni & Funari 1992)
 2.70 (selected, Lohninger 1994)
 2.09 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 1.48 (soil, 20–25°C, estimated, Hornsby et al. 1996)

Adsorption coefficient, K_d ($\text{L}\cdot\text{kg}^{-1}$):

6.4, 64 (homoionic K^+ -kaolinite, K^+ -montmorillonite clay minerals, Haderlein et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: initial rate constant $k = 1.1 \times 10^{-3} \text{ h}^{-1}$ and predicted rate constant $k = 2.6 \times 10^{-3} \text{ h}^{-1}$ from soil with $t_{1/2} = 266.5 \text{ h}$ (Thomas 1982).

Photolysis:

Oxidation:

photooxidation $t_{1/2} = 12.2\text{--}122 \text{ h}$ in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k(\text{aq.}) = (0.003\text{--}2) \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.9–5.0 and $24 \pm 1^\circ\text{C}$, with $t_{1/2} = 0.16 \text{ s}$ at pH 7 (Yao & Haag 1991).

$k(\text{calc}) = 4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in aqueous solutions at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 1032\text{--}2952 \text{ h}$, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991) and aqueous anaerobic $t_{1/2} = 96\text{--}360 \text{ h}$, based on anaerobic soil die-away test data for isopropalin (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination Constants (k_2):

Half-Lives in the Environment:

Air: $t_{1/2} = 12.2\text{--}122 \text{ h}$, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 1032\text{--}2952 \text{ h}$, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991);

measured rate constant $k = (0.003\text{--}2) \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.9–5.0 and $24 \pm 1^\circ\text{C}$, with $t_{1/2} = 0.16 \text{ s}$ at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 96\text{--}5904 \text{ h}$, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

reported $t_{1/2} = 30 \text{ d}$ (Bottoni & Funari 1992)

Sediment:

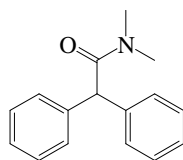
Soil: $t_{1/2} = 1032\text{--}2952 \text{ h}$, based on aerobic soil mineralization data for one soil (Doyle et al. 1978; quoted, Howard et al. 1991);

reported $t_{1/2} = 30 \text{ d}$ (Bottoni & Funari 1992);

field $t_{1/2} = 30 \text{ d}$ at $20\text{--}25^\circ\text{C}$ (estimated, Hornsby et al. 1996).

Biota:

17.1.1.31 Diphenamid



Common Name: Diphenamid

Synonym: Difenamide, Dimid, Dymid, Enide, Fenam, Rideon

Chemical Name: *N,N*-dimethyldiphenylacetamide; *N,N*-dimethyl- α -phenyl-benzeneacetamide

Uses: herbicide for pre-emergence control of annual grasses and some broadleaf weeds in cotton, sweet potatoes, tomatoes, vegetables, capsicums, okra, soybeans, groundnuts, tobacco, pome fruit, stone fruit, citrus fruit, bush fruit, strawberries, forestry nurseries, and ornamental plants, shrubs, and trees.

CAS Registry No: 957-51-7

Molecular Formula: $C_{16}H_{17}NO$

Molecular Weight: 239.312

Melting Point ($^{\circ}C$):

135 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.17 ($23.3^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

284.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.405 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0833 (mp at $135^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

240 (Melnikov 1971)

260 ($27^{\circ}C$ Spencer 1973, 1982; Khan 1980; Worthing & Walker 1987)

260 (Martin & Worthing 1977; Weber et al. 1980; Kenaga 1980)

260 ($27^{\circ}C$, Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994)

280 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

$< 1.33 \times 10^{-4}$ (Weber et al. 1980)

negligible ($20^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

4.0×10^{-6} (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Bioconcentration Factor, $\log BCF$:

1.43 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

2.32 (soil, calculated-S, Kenaga 1980)

2.32 (selected, Lohninger 1994)

2.32 (soil, 20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Photolysis: $t_{1/2} = 2.25$ h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

Half-Lives in the Environment:

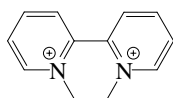
Soil: estimated persistence of 8 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

persistence under warm damp conditions is ca. 3–6 months (Herbicide Handbook 1989; Tomlin 1994)

field $t_{1/2} = 30$ d at 20–25°C (selected, Hornsby et al. 1996).

Biota:

17.1.1.32 Diquat



Common Name: Diquat

Synonym: Aquacide, Deiquat, Dextrone, Ortho, Pathclear, Preeglone, Reglone, Weedol, Weedtrine-D

Chemical Name: 1,1'-ethylene-2,2'-dipyridine

Uses: nonselective contact herbicide to control broadleaf weeds in fruit and vegetable crops.

CAS Registry No: 2764-72-9

Molecular Formula: $C_{12}H_{14}N_2$

Molecular Weight: 186.236

Melting Point ($^{\circ}C$): 335–340 (Spencer 1982)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.22–1.27 (Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

230.6 (calculated-Le Bas method at normal boiling point)

149.6 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

700000 (Khan 1980; Spencer 1982)

670000 (Weber et al. 1980)

700000 (Verschuereen 1983)

700000 (Worthing & Hance 1991; Tomlin 1994)

700000 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

< 0.00533 (Agrochemicals Handbook 1983)

< 1.3×10^{-5} (Worthing & Hance 1991; Tomlin 1994)

< 1.3×10^{-5} ($20^{\circ}C$, Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

< 6.38×10^{-9} (20 – $25^{\circ}C$, calculated-P/C, Montgomery 1993)

< 3.42×10^{-9} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

–3.05 (Garten & Trabalka 1983)

2.78 (Reinert 1989)

–4.60 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

–4.60 (Montgomery 1993)

Bioconcentration Factor, $\log BCF$:

–2.84 (calculated-S as per Kenaga 1980, this work)

–5.92 (calculated- $\log K_{ow}$ as per Mackay 1982, this work)

Sorption Partition Coefficient, $\log K_{oc}$:

2.84 (Reinert 1989)

0.420 (calculated, Montgomery 1993)

0.425 (calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 192$ h for 10 $\mu\text{g/mL}$ to degrade in distilled water under 240–260 nm light (Funderburk et al. 1960; quoted, Cessna & Muir 1991);

$t_{1/2} < 5$ wk for 4 $\mu\text{g/mL}$ to degrade in distilled water under sunlight (Slade & Smith 1967; quoted, Cessna & Muir 1991);

dry diquat photodecomposed by UV light with $t_{1/2} = 48$ h (Funderburk & Bozarth 1967; quoted, Montgomery 1993);

$t_{1/2} \sim 48$ h when associated with aerosols (Howard 1991);

$t_{1/2} = 3$ wk for 3% of 5 $\mu\text{g/mL}$ to degrade in distilled water under sunlight (Smith & Grove 1969; quoted, Cessna & Muir 1991).

Oxidation:

$k(\text{aq.}) = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.1 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(\text{aq.}) = (0.6 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 3.1 and 22°C , with a half-life of 15 h at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = (8.0 \pm 1.8) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.1 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992).

Hydrolysis: $t_{1/2} = 74$ d under simulated sunlight at pH 7 (Montgomery 1993; Tomlin 1994).

Biodegradation: $t_{1/2} \sim 50$ d to biodegrade in lake water (Hiltibrant 1972; quoted, Muir 1991);

$t_{1/2} > 158$ d for 1.5 $\mu\text{g/mL}$ of infested sediment-water microcosm to biodegrade in sediment and $t_{1/2} \sim 2$ d in water both at 25°C (derived from Simsiman & Chesters 1976; Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} \sim 50$ d to biodegrade in lake water (Hiltibrant 1972; quoted, Muir 1991);

$t_{1/2} \sim 2$ d of ^{14}C -diquat in water of a weed-infested simulated lake impoundment containing Lake Mendota sediment, the rapid disappearance is attributed to adsorption by sediments, suspended particulate matter and aquatic plants (shake flask-scintillation spectrometry, Simsiman & Chesters 1976)

measured rate constant $k = (0.6 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 3.1 and 22°C , with $t_{1/2} = 15$ h at pH 7 (Yao & Haag 1991).

Ground water:

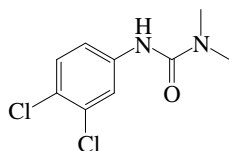
Sediment: Slow microbial degradation due to tight bonding of adsorbed Diquat to the clay minerals on the sediment (shake flask-liquid scintillation spectrometry, Simsiman & Chesters 1976)

$t_{1/2} > 158$ d for 1.5 $\mu\text{g/mL}$ of infested sediment-water microcosm to biodegrade (derived from results of Simsiman & Chesters 1976; Muir 1991).

Soil:

Biota:

17.1.1.33 Diuron



Common Name: Diuron

Synonym: AF 101, Cekiuron, Crisuron, Dailon, DCMU, Diater, dichlorofonidim, Di-on, Direx, DMU, Drexel, Duran, Dynex, Herbatox, Karmex, Marmer, NA 2767, Telvar, Unidron, Urox D, Vonduron

Chemical Name: 3-(3,4-dichlorophenyl)-1,1-dimethylurea; *N'*-(3,4-dichlorophenyl)-*N,N*-dimethylurea

Uses: pre-emergence herbicide in soils to control germinating broadleaf grasses and weeds in crops such as apples, cotton, grapes, pears, pineapple, and alfalfa; also used as sugar cane flowering depressant.

CAS Registry No: 330-54-1

Molecular Formula: $C_9H_{10}Cl_2N_2O$

Molecular Weight: 233.093

Melting Point ($^{\circ}C$):

158 (Lide 2003)

Boiling Point ($^{\circ}C$):

180 (decomposes, Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

223.8 (calculated-Le Bas method at normal boiling point)

188.0 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994a)

Dissociation Constant pK_a :

-1 to -2 (Montgomery 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

66.0 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

33.89 (DSC method, Plato & Glasgow 1969)

27.3 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0496 (mp at $158^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

42.0 (Günther et al. 1968; Melnikov 1971; Spencer 1973, 1982; Khan 1980; Ashton & Crafts 1981)

42.0 ($20^{\circ}C$, Weber 1972; Weber et al. 1980)

37.3 (shake flask-UV, Freed et al. 1976; Freed 1976)

42.0 (Martin & Worthing 1977; Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

42.4 (shake flask, Briggs 1981)

22.0 (shake flask-HPLC, Ellgehausen et al. 1981)

38.7 (generator column-HPLC/RI, Swann et al. 1983)

120 (RP-HPLC-RT correlation, Swann et al. 1983)

19.6, 40.1, 53.4 (4, 25, $40^{\circ}C$, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)

42.0 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

40.0 ($20^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.6×10^{-5} (estimated, Nex & Swezey 1954)

3.8×10^{-6} ($20^{\circ}C$, Johnson & Julin 1974)

4.1×10^{-4} ($50^{\circ}C$, Khan 1980; Ashton & Crafts 1981)

$< 1.3 \times 10^{-4}$ (20 – $25^{\circ}C$, Weber et al. 1980)

2.5×10^{-4} (Thomas 1982)

- 2.1×10^{-5} (Jury et al. 1983; quoted, Taylor & Glotfelty 1988; Taylor & Spencer 1990)
- 3.6×10^{-4} (Jury et al. 1983; quoted, Howard 1991)
- 2.7×10^{-4} (selected, Nkedi-Kizza et al. 1985)
- 4.1×10^{-4} (50°C, Hartley & Kidd 1987; Worthing & Hance 1991; Herbicide Handbook 1989)
- 2.0×10^{-4} (20°C, selected, Suntio et al. 1988)
- 5.30×10^{-4} , 1.0×10^{-2} , 0.130, 1.20, 79 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
- $\log (P_s/Pa) = 13.339 - 4953.8/(T/K)$; measured range 36.2–90.2°C (solid, gas saturation-GC, Rordorf 1989)
- $\log (P_L/Pa) = 9.800335 - 3445.24/(T/K)$; measured range not specified (liquid, gas saturation-GC, Rordorf 1989)
- 9.2×10^{-6} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.1×10^{-6} (Tomlin 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 1.4×10^{-4} (calculated-P/C, Jury et al. 1984, 1987a,b; Jury & Ghodrati 1989)
- 1.2×10^{-4} (20°C, calculated-P/C, Suntio et al. 1988)
- 1.3×10^{-4} (calculated-P/C, Taylor & Glotfelty 1988)
- 0.274 (calculated-P/C, Howard 1991)
- 2.1×10^{-5} (20°C, calculated-P/C, Muir 1991)
- 1.5×10^{-4} (20–25°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.60 (calculated-f const., Rekker 1977)
- 2.81 (Rao & Davidson 1980)
- 2.68 (shake flask-UV, Briggs 1981)
- 2.89 (shake flask-HPLC, Ellgehausen et al. 1981)
- 2.60 (Elgar 1983)
- 2.77 (Hansch & Leo 1985)
- 2.69, 2.65, 2.63 (4, 25, 40°C, shake flask-liquid scintillation spectrometer LSS, Madhun et al. 1986)
- 2.86 (shake flask, Mitsutake et al. 1986)
- 1.97–2.81 (Montgomery 1993)
- 2.78 (recommended, Sangster 1993)
- 2.45 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.80 (Aquasol Database 1994; quoted, Pinsuwan et al. 1995)
- 2.81 (shake flask, Spurlock & Biggar 1994a)
- 2.85 ± 1.70 (Tomlin 1994)
- 2.58, 2.73 (shake flask-UV, RP-HPLC- k' correlation, Liu & Qian 1995)
- 2.68 (recommended, Hansch et al. 1995)
- 2.45 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.40 (measured, Isensee 1976)
- 1.88 (calculated-S, Kenaga 1980)
- 1.34 (calculated- K_{oc} , Kenaga 1980)
- 2.16 (*Pimephales promelas*, Call et al. 1987)
- 2.41, 2.48 (cuticle/water: tomato, pepper, Chaumat et al. 1991)
- 2.41, 2.51 (cuticle/water: box tree, laurel, Chaumat et al. 1991)
- 2.55, 2.28 (cuticle/water: pear, ivy, Chaumat et al. 1991)
- 1.18, 1.64 (cuticle/water: cleavers, vanilla, Chaumat et al. 1991)
- 2.45, 2.48 (cuticle/water: tomato, pepper, Evelyne et al. 1992)

Bioaccumulation Factor, $\log \text{BF}$:

- −1.70 (adipose tissue in both male & female Albino rats, Hodge et al. 1967)

Sorption Partition Coefficient, $\log K_{oc}$:

- 2.60 (soil, Hamaker & Thompson 1972; Farmer 1976; Hance 1976)

- 2.75 (soil, calculated-S as per Kenaga & Goring 1977, Kenaga 1980)
- 2.59 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
- 2.15–2.52 (Peck et al. 1980)
- 2.21 (soil, converted from reported K_{OM} multiplied 1.724, Briggs 1981)
- 3.06, 2.41 (estimated-S, solubility and mp, Karickhoff 1981)
- 1.58, 2.42 (estimated- K_{OW} , Karickhoff 1981)
- 2.58 (average of 84 soils, Rao & Davidson 1982)
- 2.18 (soil, Thomas 1982)
- 2.83 (Webster soil, Nkedi-Kizza 1983)
- 2.49 (soil slurry method, Swann et al. 1983)
- 2.48 (RP-HPLC-RT correlation, Swann et al. 1983)
- 3.03, 2.94 (4°C, 25°C, Semiahmoo soil, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.82, 2.68 (4°C, 25°C, Adkins soil, batch equilibrium method-LSS, Madhun et al. 1986)
- 2.86, 2.44, 2.48; 2.81, 2.74, 2.44 (estimated- K_{OW} ; solubility, Madhun et al. 1986)
- 2.50 (calculated-MCI χ , Gerstl & Helling 1987)
- 2.58 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 2.35, 2.57 (2 subsurface soils from Oklahoma, Bouchard & Wood 1988)
- 2.94, 2.68 (mucky peat soil, loam sand soil, quoted, Howard 1991)
- 2.18, 2.48–2.49, 2.59, 2.66 (soil, quoted values, Bottoni & funari 1992)
- 2.68 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.21–2.87 (Montgomery 1993)
- 2.68 (selected, Lohninger 1994)
- 2.60 (Tomlin 1994)
- 2.70 (calculated- K_{OW} , Liu & Qian 1995)
- 2.40 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.07, 2.37, 2.82, 2.51, 2.96 (calculated- K_{OW} ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 2.48, 2.42 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.44, 2.43, 2.57 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
- 2.78^c (sediment: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization: $2.5 \times 10^{-3} \text{ h}^{-1}$ (initial) and $5.3 \times 10^{-4} \text{ h}^{-1}$ (predicted) from soil with $t_{1/2} = 1307 \text{ h}$ (Thomas 1982); the calculated $t_{1/2} = 1918 \text{ d}$ due to volatilization from soil when incorporated into 1 cm of soil (Jury et al. 1983; quoted, Howard 1991).
- Photolysis: $t_{1/2} = 2.25 \text{ h}$ for 80–84% of 40 $\mu\text{g/mL}$ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991); in surface waters should be photolyzed within a few days (Howard 1991).
- Oxidation: photooxidation $t_{1/2} = 0.12 \text{ d}$ in air, based on estimation for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).
- Hydrolysis: $t_{1/2} > 4$ months for 4660 $\mu\text{g/mL}$ to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).
- Biodegradation: $t_{1/2} = 328 \text{ d}$ for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a);
- $t_{1/2} = 3–10 \text{ d}$ for 40 $\mu\text{g/mL}$ to biodegrade in pond sediment of anaerobic media at 30°C (Attaway et al. 1982a quoted, Muir 1991);
- $t_{1/2} < 17 \text{ d}$ for 40 $\mu\text{g/mL}$ to biodegrade in pond sediment at 30°C (Attaway et al. 1982b; quoted, Muir 1991);
- 67–99% will be degraded in 10 wk under aerobic conditions by mixed cultures isolated from pond water and sediments forming 6–7 products (Ellis & Camper 1982; quoted, Howard 1991; Muir 1991);
- $t_{1/2} < 70 \text{ d}$ at 30°C (Ellis & Camper 1982; quoted, Muir 1991; Montgomery 1993);
- $t_{1/2} \sim 5 \text{ d}$ for 0.22 $\mu\text{g/mL}$ to biodegrade in pond sediment of anaerobic media (Stepp et al. 1985; quoted, Muir 1991);
- $t_{1/2}(\text{aerobic}) \sim 20 \text{ d}$ for 0.0005–10 $\mu\text{g/mL}$ to biodegrade in filtered sewage water at 20°C (Wang et al. 1985; quoted, Muir 1991).

Biotransformation: ~ 7% of a selection of 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted over 50% of diuron (20 mg/L) in 5-d experiment (Vroumsia et al. 1996)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.12 d, based on estimation for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water: should be photolyzed within a few days (Howard 1991).

Ground water: reported half-lives or persistence, $t_{1/2}$ = 20–70, 90–180, 200, and 328 d (Bottoni & Funari 1992)

Sediment: $t_{1/2}$ = 3–10 d for 40 µg/mL to biodegrade in pond sediment of anaerobic media at 30°C (Attaway et al. 1982a; quoted, Muir 1991);

$t_{1/2}$ < 17 d for 40 µg/mL to biodegrade in pond sediment at 30°C (Attaway et al. 1982b);

$t_{1/2}$ ~ 5 d for 0.22 µg/mL to biodegrade in pond sediment of anaerobic media (Stepp et al. 1985)

Soil: estimated persistence of 10 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987);

persistence of 8 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2}$ = 7.0 months at 15°C and $t_{1/2}$ = 5.5 months at 30°C in soils (Freed & Haque 1973);

persistence of 10 months (Wauchope 1978);

rate constant k = 0.0031 d⁻¹ with $t_{1/2}$ = 328 d under field conditions (Rao & Davidson 1980);

calculated $t_{1/2}$ = 1918 d due to volatilization from soil when incorporated into 1 cm of soil (Jury et al. 1983; quoted, Howard 1991);

$t_{1/2}$ ~ 200–4000 d in loamy sand and peat at 25–35°C as follows (Madhum & Freed 1987):

$t_{1/2}$ = 705, 414, and 225 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg, while $t_{1/2}$ = 1392, 630, and 406 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in an Adkins loamy sand; however, the half-lives were considerable higher in peat. $t_{1/2}$ = 3991, 2164, and 1165 d at 25, 30, and 35°C, respectively, at herbicide concn at 5 µg/kg while $t_{1/2}$ = 3416, 1832, and 896 d at 25, 30, and 35°C, respectively, at herbicide concn at 100 µg/kg in a Semiahoo mucky peat (Madhun & Freed 1987)

$t_{1/2}$ = 328 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

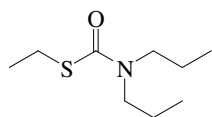
reported $t_{1/2}$ = 20–70 d, 90–180 d, 200 d and 328 d (Bottoni & Funari 1992);

$t_{1/2}$ = 75–102 d in 0–40 cm soil cores taken, from cultivated field, $t_{1/2}$ = 55–65 d from meadow and $t_{1/2}$ = 29–35 d from gravel track (Hassink et al. 1994);

selected field $t_{1/2}$ = 90 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical $t_{1/2}$ = 328 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

17.1.1.34 EPTC



Common Name: EPTC

Synonym: Eptam, Eradicane, FDA 1541, R 1608, Torbin

Chemical Name: carbamic acid, dipropylthio-, *S*-ethyl ester; *S*-ethyldipropyl(thiocarbamate); *S*-ethyldipropylcarbamo-thioate

Uses: selective systemic herbicide for pre-emergence control of perennial and annual grasses, broadleaf weeds.

CAS Registry No: 759-94-4

Molecular Formula: $C_9H_{19}NOS$

Molecular Weight: 189.318

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

235.0 (Khan 1980; Herbicide Handbook 1989)

127.0 (at 20 mmHg, Hartley & Kidd 1987; Budavari 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

0.9546 ($30^{\circ}C$, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

0.960 ($25^{\circ}C$, Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

236.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

375 (shake flask-GC, Freed et al. 1967)

365 (Martin & Worthing 1977)

370 ($20^{\circ}C$, Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)

370–375 (Weber et al. 1980)

375 ($20^{\circ}C$, Spencer 1982)

370 (Beste & Humburg 1983; Jury et al. 1983, 1984)

375 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

375 ($24^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991)

365 ($20^{\circ}C$, Budavari 1989; Milne 1995)

344 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996; Lohninger 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

4.666 (extrapolated, Patchett et al. 1964)

20.66 (Bailey & White 1965)

1.84 ($20^{\circ}C$, effusion method, Hamaker & Kerlinger 1971)

2.16, 2.63, 3.69, 8.266 (23, 24, 28, $40^{\circ}C$, Hamaker 1972)

4.532 (Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)

2.62 ($20^{\circ}C$, volatilization rate, Burkhard & Guth 1981)

2.80 (Patchett et al. 1983)

0.612 ($20^{\circ}C$, GC-RT correlation, Kim 1985)

4.70 (Hartley & Kidd 1987)

2.00 ($20^{\circ}C$, selected, Suntio et al. 1988)

4.532 ($35^{\circ}C$, Budavari 1989)

4.50 (Worthing & Hance 1991)

- 4.532 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 4.532 (20°C, Montgomery 1993)
 0.00001 (Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 1.32 (20°C, volatilization rate, Burkhard & Guth 1981)
 1.463 (calculated-P/C, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989)
 1.02 (20°C, calculated-P/C, Suntio et al. 1988)
 1.463 (calculated-P/C, Taylor & Glotfelty 1988)
 1.013 (20–25°C, calculated-P/C, Montgomery 1993)
 1.023 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

- 1.76 (selected, Dao et al. 1983)
 3.21 (shake flask, Log P Database, Hansch & Leo 1987)
 3.20 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)
 3.21 (recommended, Sangster 1993)
 3.21 (recommended, Hansch et al. 1995)
 3.45 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.34 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 1.08 (calculated-K_{OC}, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC}:

- 2.38 (soil, Hamaker & Thompson 1972)
 2.45 (soil, Hamaker & Thompson 1972)
 2.23 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 2.58 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
 2.23–2.38, 2.45 (quoted values, Bottoni & Funari 1992)
 2.30 (soil, 20–25°C, selected, Wauchope et al. 1992)
 2.38 (Montgomery 1993)
 2.30 (selected, Lohninger 1994)
 2.45 (selected, Wienhold & Gish 1994)
 2.38 (soil, calculated-MCI ¹χ, Sabljic et al. 1995)
 2.23, 1.98 (soil, estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 2.03, 2.00 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization: t_{1/2} = 3.7 d (Jury et al. 1983).

Photolysis: rate constant k = 5.2 × 10⁻³ s⁻¹ for a light intensity corresponding to a 12-h average NO₂ photolysis rate with a black lamp spectral distribution (Kwok et al. 1992);

photodegradation t_{1/2} = 14.0 and 18.5 min in water solution under irradiation with UV light at 254 nm (Abu-Qare & Duncan 2002).

Oxidation: second order rate constants k_{OH} = (3.10–3.40) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for gas-phase reaction with OH radical, k_{NO₃} = 0.92 × 10⁻¹⁴ cm³ molecule⁻¹ s⁻¹ with NO₃ radical and k_{O₃} < 1.3 × 10⁻¹⁹ cm³ molecule⁻¹ s⁻¹ with O₃ at 298 K (Kwok et al. 1992);

calculated lifetime of 6 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Hydrolysis:

Biodegradation: t_{1/2} = 30 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Nash 1980; quoted, Jury et al. 1983, 1984, 1987a; quoted, Grover 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetimes are: > 8 h due to photolysis, 5.8 d due to reaction with OH radical, 5.0 d with NO_3 radical and > 125 d with O_3 (Kwok et al. 1992);

calculated lifetime of 6 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Surface water: $t_{1/2} = 14.0$ and 18 min for elimination in water under irradiation with UV light at 254 nm (Abu-Qare & Duncan 2002).

Ground water: reported half-lives or persistence, $t_{1/2} = 7$ and 30 d (Bottoni & Funari 1992)

Sediment:

Soil: estimated persistence of 4 months in soil (Kearney et al. 1969; quoted, Jury et al. 1987a);

$t_{1/2} = 30$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);

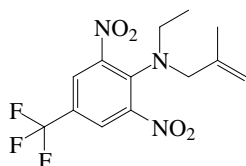
$t_{1/2} \sim 1$ wk in moist loam soil at 21 to 27°C (Herbicide Handbook 1974, 1989);

reported $t_{1/2} = 7, 30$ d (Bottoni & Funari 1992);

selected field $t_{1/2} = 6$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996).

Biota: biochemical $t_{1/2} = 30$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989)

17.1.1.35 Ethalfluralin



Common Name: Ethalfluralin

Synonym: Benzenamine, Somilan, Sonalan, Sonalen

Chemical Name: *N*-ethyl-*N*-(2-methyl-2-propenyl)-2,6-dinitro-(trifluoromethyl)-benzenamine

CAS Registry No: 55283-68-6

Uses: herbicide

Molecular Formula: $C_{13}H_{14}F_3N_3O_4$

Molecular Weight: 333.263

Melting Point ($^{\circ}C$):

57 (Lide 2003)

Boiling Point ($^{\circ}C$):

256 (decomposes, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.32 (Ashton & Crafts 1981; Herbicide Handbook 1989)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.485 (mp at $57^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.21 (Ashton & Crafts 1981)

0.20 (pH 7, Spencer; Hartley & Kidd 1987; Worthing & Walker 1987)

0.30 (pH 7, Herbicide Handbook 1989)

0.30 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.30 (pH 7, Tomlin 1994; Milne 1995)

0.40 (Majewski & Capel 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.10×10^{-4} (Worthing & Walker 1983, 1987; Hartley & Kidd 1987)

0.0109 (Spencer 1982; Herbicide Handbook 1989)

0.0117 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0117 (Tomlin 1994)

2.22×10^{-4} (20 – $25^{\circ}C$, Majewski & Capel 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.183 (calculated-P/C, Majewski & Capel 1995)

13 (calculated-P/C, Wolt 1997)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.11 (pH 7, Tomlin 1994; Milne 1995)

4.92 (quoted values; selected, Wolt 1997)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.60 (selected, soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.60–3.90 (soil, Tomlin 1994)
- 3.61–3.92 (soil, Wolt 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 6.3$ h in aqueous phase and $t_{1/2} = 2$ h in vapor phase (Tomlin 1994);

Aqueous photolysis $t_{1/2} = 6.3$ h in pH 5 sterile buffer solution; soil photolysis $t_{1/2} = 14.2$ d in air-dry sandy loam soil when exposed to a xenon light source; air photolysis $t_{1/2} = 2$ h when exposed to a light source simulating summer sunlight at 34°C (Wolt 1997).

Oxidation:

Hydrolysis: no hydrolysis after 33 d at pH 3, 6 and 9 (51°C, Tomlin 1994); stable in sterile, buffered solutions across a range of pH (Wolt 1997).

Biodegradation:

Biotransformation: $t_{1/2} = 45$ d for aerobic metabolism in sandy loam soils and $t_{1/2} = 14$ d for more rapid metabolism anaerobically in the same soil (quoted, Tomlin 1994; Wolt 1997).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: air photolysis $t_{1/2} = 2$ h when exposed to a light source simulating summer sunlight at 34°C (Wolt 1997).

Surface water: water photolysis $t_{1/2} = 6.3$ h in pH 5 sterile buffer solution; $t_{1/2} = 2$ d for dissipation from the water column in a pond water-sediment system under outdoor conditions (Wolt 1997).

Ground water:

Sediment: $t_{1/2} = 38$ h in anaerobic pond water sediment system (Wolt 1997).

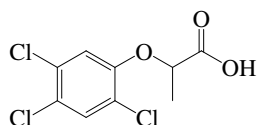
Soil: reported field $t_{1/2} = 30$ –60 d, 60 d, 25–46 d; recommended $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 45$ d for aerobic metabolism in sandy loam soils and $t_{1/2} = 14$ d for more rapid metabolism anaerobically in the same soil (Tomlin 1994);

terrestrial field dissipation $t_{1/2} = 4$ –146 d, $t_{1/2} = 45$ d in moist aerobic soil, $t_{1/2} = 14$ d in anaerobic soil shifted to anaerobic conditions (Wolt 1997).

Biota:

17.1.1.36 Fenoprop



Common Name: Fenoprop

Synonym: Silvex, 2,4,5-TP, Kuron, Kurosol, Fruitone T

Chemical Name: 2-(2,4,5-trichlorophenoxy) propionic acid

CAS Registry No: 93-72-1

Uses: herbicide/growth regulator

Molecular Formula: $C_9H_7Cl_3O_3$

Molecular Weight: 269.509

Melting Point ($^{\circ}C$):

181.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

2.84 (Worthing 1983, 1987; Augustijn-Beckers et al. 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

75.75 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

44.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0291 (mp at $181.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

140 (Kenaga & Goring 1980, Kenaga 1980a,b, Spencer 1982)

140 (Worthing & Walker 1983, 1987; Budavari 1989)

200 (Verschuere 1983)

176 (Hartley & Kidd 1987)

12.0 (calculated-MCI χ , Patil 1994)

140 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.30×10^{-3} , 4.40×10^{-2} , 0.55, 4.90, 34.0 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 13.953 - 4948/(T/K)$; measured range 85.4 – $181^{\circ}C$ (gas saturation-GC, Rordorf 1989)

$\log(P_l/Pa) = 11.727 - 3956.9/(T/K)$; measured range 181 – $211^{\circ}C$ (gas saturation-GC, Rordorf 1989)

$< 1.33 \times 10^{-6}$ (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.44 (Kenaga 1980a)

3.86 (estimated, Garten & Trabalka 1983)

3.13 (counter-current chromatography, Ilchmann et al. 1993)

2.75 (calculated-MCI χ , Patil 1994)

3.80 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.76 (calculated, Kenaga 1980a)

1.58, 2.23 (calculated-solubility, K_{ow} , Kenaga 1980b)

- 1.76 (fish, flowing water, Garten & Grabalka 1983)
2.35 (Isensee 1991)

Sorption Partition Coefficient, log K_{OC} :

- 3.41 (soil, Kenaga & Goring 1980)
2.46 (calculated- K_{OW} , Kenaga 1980b)
1.91 (soil: calculated-MCI χ , Meylan et al. 1992)
2.48 (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
3.28 (soil, calculated-MCI χ , Sabljic et al. 1995)

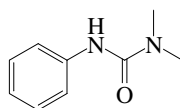
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: $t_{1/2} > 205$ d for ring cleavage in soil suspensions (Verschueren 1983)

Half-Lives in the Environment:

Soil: persistence 47–205 d in soil (Alexander et al. 1961)
degradation $t_{1/2} = 21$ d and 14 d in Quachita Highlands' forest and grassland soil respectively, $t_{1/2} = 15$ d in gross timbers forest soil, average $t_{1/2} = 17$ d in 3 soils (Altom & Stritzke 1973);
 $t_{1/2} = 5$ –11 d in a microagroecosystem study (Nash 1983);
 $t_{1/2} > 205$ d for ring cleavage in soil suspensions (Verschueren 1983);
field $t_{1/2} = 21$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

17.1.1.37 Fenuron



Common Name: Fenuron

Synonym: Dozer, Dybar, Falisilvan, Fenidim, Fenulon, Urab

Chemical Name: 1,1-dimethyl-3-phenylurea; *N,N*-dimethyl-*N'*-phenylurea

Uses: herbicide to control woody plants and deep-rooted perennial weeds, often used in combination with chlorpropham to extend its weed control spectrum and range of crops.

CAS Registry No: 101-42-8

Molecular Formula: $C_9H_{12}N_2O$

Molecular Weight: 164.203

Melting Point ($^{\circ}C$):

132 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.13 ($25^{\circ}C$, Hartley & Kidd 1987)

1.08 (Worthing & Hance 1991; Tomlin 1994)

Molar Volume (cm^3/mol):

182.0 (calculated-Le Bas method at normal boiling point)

159.0 (modified Le Bas method, Spurlock & Biggar 1994a)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.267 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0892 (mp at $132^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2600 (Freed 1966)

2400 (Günther et al. 1968)

3850 (Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Verschueren 1983)

3850 (Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Willis & McDowell 1982)

3700 (shake flask-HPLC, Ellgehausen et al. 1981)

3850 (Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991; Tomlin 1994)

3000 ($20^{\circ}C$, selected, Suntio et al. 1988)

3900 (Spurlock 1992; Spurlock & Biggar 1994b)

3850 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0213 ($60^{\circ}C$, Khan 1980; Verschueren 1983)

0.0210 ($60^{\circ}C$, Hartley & Kidd 1987)

0.0050 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.0210 ($60^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

0.0267 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.00027 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.98 (shake flask-UV, Hansch & Anderson 1967)

1.00 (Leo et al. 1971)

1.00 (shake flask-UV, Lord et al. 1980)

0.96	(shake flask-UV, Briggs 1981; Karickhoff 1981)
0.88	(shake flask-HPLC, Ellgehausen et al. 1981)
0.62	(HPLC- k' correlation, McDuffie 1981)
0.70	(Elgar 1983)
1.18	(RP-HPLC- k' correlation, Braumann et al. 1983)
1.00	(shake flask-HPLC, Spurlock & Biggar 1994a)
0.98	(recommended, Sangster 1993)
1.18	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
0.98	(recommended, Hansch et al. 1995)
1.18	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

0.778	(calculated-S, Kenaga 1980)
0.0	(calculated- K_{OC} , Kenaga 1980)
1.34	(earthworms, Lord et al. 1980)
0.699, 0.602	(cuticle/water: tomato, pepper, Evelyne et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

1.43	(soil, Hamaker & Thompson 1972)
1.67	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
0.88	(reported as log K_{OM} , Briggs 1981)
0.61	(estimated- K_{OW} , Karickhoff 1981)
1.80, 1.86	(estimated-S, Karickhoff 1981)
0.72, 0.84	(estimated-S and mp, Karickhoff 1981)
1.74	(calculated-MCI χ , Gerstl & Helling 1987)
1.62	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
1.40	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.40; 1.40, 1.70	(soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
1.42, 1.41	(soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: aerobic $t_{1/2} \geq 10$ d for 0.01 $\mu\text{g/mL}$ to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991).

Half-Lives in the Environment:

Air:

Surface water: aerobic $t_{1/2} \geq 10$ d for 0.01 $\mu\text{g/mL}$ to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);
persistence of up to 4 weeks in river water (Eichelberger & Lichtenberg 1971).

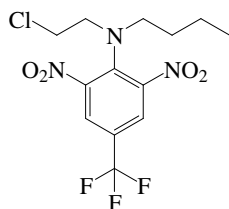
Ground water:

Sediment:

Soil: $t_{1/2} = 4.5$ months at 15°C and 2.2 months at 30°C in soils (Freed & Haque 1973);
persistence of 8 months in soil (Edwards 1973; quoted, Morrill et al. 1982);
selected field $t_{1/2} = 60$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

17.1.1.38 Fluchloralin



Common Name: Fluchloralin

Synonym: BAS-392H, Basalin

Chemical Name: *N*-(2-chloroethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzenamine; *N*-(2-chloroethyl) α,α,α -trifluoro-2,6-dinitro-*N*-propyl-*p*-toluidine

Uses: herbicide for pre-plant or pre-emergence control of annual grass and broadleaf weeds in cotton, groundnuts, jute, potatoes, rice soybeans, and sunflowers, etc.

CAS Registry No: 33245-39-5

Molecular Formula: $C_{12}H_{13}ClF_3N_3O_4$

Molecular Weight: 355.697

Melting Point ($^{\circ}C$):

42 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

326.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.681 (mp at $42^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.00	($20^{\circ}C$, Weber 1972; Ashton & Crafts 1981)
1.00	(Edwards 1977)
< 1.0	(Martin & Worthing 1977; Herbicide Handbook 1978, 1989)
0.70	($20^{\circ}C$, Spencer 1982)
< 1.0	(Worthing & Walker 1987, 1991; Tomlin 1994)
10	(Budavari 1989; Milne 1995)
0.90	(20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.50	(selected, Lohninger 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0033	($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)
0.373	($20^{\circ}C$, Ashton & Crafts 1981)
0.0008, 0.0033, 0.0133, 0.533	($20, 30, 40, 50^{\circ}C$, gas saturation, Spencer 1982)
0.0035	(Herbicide Handbook 1983; quoted, Nash 1988)
0.0037, 0.0033	($20^{\circ}C, 30^{\circ}C$, Herbicide Handbook 1989)
0.004	($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)
0.004	(20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

1.174	($20^{\circ}C$, calculated-P/C, Muir 1991)
1.343	calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.63	(selected, Magee 1991)
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4.70 (CLOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

> 2.79, 2.40 (calculated-S, calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

3.56 (soil, Harvey 1974)

3.60 (soil, Kenaga 1980)

> 3.64 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)

4.25 (calculated-MCI χ , Bahnick & Doucette 1988)

3.56; 3.58 (reported as log K_{OM} , estimated as log K_{OM} , Magee 1991)

3.48 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

3.80 (estimated-chemical structure, Lohninger 1994)

3.55 (soil, calculated-MCI χ , Sabljic et al. 1995)

3.55; 4.02 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 1$ d from 1 m depth of water (20°C, Muir 1991).

Photolysis: $t_{1/2} = 13$ d for 84% of 5 $\mu\text{g/mL}$ to degrade in distilled water under sunlight (Nilles & Zabik 1974; quoted, Cessna & Muir 1991);

$t_{1/2} = 8$ h for 50% of 2000 $\mu\text{g/mL}$ to degrade in methanol under sunlight (Plimmer & Klingebiel 1974; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} = 8$ d for 0.5 $\mu\text{g/mL}$ to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991);

$t_{1/2} = 3.6$ wk for 2.0 $\mu\text{g/mL}$ to biodegrade in soil at 25°C (Brewer et al. 1982; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} = 8$ d for 0.5 $\mu\text{g/mL}$ to biodegrade in soil at 20–42°C (Savage 1978; quoted, Muir 1991);

$t_{1/2} = 1.5$ d on Bosket silt loam, $t_{1/2} = 4$ d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with $t_{1/2} = 13$ d on Bosket silt loam, $t_{1/2} = 8$ d on Sharkey clay (Savage & Jordon 1980)

measured dissipation rate $k = 0.099\text{--}0.13$ d^{-1} (derived from Savage & Jordan 1980, Nash 1988);

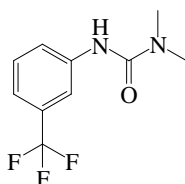
field studies, $t_{1/2} = 12.2$ wk - 1978 first study; $t_{1/2} = 13.0$ wk -1978 second study; $t_{1/2} = 17.6$ wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)

Laboratory studies: $t_{1/2} = 28.7$ wk at 4°C, 10.5 wk at 25°C for soils of field capacity moisture (27% w/w for Crowley silt loam) and $t_{1/2} = 20.8$ wk at 4°C, $t_{1/2} = 8.4$ wk at 25°C for flooded soil of Crowley silt loam; $t_{1/2} = 29.3$ wk at 4°C, $t_{1/2} = 10.5$ wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay) and $t_{1/2} = 20.8$ wk at 4°C and $t_{1/2} = 4.3$ wk at 25°C for flooded soil, Sharkey silty clay (Brewer et al. 1982);

$t_{1/2} = 3.6$ wk for 2.0 $\mu\text{g/mL}$ to biodegrade in soil at 25°C (derived from Brewer et al. 1982, Muir 1991); estimated dissipation rate $k = 0.29$, and 0.120 d^{-1} (Nash 1988);

estimated field $t_{1/2} \sim 60$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.39 Fluometuron



Common Name: Fluometuron

Synonym: CIBA 2059, Cotoran, Cottonex, Higalcoton, Lanex, Meturon, Pakhtaran

Chemical Name: 1,1-dimethyl-3-(α,α,α -trifluoro-*m*-tolyl)urea; N,N-dimethyl-N'-[3-(trifluoromethyl)phenyl]urea

Uses: herbicide to control many annual broadleaf weeds in sugar cane and cotton.

CAS Registry No: 2164-17-2

Molecular Formula: $C_{10}H_{11}F_3N_2O$

Molecular Weight: 232.201

Melting Point ($^{\circ}C$):

163–164.5 (Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

164 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.390 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

229.7 (calculated-Le Bas method at normal boiling point)

167.1 (calculated-density)

Dissociation Constant pK_a :

–1.00 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

29.706 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0433 (mp at $164^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

90 (Melnikov 1971; Spencer 1973, 1982; quoted, Wauchope 1978; Khan 1980; Weber et al. 1980)

90 ($20^{\circ}C$, Martin & Worthing 1977; Herbicide Handbook 1978,89)

106 (shake flask-UV, Briggs 1981)

90 (Herbicide Handbook 1983)

105 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987, 1991)

110 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

80 (Montgomery 1993)

110 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

6.70×10^{-5} (20 – $25^{\circ}C$, Weber et al. 1980)

6.70×10^{-5} (Herbicide Handbook 1983)

6.70×10^{-5} ($20^{\circ}C$, Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993)

6.60×10^{-5} ($20^{\circ}C$, Worthing & Hance 1991)

1.25×10^{-4} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.25×10^{-4} (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

< 0.283 (20 – $25^{\circ}C$, calculated-P/C, Montgomery 1993)

1.73×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

- 1.34 (Briggs 1969)
- 2.42 (shake flask-UV, Briggs 1981)
- 1.88 (shake flask-UV, pH 5, Barak et al. 1983)
- 2.40 (selected, Gerstl & Helling 1987)
- 2.23 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
- 2.23, 2.38 (Montgomery 1993)
- 2.03 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.20 (recommended, Sangster 1993)
- 2.42 (recommended, Hansch et al. 1995)
- 2.03 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.67 (calculated-S, Kenaga 1980)
- 0.954 (calculated- K_{oc} , Kenaga 1980)

Sorption Partition Coefficient, log K_{oc} :

- 2.24 (soil, Abernethy & Davidson 1971; Davidson & McDougal 1973; Savage & Wauchope 1974; Carringer et al. 1975; Wood & Davidson 1975)
- 2.30 (soil, Kenaga 1980)
- 2.57 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 1.82 (soil, converted from reported K_{om} multiplied by 1.724, Briggs 1981)
- 2.30 (calculated-MCI χ , Gerstl & Helling 1987)
- 2.00 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.46–2.08 (Montgomery 1993)
- 2.00 (estimated-chemical structure, Lohninger 1994)
- 1.49–2.07 (Tomlin 1994)
- 2.00 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 2.33; 2.66., 2.03, 2.64, 2.36, 1.94 (quoted lit., calculated- K_{ow} ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
- 2.14, 2.51 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = (11 \pm 2 \text{ h})$ in 10 ppm aqueous solutions under summer sunlight of 9.1 h/d exposure and $t_{1/2} = (33 \pm 16) \text{ h}$ under spring sunlight of 3.7 h/d exposure (Burkhard et al. 1975).

Oxidation:

Hydrolysis: $t_{1/2} = 1.6 \text{ yr}$ at 20°C and pH 1, $t_{1/2} = 2.4 \text{ yr}$ at pH 5, and $t_{1/2} = 2.8 \text{ yr}$ at pH 9 (Montgomery 1993).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 730\text{--}1010 \text{ d}$ at pH 5–9 and 20°C in aqueous solutions (Herbicide Handbook 1989).

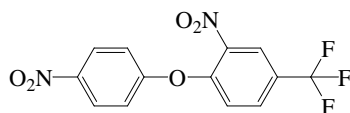
Ground water:

Sediment:

Soil: measured dissipation rate $k = 0.023\text{--}0.043 \text{ d}^{-1}$ (Horowitz & Herzlinger 1974: quoted, Nash 1988); estimated dissipation rate $k = 0.0012$, and 0.011 d^{-1} (Nash 1988); persistence of 4 months in soil (Wauchope 1978); selected field $t_{1/2} = 85 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996); soil $t_{1/2} = 30 \text{ d}$ (Pait et al. 1992); median $t_{1/2} \sim 30 \text{ d}$ in soil (Herbicide Handbook 1989; Tomlin 1994).

Biota:

17.1.1.40 Fluorodifen



Common Name: Fluorodifen

Synonym: Preforan, Soyex

Chemical Name: 4-nitrophenyl α,α,α -trifluoro-2-nitro-*p*-tolyl ether

Uses: herbicide.

CAS Registry No: 15457-05-3

Molecular Formula: $C_{13}H_7F_3N_2O_5$

Molecular Weight: 328.200

Melting Point ($^{\circ}C$):

94 (Spencer 1982; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

282.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.210 (mp at $94^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2.0 ($20^{\circ}C$, Spencer 1973, 1982)

< 2.0 (Weber et al. 1980)

2.0 (shake flask-HPLC, Ellgehausen et al. 1981)

2.0 ($20^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

9.33×10^{-6} ($20^{\circ}C$, Spencer 1982)

Henry's Law Constant (Pa- m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.30 (shake flask-HPLC, Ellgehausen et al. 1980; Geyer et al. 1991)

4.40 ($20 \pm 2^{\circ}C$, shake flask-UV, Briggs 1981)

3.65 (shake flask-HPLC, Ellgehausen et al. 1981)

3.60 (HPLC-RT correlation, Nandihalli et al. 1993)

3.65 (recommended, Sangster 1993)

3.65 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.019 (algae, $\log BF$ -bioaccumulation factor, Ellgehausen et al. 1980)

2.386 (catfish, $\log BF$ -bioaccumulation factor, Ellgehausen et al. 1980)

1.178 (daphnids, $\log BF$ -bioaccumulation factor, Ellgehausen et al. 1980)

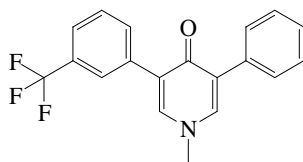
Sorption Partition Coefficient, $\log K_{oc}$:

3.13 (calculated-MCI χ , Gerstl & Helling 1987)

Environmental Fate Rate Constants, k , or Half-Lives. $t_{1/2}$:

Half-Lives in the Environment:

17.1.1.41 Fluridone



Common Name: Fluridone

Synonym: Brake, EL-171, Fluridon, Pride, Sonar

Chemical Name: 1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl] 4(1H)-pyridinone; 1-methyl-3-phenyl-5-(α,α,α -trifluorom-tolyl)-4-pyridone

Uses: herbicide to control annual grass and broadleaf weeds and certain perennial species in cotton; also used to control aquatic weeds and plants in lakes, ponds, ditches, etc.

CAS Registry No: 59756-60-4

Molecular Formula: $C_{19}H_{14}F_3NO$

Molecular Weight: 329.315

Melting Point ($^{\circ}C$):

155 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

333.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

12.3 (pK_b , Wauchope et al. 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0530 (mp at $155^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

12.0 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

12.0 (Kenaga 1980)

12.0 (Herbicide Handbook 1983, 1989; Budavari 1989; Milne 1995)

12.0 (Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)

10.0 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

10.0 (selected, Lohninger 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.31×10^{-5} ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

1.00×10^{-5} (Herbicide Handbook 1983)

0.013 (Hartley & Kidd 1987; Worthing & Hance 1991)

1.33×10^{-5} (Herbicide Handbook 1989)

1.33×10^{-5} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.30×10^{-5} (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

3.59×10^{-4} ($20^{\circ}C$, calculated-P/C, Muir 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.87 (Reinert 1989)

1.87 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)

2.98 (shake flask, Takahashi et al. 1993; quoted, Sangster 1993)

3.16 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

- 2.18 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 0.778 (measured, West et al. 1983; quoted, Isensee 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 1.60 (soil, Kenaga 1980)
 2.97–3.39 (pond sediment, Muir et al. 1980)
 3.36, 2.95 (lake and river sediment, Muir et al. 1980)
 2.94 (Reinert 1989)
 2.90, 3.81, 3.03 (Norfolk sand pH 6.0, Norfolk with montmorillonite pH 5.9, Norfolk sand with added organic matter pH 5.3, Reinert 1989)
 3.43, 2.57, 2.43 (California soil at pH 6, 7, 7.3, Reinert 1989)
 3.00 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 3.00 (selected, Lohninger 1994)
 2.85 (soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2}$ = 10,000 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: $t_{1/2}$ ~ 23 h to degrade in distilled water under > 290 nm light (West et al. 1979; quoted, Cessna & Muir 1991);

$t_{1/2}$ ~ 6 h for 5 µg/mL to degrade in nonsterile pond water under sunlight (Muir & Grift 1982; quoted, Cessna & Muir 1991);

$t_{1/2}$ = 27 d for 85% of 10 µg/mL to degrade in distilled water and for 85% of 10 µg/mL to degrade in lake water at pH 8.4 both under sunlight (Sanders & Mosier 1983; quoted, Cessna & Muir 1991; Howard et al. 1991)

resistance to decomposition by UV light with $t_{1/2}$ = 23 h in deionized water (Herbicide Handbook 1989).

Oxidation: photooxidation $t_{1/2}$ = 0.359–3.20 h, based on estimated rate constant for reaction with hydroxyl radicals (Atkinson 1987; quoted, Howard et al. 1991) and ozone (Atkinson & Carter 1984; quoted, Howard et al. 1991).

Hydrolysis: $t_{1/2}$ > 113 d for 1 µg/mL to hydrolyze in pond water at 4°C (Ghassemi et al. 1981; quoted, Muir 1991); $t_{1/2}$ = 23 h in water (Tomlin 1994).

Biodegradation: aqueous aerobic $t_{1/2}$ = 44–192 d, based on soil die-away test data and field study soil persistence (Banks et al. 1979; quoted, Howard et al. 1991);

$t_{1/2}$ = 12 months for 5 µg/mL to biodegrade in static sediment and water, and $t_{1/2}$ ~ 9 months in aerobic and anaerobic sediment and water all at 25°C (Muir & Grift 1982; quoted, Muir 1991);

aqueous anaerobic $t_{1/2}$ = 176 d to 2.1 yr, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

microbial degradation $t_{1/2}$ > 343 d at pH 7.3 with 2.6% organic matter in a silt loam soil (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 0.9–1.3 h⁻¹ (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 0.70–5.6 h⁻¹ (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 1.7–3.40 h⁻¹ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

k_1 = 1.7–2.1 h⁻¹ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

k_2 = 0.052 h⁻¹ (*Chironomus tentans* larvae in pond sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.118 h⁻¹ (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)

k_2 = 0.055 h⁻¹ (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.041 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.359\text{--}3.20 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radicals (Atkinson 1987; quoted, Howard et al. 1991) and ozone (Atkinson & Carter 1984; quoted, Howard et al. 1991).

Surface water: $t_{1/2} \sim 21 \text{ d}$ in water (Hartley & Kidd 1987);

$t_{1/2} = 288\text{--}864 \text{ h}$, based on estimated photolysis half-life in water (Howard et al. 1991);

anaerobic $t_{1/2} = 9 \text{ months}$ and aerobic $t_{1/2} \sim 20 \text{ d}$ (Tomlin 1994).

Ground water: $t_{1/2} = 2112\text{--}9216 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} = 12 \text{ months}$ for $5 \mu\text{g/mL}$ to biodegrade in static sediment and water, and $t_{1/2} \sim 9 \text{ months}$ in aerobic and anaerobic sediment and water all at 25°C (Muir & Grift 1982; quoted, Muir 1991).

Soil: measured dissipation rate $k = 0.0041 \text{ d}^{-1}$ (Banks et al. 1979; quoted, Nash 1988) with estimated $t_{1/2} = 44\text{--}192 \text{ d}$ (Banks et al. 1979; quoted, Howard et al. 1991);

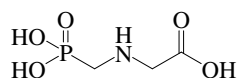
estimated dissipation rate $k = 0.0067 \text{ and } 0.025 \text{ d}^{-1}$ (Nash 1988);

selected field $t_{1/2} = 21 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} \sim 90 \text{ d}$ in the hydrosol (Tomlin 1994).

Biota: elimination $t_{1/2} = 13.2 \text{ h}$ in pond sediment-water, $t_{1/2} = 5.9 \text{ h}$ in river water, $t_{1/2} = 12.5 \text{ h}$ in river sediment-water, $t_{1/2} = 16.9$ in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

17.1.1.42 Glyphosate



Common Name: Glyphosate

Synonym: Mon-0573, 0468, 2139; Polado, Roundup

Chemical Name: *N*-(phosphoromethyl)glycine

Uses: nonselective, post-emergent, broad spectrum herbicide to control annual and perennial grasses, sedges, broadleaf, and emerged aquatic weeds; also used to control insects on fruit trees.

CAS Registry No: 1071-83-6

Molecular Formula: $C_3H_8NO_3P$

Molecular Weight: 169.074

Melting Point ($^{\circ}C$):

230 (dec., Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.74 (Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

5.70 (Worthing & Hance 1991)

2.60, 5.90, 10.40 (pK_1 , pK_2 , pK_3 , Yao & Haag 1991; Haag & Yao 1992)

2.32, 5.86, 10.86 (pK_1 , pK_2 , pK_3 , Montgomery 1993; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F : 0.0097 (mp at $230^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

10000 (Spencer 1973, 1982; Herbicide Handbook 1978; Ashton & Crafts 1981)

12000 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)

15700 (Herbicide Handbook 1989)

12000 (Budavari 1989; Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

2.59×10^{-5} ($45^{\circ}C$, Herbicide Handbook 1989)

4.00×10^{-5} (Worthing & Hance 1991)

0.001 (Montgomery 1993; quoted, Majewski & Capel 1995)

negligible (Tomlin 1994)

0.0 (selected, Halfon et al. 1996)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1.41×10^{-5} (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

-1.70 (shake flask, pH 5.3, Martin & Edgington 1981)

-4.10 (shake flask, pH 2.5, Stevens et al. 1988)

-3.25 (Reinert 1989)

-4.59 (Worthing & Hance 1991)

-1.60 (Montgomery 1993)

-4.10, -1.70 (pH 2.5, pH 5.3, quoted, Sangster 1993)

-1.70 (pH 5.3, selected, Hansch et al. 1995)

0.94 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

0.477	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
2.26	(calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

3.42	(soil, Sprankle et al. 1975; Hance 1976; Nomura & Hilton 1977)
1.40	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.22	(selected, USDA 1989; quoted, Neary et al. 1993)
-0.43	(Reinert 1989)
3.69, 3.53, 3.42	(3 agricultural soils: Houston clay loam at pH 7.5, Muskingum silt loam at pH 5.8, Sassafras sandy loam at pH 5.6, Reinert 1989)
4.38	(organic carbon, Wauchope et al. 1991)
3.43–3.69	(Montgomery 1993)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 48$ h for 0% of 168 $\mu\text{g/mL}$ to degrade in distilled water under > 290 nm light (Rueppel et al. 1977; quoted, Cessna & Muir 1991);
 $t_{1/2} = 9$ wk for $> 90\%$ of 2 $\mu\text{g/mL}$ to degrade in distilled water under sunlight (Lund-Høie & Friestad 1986; quoted, Cessna & Muir 1991);
 $t_{1/2} = 4.0$ d and 3–4 wk for aqueous solutions of 1.0 and 2000 ppm under indoor UV light (Lund-Høie & Friestad 1986; quoted, Montgomery 1993).

Oxidation:

$k(\text{aq.}) = 7.3 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to glycolic acid) with hydroxyl radical in aqueous solutions at pH 3.8 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
 $k(\text{aq.}) = (0.027\text{--}8.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.8–7.0 and $22 \pm 2^\circ\text{C}$, with a half-life of 4.0 s at pH 7 (Yao & Haag 1991).
 $k(\text{aq.}) = (1.8 \pm 0.5) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to glycolic acid) with hydroxyl radical in aqueous solutions at pH 3.8 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992).

Hydrolysis: $t_{1/2} = 7$ d for 10 $\mu\text{g/mL}$ to hydrolyze in sterile water + soil (Rueppel et al. 1977; quoted, Muir 1991);
 $t_{1/2} = 32$ d for 25 and 250 $\mu\text{g/mL}$ to hydrolyze in sterile distilled water at pH 3, 6 and 9 in the dark at 5 and 35°C (Ghassemi et al. 1981; quoted, Muir 1991)

Biodegradation: $t_{1/2} < 28$ d for 10 $\mu\text{g/mL}$ to biodegrade in soil-water suspension (Rueppel et al. 1977; quoted, Muir 1991);

$t_{1/2} > 9$ wk for 2 $\mu\text{g/mL}$ to biodegrade in polluted lake water (Rueppel et al. 1977; quoted, Muir 1991);
rate constant $k = 0.1 \text{ d}^{-1}$ from soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
 $t_{1/2} = 70$ d in pond water at pH 7.2, $t_{1/2} = 63$ d in swamp water at pH 6.3 and $t_{1/2} = 49$ d in Sphagnum bog water at pH 4.2 (Ghassemi et al. 1981; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} > 9$ wk for 2 $\mu\text{g/mL}$ to biodegrade in polluted lake water (Rueppel et al. 1977; quoted, Muir 1991);
 $t_{1/2} = 70$ d in pond water at pH 7.2, $t_{1/2} = 63$ d in swamp water at pH 6.3 and $t_{1/2} = 49$ d in Sphagnum bog water at pH 4.2 (Ghassemi et al. 1981; quoted, Muir 1991);
measured rate constant $k = (0.027 - 8.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.8–7.0 and $22 \pm 2^\circ\text{C}$, with $t_{1/2} = 4.0$ s at pH 7 (Yao & Haag 1991).

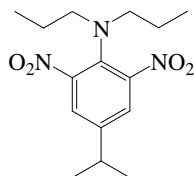
Ground water:

Sediment:

Soil: $t_{1/2} < 28$ d for 10 $\mu\text{g/mL}$ to biodegrade in soil-water suspension (Rueppel et al. 1977; quoted, Muir 1991); estimated first-order $t_{1/2} = 7$ d from biodegradation rate constant $k = 0.1 \text{ d}^{-1}$ from soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982); moderately persistent in soil with $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982); average $t_{1/2} < 60$ d (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993); selected $t_{1/2} = 47$ d (Wauchope et al. 1991; quoted, Dowd et al. 1993; Halfon et al. 1996).

Biota: average $t_{1/2} = 60$ d in the forest (USDA 1989; quoted, Neary et al. 1993).

17.1.1.43 Isopropalin



Common Name: Isopropalin

Synonym: EL 179, Isopropaline, Isopropalin solution, Paarlan

Chemical Name: 4-(1-methylethyl)-2,6-dinitro-*N,N*-dipropylaniline; 4-(1-methylethyl)-2,6-dinitro-*N,N*-dipropylbenzenamine; 2,6-dinitro-*N,N*-dipropylcumidine

Uses: herbicide used pre-planting and incorporated with soil preparation to control broadleaf weeds and grasses in transplanted tobacco, and in direct-seeded tomatoes and capsicums.

CAS Registry No: 33820-53-0

Molecular Formula: $C_{15}H_{23}N_3O_4$

Molecular Weight: 309.362

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

361.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.11	(Martin & Worthing 1977; Herbicide Handbook 1978)
1.10	(Ashton & Crafts 1981)
0.10	(Spencer 1982; Hartley & Kidd 1987; Budavari 1989; Milne 1955)
0.10	(Worthing & Walker 1987, Worthing & Hance 1991)
0.08	(Herbicide Handbook 1989)
0.10	(20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.02	(predicted-AQUAFAC, Lee et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0019	($30^{\circ}C$, Ashton & Crafts 1981)
0.0019	($30^{\circ}C$, Hartley & Kidd 1987)
0.0040	($25.6^{\circ}C$, Herbicide Handbook 1989)
0.0012	(20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.34	(calculated-P/C, this work)
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Octanol/Water Partition Coefficient, $\log K_{ow}$:

Bioconcentration Factor, $\log BCF$:

3.50	(calculated-S, Kenaga 1980; quoted, Isensee 1991)
3.88	(calculated- K_{oc} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

4.88	(soil, Harvey 1974)
4.17	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
4.17–4.88	(soil, quoted values, Bottoni & Funari 1992)

4.00	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
4.00	(selected, Lohninger 1994)
3.50	(soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmosphere photolysis $t_{1/2} = 288\text{--}864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); aqueous photolysis $t_{1/2} = 288\text{--}864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 0.743\text{--}74.3$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Abiotic Transformation: Degradation by abiotic reductive transformations:

$k = 1.71 \text{ M}^{-1} \text{ s}^{-1}$ in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 0.94 \times 10^{-3} \text{ h}^{-1}$ at pH 6.5, $k = 0.36 \times 10^{-2} \text{ h}^{-1}$ at pH 7.0, $k = 0.057 \text{ h}^{-1}$ at pH 7.4, and $k = 1.76 \text{ h}^{-1}$ at pH 7.8 for aqueous ferrous ion system;

$k = 0.297 \text{ h}^{-1}$ at pH 6.5, $k = 0.586 \text{ h}^{-1}$ at pH 6.7, $k = 1.28 \text{ h}^{-1}$ at pH 7.0, and $k = 6.90 \text{ h}^{-1}$ at pH 7.3 for Fe(II)/goethite system;

$k = 9.91 \times 10^{-3} \text{ h}^{-1}$ at pH 6.5, $k = 8.45 \times 10^{-3} \text{ h}^{-1}$ at pH 7.0, $k = 7.45 \times 10^{-3} \text{ h}^{-1}$ at pH 7.4 and $k = 6.96 \times 10^{-2} \text{ h}^{-1}$ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 408\text{--}2520$ h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 96\text{--}360$ h, based on anaerobic soil die-away test that tested one soil (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.743\text{--}74.3$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 288\text{--}864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 96\text{--}5040$ h, based on estimated unacclimated aqueous aerobic and anaerobic degradation half-lives (Howard et al. 1991)
reported $t_{1/2} < 180$ d (Bottoni & Funari 1992)

Sediment:

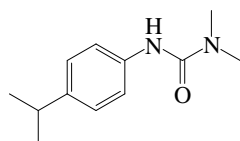
Soil: $t_{1/2} = 408\text{--}2520$ h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991);

selected field $t_{1/2} = 100$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} < 180$ d (Bottoni & Funari 1992).

Biota:

17.1.1.44 Isoproturon



Common Name: Isoproturon

Synonym: Alon, Arelon, CGA 18731, Gramion, Graminon, Hoe 16410, Hytane, IP 50, IP flo, Tolkan

Chemical Name: 3-(4-isopropylphenyl)-1,1-dimethylurea; 3-*p*-cumenyl-1,1-dimethylurea

Uses: herbicide used for pre- and post-emergence control of annual grasses and broadleaf weeds in spring and winter wheat (except durum wheat), spring and winter barley, winter rye, and triticale.

CAS Registry No: 34123-59-6

Molecular Formula: C₁₂H₁₈N₂O

Molecular Weight: 206.284

Melting Point (°C):

155–156 (Worthing & Hance 1991)

158 (Tomlin 1994)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.16 (Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm³/mol):

259.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

60 (Martin & Worthing 1977)

70 (20°C, Spencer 1982)

72 (20°C, Hartley & Kidd 1987)

55 (Worthing & Walker 1987, Worthing & Hance 1991)

55.9 (Chaumat et al. 1991)

65 (22°C, Tomlin 1994; quoted, Otto et al. 1997)

65 (20°C, selected, Traub-Eberhard et al. 1994)

Vapor Pressure (Pa at 25°C or as indicated):

3.3 × 10⁻⁶ (20°C, Spencer 1982; Hartley & Kidd 1987)

3.3 × 10⁻⁶ (20°C, Worthing & Hance 1991)

3.3 × 10⁻⁶, 3.15 × 10⁻², 0.172 (20, 77, 150°C, Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

1.05 × 10⁻⁵ (calculated-P/C, Otto et al. 1997)

1.24 × 10⁻⁵ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} at 25°C or as indicated:

2.87 (shake flask, Log P Database, Hansch & Leo 1987)

2.25 (Worthing & Hance 1991)

2.30 (shake flask, pH 7, Baker et al. 1992)

2.537 (calculated, Evelyne et al. 1992)

2.30 (Behrendt & Bruggemann 1993)

2.87 (recommended, Sangster 1993)

2.87 (recommended, Hansch et al. 1995)

- 2.50 (pH 7, 22°C, Tomlin 1994)
 2.40 (quoted Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:

- 1.79 (calculated-S, Kenaga 1980)
 1.76, 1.82 (cuticle/water: tomato, pepper; Chaumat et al. 1991)
 1.71, 1.90 (cuticle/water: box tree, pear; Chaumat et al. 1991)
 1.52, 1.20 (cuticle/water: ivy, vanilla; Chaumat et al. 1991)
 1.76, 1.82 (cuticle/water: tomato, pepper; Evelyne et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

- 2.66 (soil, calculated-S, Kenaga 1980)
 1.86 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993)
 2.11 (soil, quoted from Kördel et al. 1993, Traub-Eberhard et al. 1994)
 1.86; 2.40 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 2.57, 1.71, 1.78, 1.73, 2.34 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
 1.86, 2.31; 2.81, 2.24, 2.83, 2.35, 1.93 (quoted lit., calculated- K_{OW} ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
 2.155, 1.918, 1.790, 1.719, 2.367 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 1999)
 2.155, 1.918, 1.790, 1.719, 2.367 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
 1.78, 2.10 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmosphere photolysis $t_{1/2} = 288\text{--}864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991);

aqueous photolysis $t_{1/2} = 288\text{--}864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991);

$t_{1/2} = 1.5$ h for 215 $\mu\text{g/mL}$ to degrade in distilled water under 254 nm light (Kulshrestha & Mukerjee 1986; quoted, Cessna & Muir 1991).

Oxidation: photooxidation $t_{1/2} = 0.743\text{--}74.3$ h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 408\text{--}2520$ h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}360$ h, based on anaerobic soil die-away test which tested one soil (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991)

Biotransformation: ~ 11% of a selection of 90 strains of micromycetes mostly isolated from soil-soil fungi, depleted over 50% of isoproturon (100 mg/L) in 5-d experiment (Vroumsia et al. 1996)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.743\text{--}74.3$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

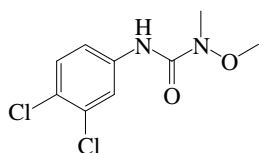
Surface water: $t_{1/2} = 288\text{--}864$ h, based on observed photolysis on soil TLC plates under summer sunlight (Helling 1976; quoted, Howard et al. 1991) and adjusted for relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 96\text{--}5040$ h, based on estimated unacclimated aqueous aerobic and anaerobic degradation half-lives (Howard et al. 1991)
 reported half-lives or persistence, $t_{1/2} = 12\text{--}29$ and 60–120 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 408\text{--}2520$ h, based on aerobic soil die-away test data for one soil at 15°C and 30°C (Gingerich & Zimdahl 1976; quoted, Howard et al. 1991);
reported $t_{1/2} = 12\text{--}29$ d and 60–120 d (Bottoni & Funari 1992);
 $t_{1/2} = 15\text{--}21$ d in sandy loam, $t_{1/2} = 11$ d in silt loam at 20°C (Traub-Eberhard et al. 1994)
Degradation and mineralization $t_{1/2} = 16$ d, 24 d and 34 d for pelosol, brown calcareous soil and brown acid soil, respectively, over 120 days under controlled laboratory conditions (Pieuchot et al. 1996)
estimated $t_{1/2} \sim 14.6$ d under conventional tillage, $t_{1/2} = 7.99$ d under ridge tillage and $t_{1/2} = 12.17$ d with no tillage (Otto et al. 1997).

17.1.1.45 Linuron



Common Name: Linuron

Synonym: Afalon, Cephalon, Garnitan, Herbicide 326, Hoe 2810, Linex 4L, Linorox, Linurex, Lorox, Methoxydiuron, Premalin, Scarclex, Sinuron

Chemical Name: 3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea; *N'*-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methylurea

Uses: selective pre-emergence and post-emergence herbicide used on a wide variety of food crops to control many annual broadleaf and grass weeds.

CAS Registry No: 330-55-2

Molecular Formula: $C_9H_{10}Cl_2N_2O_2$

Molecular Weight: 249.093

Melting Point ($^{\circ}C$):

93 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

232.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

90.23 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.66 (DSC method, Plato & Glasgow 1969)

25.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.215 (mp at $93^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

75 (Woodford & Evans 1963; Bailey & White 1965; Hartley & Graham-Bryce 1980; Kenaga 1980; Kenaga & Goring 1980; Beste & Humburg 1983)

75 (Melnikov 1971; Spencer 1973, 1982; Wauchope 1978; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Briggs 1981)

75 (Martin & Worthing 1977; Worthing & Walker 1983, 1987; Herbicide Handbook 1978, 1989)

81 (Hartley & Kidd 1987; Milne 1995)

81 ($24^{\circ}C$, Worthing & Hance 1991)

75 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

75–81 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00147 ($20^{\circ}C$, Quellette & King 1977)

0.0012 ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

0.002 ($24^{\circ}C$, Khan 1980)

0.002 (20 – $25^{\circ}C$, Weber et al. 1980)

0.002 ($24^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

0.0014 ($20^{\circ}C$, selected, Suntio et al. 1988)

3.50×10^{-4} , 1.10×10^{-2} , 0.22, 2.90, 28.0 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 16.074 - 5824.2/(T/K)$; measured range 40.5 – $92^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 12.989 - 4713.7/(T/K)$; measured range 92.7 – $160^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

0.0011 ($20^{\circ}C$, selected, Taylor & Spencer 1990)

0.0023 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0027 (selected, Halfon et al. 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.0054 (20°C , calculated-P/C, Suntio et al. 1988)
 0.004 (Taylor & Glotfelty 1988)
 0.0062 ($20\text{--}25^\circ\text{C}$, calculated-P/C, Montgomery 1993)
 0.00465 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.19 (Briggs 1969)
 3.20 (shake flask-UV, Erkell & Walum 1979)
 2.76 (shake flask-UV, Briggs 1981)
 3.11 (shake flask, Mitsutake et al. 1986)
 2.48 (selected, Gerstl & Helling 1987)
 3.00 (Worthing & Hance 1991; Milne 1995)
 2.19, 3.00 (Montgomery 1993)
 2.75 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
 3.20 (recommended, Sangster 1993)
 3.20 (recommended, Hansch et al. 1995)
 3.18 (Pomona-database, Müller & Kördel 1996)
 2.75 (RP-HPLC-RT correlation, Finizio et al. 1997)
 2.72 (RP-HPLC-RT correlation, Yu et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

1.73 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 1.68 (calculated- K_{OC} , Kenaga 1980)
 1.73 (calculated, Pait et al. 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.91 (soil, Hamaker & Thompson 1972)
 2.61 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 2.93 (average soils/sediments, Rao & Davidson 1980)
 2.43 (soil, converted form reported K_{OM} multiplied by 1.724, Briggs 1981)
 2.93, 2.80, 1.80 (estimated-S, calculated-S and mp, calculated- K_{OW} , Karickhoff 1981)
 3.83 (Means & Wijayarathne 1982)
 2.99, 2.58; 2.62, 2.80 (estimated- K_{OW} , S, Madhun et al. 1986)
 2.76, 2.64 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
 2.94 (screening model calculations, Jury et al. 1987b)
 2.61–2.91, 2.83, 2.93 (soil, quoted values, Bottoni & Funari 1992)
 2.60 (soil, $20\text{--}25^\circ\text{C}$, selected, Wauchope et al. 1992;)
 2.70–2.78 (Montgomery 1993)
 2.59 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a)
 2.59 (soil, HPLC-screening method, Kördel et al. 1993, 1995b)
 2.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.59; 2.54 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.28, 2.39, 2.46, 2.29, 3.12 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
 2.884, 2.58, 2.45, 1.33, 3.18 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
 2.884, 2.578, 2.450, 2.336, 3.183 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
 2.70; 2.55, 2.61 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 2.65, 2.64 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, average, Delle Site 2001)

2.78 (average values for sediment OC $\geq 0.5\%$, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 2$ months for 31% of $55 \mu\text{g mL}^{-1}$ to degrade in distilled water under sunlight (Rosen et al. 1969; quoted, Cessna & Muir 1991);

$t_{1/2} = 2.25$ h for 67–75% of $75 \mu\text{g mL}^{-1}$ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

atmosphere photolysis $t_{1/2} = 1344\text{--}4032$ h, based on measured rate constant for summer sunlight photolysis in distilled water (Rosen et al. 1969; quoted, Howard et al. 1991) and adjusted to relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991); aqueous photolysis $t_{1/2} = 1344\text{--}4032$ h, based on measured rate constant for summer sunlight photolysis in distilled water (Rosen et al. 1969; quoted, Howard et al. 1991) and adjusted to relative winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 0.49\text{--}4.90$ h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $t_{1/2} > 4$ months for $4980 \mu\text{g mL}^{-1}$ to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-dib & Aly 1976; quoted, Muir 1991).

Biodegradation: $t_{1/2} = 78$ d in soil (Moyer et al. 1972; quoted, Means et al. 1983),

$t_{1/2} = 87$ d in soil (Hance 1974; quoted, Means et al. 1983),

$t_{1/2} = 58$ and 180 d in soil (Urosol & Hance 1974; quoted, Means et al. 1983);

aqueous aerobic $t_{1/2} = 672\text{--}4272$ h, based on soil die-away test data (Walker 1978; Walker & Zimdahl 1981; quoted, Howard et al. 1991);

rate constant $k = 0.0096 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

aerobic $t_{1/2} \sim 40$ d for $1 \mu\text{g mL}^{-1}$ to biodegrade in lake sediment and $t_{1/2} \sim 60$ d for $4 \mu\text{g mL}^{-1}$ to biodegrade in lake sediment and water (Huber & Gemes 1981; quoted, Muir 1991);

aerobic $t_{1/2} \sim 20$ d for $0.22 \mu\text{g mL}^{-1}$ to biodegrade in pond sediment plus aerobic salts medium of 34 g L^{-1} (Stepp et al. 1985; quoted, Muir 1991);

aqueous anaerobic $t_{1/2} = 2688\text{--}17088$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

degradation rate constant $k = (3.48 \pm 0.156) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 19.9$ d in control soil and $k = (23.2 \pm 2.07) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 2.99$ d in pretreated soil in the field; $k = (3.73 \pm 0.208) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 18.6$ d in control soil and $k = (18.8 \pm 2.76) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 3.68$ d in pretreated soil once only in the laboratory (Walker & Welch 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.49\text{--}4.90$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 672\text{--}4272$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}8544$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

reported half-lives or persistence, $t_{1/2} = 38\text{--}69$ and 75 d (Bottoni & Funari 1992).

Sediment: degradation $t_{1/2} = 12$ d in estuarine sediment ($12^\circ/\infty$) system (Cunningham et al. 1981; quoted, Means et al. 1983);

degradation $t_{1/2} = 6$ d in estuarine sediment ($18^\circ/\infty$) system (Means et al. 1983).

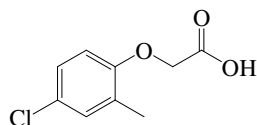
Soil: estimated persistence of 4 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

$t_{1/2} = 672\text{--}4272$ h, based on soil die-away test data (Walker 1978; Walker & Zimdahl 1981; quoted, Howard et al. 1991);

persistence of 4 months (Wauchope 1978);

correlated $t_{1/2} = 57$ d at pH 5.1–5.8, $t_{1/2} = 22$ d at pH 6.3–7.0 and $t_{1/2} = 19$ d at pH 7.7–8.2 (Boddington Barn soil, Hance 1979) and $t_{1/2} = 67$ d at pH 4.6–5.2, $t_{1/2} = 53$ d at pH 5.3–6.1, and $t_{1/2} \sim 20$ d at pH 6.3–8.0 (Triangle soil, Hance 1979);
estimated first-order $t_{1/2} = 72$ d from biodegradation rate constant $k = 0.0096 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);
decomposition $t_{1/2} = 11$ d in fresh soil and $t_{1/2} = 12$ d in air dried soil both in polyethylene bags, $t_{1/2} = 49$ d in undisturbed cores and $t_{1/2} = 40$ d in perfusion (Hance & Haynes 1981);
moderately persistent in soil with $t_{1/2} = 20$ –100 d (Willis & McDowell 1982);
 $t_{1/2} = 2$ to 5 months under field conditions (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993);
 $t_{1/2} = 75$ d from screening model calculations (Jury 1987b);
 $t_{1/2} = 60, 35, 35, 30$ d in plots treated, i.e., repeated application of pesticide, for the first, second, third and fourth time, respectively, in the field; in the laboratory $t_{1/2}$ reduced from 19 d to 3–7 d in a single pretreatment in moist soil at 20°C (Walker & Welch 1991)
reported $t_{1/2} = 38$ –69 d and 75 d (Bottoni & Funari 1992);
selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; quoted, Halfon et al. 1996; Hornsby et al. 1996);
soil $t_{1/2} = 60$ d (Pait et al. 1992);
soil $t_{1/2} = 29$ –67 d (Di Guardo et al. 1994).
Biota: biochemical $t_{1/2} = 75$ d from screening model calculations (Jury et al. 1987b).

17.1.1.46 MCPA



Common Name: MCPA

Synonym: Agritox, Agroxohe, Agroxone, Anicon Kombi, Bordermaster, Chiptox, Chwastox, Cornox, Ded-weed, Dicopur-M, Dicotex, Dikotes, Emcepan, Empal, Hedapur M 52, Hederax M, Herbicide M, Hedonal, Hormotuho, Kilsem, Krezone, Legumex DB, Leuna M, Leyspray, Linormone, MCP, metaxon, Methoxone, Netazol, Okultin M, Phenoxyline Plus, Raphone, Razol dock killer, Rhomenc, Rhonox, Shamrox, Seppic MMD, Trasan, Ustinex, Vacate, Verdone, Weedar, Weed-rhap, Zelan

Chemical Name: (4-chloro-2-methylphenoxy)acetic acid; 4-chloro-*o*-tolylxyacetic acid

Uses: systemic post-emergence herbicide to control annual and perennial weeds in cereals, rice, flax, vines, peas, potatoes, asparagus, grassland and turf.

CAS Registry No: 94-74-6

Molecular Formula: $C_9H_9ClO_3$

Molecular Weight: 200.618

Melting Point ($^{\circ}C$):

120 (Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.56 ($25^{\circ}C$, Que Hee et al. 1981; Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

211.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

3.05 (potentiometric titration, Nelson & Faust 1969)

3.125 (Cessna & Grover 1978)

3.07 (Worthing & Hance 1991)

3.05–3.13 (Montgomery 1993)

3.12 (Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.117 (mp at $120^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1605 (shake flask-UV, Leopold et al. 1960)

1605 (Bailey & White 1965)

< 1000 (Khan 1980)

630 ($20^{\circ}C$, Melnikov 1971)

825 (Martin & Worthing 1977; Weber et al. 1980; Milne 1995)

1500 (selected, Seiber et al. 1986)

825 (room temp., Hartley & Kidd 1987; Worthing & Hance 1991)

817 (selected, Gerstl & Helling 1987)

835 (room temp., Worthing & Walker 1987)

730–825 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

7.9×10^{-4} (measured-volatilization rate, Seiber et al. 1986)

2.0×10^{-4} ($20^{\circ}C$, Hartley & Kidd 1987)

2.0×10^{-4} ($21^{\circ}C$, Worthing & Walker 1987, 1991)

2.3×10^{-5} ($20^{\circ}C$, Tomlin 1994)

2.0×10^{-4} ($20^{\circ}C$, Milne 1995)

2.0×10^{-4} (selected, Halfon et al. 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 1.0×10^{-4} (calculated-P/C, Seiber et al. 1986)
- 4.86×10^{-4} (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
- < 0.010 (estimated, Mabury & Crosby 1996)
- 2.5×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.69 (selected, Dao et al. 1983)
- 2.30 (RP-HPLC- k' correlation, Braumann et al. 1983)
- 1.41 (selected, Gerstl & Helling 1987)
- 0.57 (shake flask-UV, pH 7, Stevens et al. 1988)
- 3.25 (countercurrent LC, Ilchmann et al. 1993)
- 1.37-1.43 (calculated, Montgomery 1993)
- 0.57, 3.25 (quoted, Sangster 1993)
- 2.68 (MedChem Master file or ClogP program, Sabljic et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.15 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.04 (soil, calculated-S, Kenaga 1980; quoted, Bottoni & Funari 1992)
- 1.95 (calculated-MCI χ , Gerstl & Helling 1987)
- 2.03-2.07 (calculated, Montgomery 1993)
- 1.73 (calculated-QSAR MCI χ , Sabljic et al. 1995)
- 2.49; 1.58., 3.27, 3.17, 1.85, 2.19 (calculated- K_{OW} ; HPLC-screening method with different LC-columns, Szabo et al. 1999)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $k = 9.78 \times 10^{-7} \text{ h}^{-1}$ at pH 3.5 (Seiber et al. 1986).

Photolysis: $t_{1/2} = 71 \text{ h}$ for $< 10\%$ of $50 \mu\text{g mL}^{-1}$ to degrade in NaOH solution at pH 9.8 under $> 290 \text{ nm}$ light (Soderquist & Crosby 1975; quoted, Cessna & Muir 1991);

$t_{1/2} = 245 \text{ h}$ for 17-98.5% of $9 \mu\text{g mL}^{-1}$ to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Muir 1991);

$t_{1/2} = 4.6 \text{ d}$ for $14,700 \mu\text{g mL}^{-1}$ to degrade in droplets of spray solution suspended in air under sunlight (Freiberg & Crosby 1986; quoted, Cessna & Muir 1991).

Oxidation: degradation by ozone in dilute aqueous solutions (Benoit-Guyod et al. 1986) as follows:-

$t_{1/2} = 9.4 \text{ min}$ - dark with O_3 in air; $t_{1/2} = 8.4 \text{ min}$ - light with O_3 in air, $t_{1/2} = 500 \text{ min}$ - light, air only, at initial pH of 3.55; MCPA concn of $224 \mu\text{M L}^{-1}$, ozone input at $246 \mu\text{M h}^{-1}$;

$t_{1/2} = 10.4 \text{ min}$ - dark with O_3 in air; $t_{1/2} = 9.0 \text{ min}$ - light with O_3 in air, at initial pH of 8.0,

$t_{1/2} = 11.5 \text{ min}$ - dark with O_3 in air; $t_{1/2} = 11.3 \text{ min}$ - light with O_3 in air, at initial pH of 7.0,

$t_{1/2} = 8.4 \text{ min}$ - dark with O_3 in air; $t_{1/2} = 9.4 \text{ min}$ - light with O_3 in air, at initial pH of 7.0,

$t_{1/2} = 4.2 \text{ min}$ - dark with O_3 in air; $t_{1/2} = 4.2 \text{ min}$ - light with O_3 in air, $t_{1/2} = 150 \text{ min}$ - light, air only, at initial pH of 8.0; MCPA concn of $5 \mu\text{M L}^{-1}$, ozone input at $246 \mu\text{M h}^{-1}$;

$t_{1/2} = 176 \text{ min}$ - dark with O_3 in air; $t_{1/2} = 63 \text{ min}$ - light with O_3 in air, at initial pH of 8.0, MCPA concn of $224 \mu\text{M L}^{-1}$, ozone input at $4.6 \mu\text{M h}^{-1}$;

$t_{1/2} = 300 \text{ min}$ - dark with O_3 in air; $t_{1/2} = 162 \text{ min}$ - light with O_3 in air, at initial pH of 8.0; MCPA concn of $224 \mu\text{M L}^{-1}$, ozone input at $0.2 \mu\text{M h}^{-1}$ (Benoit-Guyod et al. 1986).

measured rate constant $k_{\text{OH}}(\text{aq.}) = 1.70 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with hydroxyl radical, in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

Hydrolysis:

Biodegradation: $t_{1/2} > 168 \text{ h}$ for $1 \mu\text{g mL}^{-1}$ to degrade in activated sludge (Schmidt 1975; quoted, Muir 1991);

aerobic $t_{1/2} \sim 9 \text{ d}$ for $1 \mu\text{g mL}^{-1}$ to degrade in natural water in absence of sunlight (Soderquist & Crosby 1975; quoted, Muir 1991);

$t_{1/2} > 12 \text{ d}$ for $0.045\text{--}0.156 \mu\text{g mL}^{-1}$ to degrade in water after application to model crop and washoff (Virtanen et al. 1979; quoted, Muir 1991);

$t_{1/2} = 15\text{--}25$ d for $10\text{ }\mu\text{g mL}^{-1}$ to degrade in flooded soils (Duah-Yentumi & Kuwatsuka 1980; quoted, Muir 1991);

first order microbial degradation $k = 0.01393\text{ d}^{-1}$ with $t_{1/2} = 50$ d at room temp, $k = 0.01687\text{ d}^{-1}$ with $t_{1/2} = 41$ d at 35°C in sandy clay soil from Finland; $k = 0.02999\text{ d}^{-1}$ with $t_{1/2} = 23$ d at room temp, $k = 0.03397\text{ d}^{-1}$ with $t_{1/2} = 20$ d at 35°C in sandy loam soil from Bangladesh (Sattar & Paasivirta 1980)

$t_{1/2} > 25$ d for $10\text{ }\mu\text{g mL}^{-1}$ to degrade in flooded soils (Ursin 1985; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: dissipation $t_{1/2} \sim 4$ d in rice field; $t_{1/2} = 17$ d in dilute aqueous solution under laboratory irradiation (Soderquist & Crosby 1975);

degradation $t_{1/2} = 4.2\text{--}300$ min by ozone and light ($\text{UV} > 300\text{ nm}$) in dilute aqueous solution, depending on pH, concn of MCPA and ozone (shake flask-GC, Benoit-Guyod et al. 1986)

degraded rapidly with $t_{1/2} = 9$ d in rice paddy water held under darkened conditions (Muir 1991)

field dissipation $t_{1/2} = 28.8$ h in water (Mabury & Crosby 1996)

Ground water: reported $t_{1/2} < 7$ and $t_{1/2} = 20\text{--}25$ d (Bottoni & Funari 1992)

Sediment: $t_{1/2} = 80$ to 400 d of MCPA at low concentrations in marine sediments (Muir 1991).

Soil: degradation $t_{1/2} = 50$ d at room temp., $t_{1/2} = 41$ d at 35°C in Finland sandy clay soil; degradation $t_{1/2} = 23$ d at room temp., $t_{1/2} = 20$ d at 35°C in Bangladesh loam soil from first-order rate constant obtained by linear regression (Sattar & Paasivirta 1980);

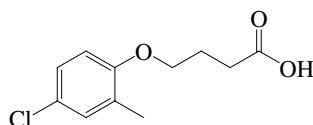
persistence of 3 months in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2} = 25$ d in flooded soils (Muir 1991);

$t_{1/2} = 15$ d (selected, Halfon et al. 1996).

Biota:

17.1.1.47 MCPB



Common Name: MCPB

Synonym: Bexane, Can-Trol, Legumex, Thistrol, Thitrol, Triflex, Tropotox

Chemical Name: 4-(4-chloro-2-methylphenoxy)butanoic acid; 4-(4-chloro-2-methylphenoxy)-butyric acid

Uses: herbicide for post-emergence control of annual and perennial broadleaf weeds in cereals, clovers, sainfoin, groundnuts, peas, etc. and also used to control broadleaf and woody weeds in forestry.

CAS Registry No: 94-81-5

Molecular Formula: $C_{11}H_{13}ClO_3$

Molecular Weight: 228.672

Melting Point ($^{\circ}C$):

100 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

> 280 (Tomlin 1994)

Density (g/cm^3 at $22^{\circ}C$):

1.254 (Tomlin 1994)

Molar Volume (cm^3/mol):

255.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

4.80 (potentiometric titration, Nelson & Faust 1969)

4.84 (Worthing & Hance 1991; Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

34.31 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.184 (mp at $100^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

41 (shake flask-UV, Leopold et al. 1960)

44 (rm. temp., Melnikov 1971)

44 (Bailey & White 1965; Martin & Worthing 1977; Hartley & Kidd 1987)

44 (rm. temp., Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

5.77×10^{-5} , 9.83×10^{-5} (20, $25^{\circ}C$, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.22×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.60 (selected, Dao et al. 1983)

3.53 (RP-HPLC- k' correlation, Braumann et al. 1983)

3.473 (countercurrent LC, Ilchmann et al. 1993)

2.79 (Tomlin 1994)

3.43 (selected, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.86 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{OC}$:

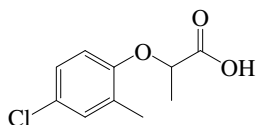
2.73 (soil, calculated-S, Kenaga 1980)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: duration of residual activity in soil is ca. 3–4 months (Hartley & Kidd 1987; Tomlin 1994).

17.1.1.48 Mecoprop



Common Name: Mecoprop

Synonym: Compitox, Duplosan, Hedonal, Iso-Cornox, Kilprop, MCP, Mecopex, Mepro, Methoxone, Propal

Chemical Name: (±)-2-(4-chloro-2-methylphenoxy)propanoic acid; (±)-2-(4-chloro-*o*-tolyl-oxy)propionic acid

Uses: herbicide for post-emergence control of broadleaf weeds in wheat, barley, rye, herbage seed crops, grassland, and under fruit trees and vines, etc.

CAS Registry No: 7085-19-0

Molecular Formula: C₁₀H₁₁ClO₃

Molecular Weight: 214.645

Melting Point (°C):

94–95 (Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

233.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

3.75 (Bailey & White 1965; quoted, Que Hee et al. 1981)

3.105 (Cessna & Grover 1978)

3.78 (Worthing & Hance 1991)

3.11 (Armbrust 2000)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.87 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

895 (Martin 1961; Bailey & White 1965)

891 (Bailey & White 1965)

620 (20°C, Melnikov 1971; Ashton & Crafts 1981; Herbicide Handbook 1989)

620 (Martin & Worthing 1977)

620 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)

734 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

< 1.0 × 10⁻⁵ (20°C, Hartley & Kidd 1987)

3.10 × 10⁻⁴ (20°C, Worthing & Hance 1991)

0.0 (selected, Halfon et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C):

7.43 × 10⁻⁵ (calculated-P/C, this work)

1.11 × 10⁻⁵ (quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, log K_{ow}:

3.94 (selected, Dao et al. 1983)

2.83 (RP-HPLC-k' correlation, Braumann et al. 1983)

0.10 (Worthing & Hance 1991)

0.09; 3.126 (quoted; countercurrent LC, Ilchmann et al. 1993)

3.13 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.20 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

2.11 (soil, calculated, Kenaga 1980, quoted, Bottoni & Funari 1992)

1.30 (selected, Lohninger 1994)

1.30 (quoted lit., Armbrust 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodegradation $t_{1/2} < 10$ –15 d on 3 Spanish natural dry soils; $t_{1/2} = 15$ –50 d on 10% peat-amended dry soils; degradation $t_{1/2} \sim 2$ –5.5 d on moist soils at field capacity and saturated soils for degradation at 0, 1 and 2 exposures days; and $t_{1/2} = 13$ –32 d on moist soils at field capacity and saturated soils for degradation at 2, 4 and 10 exposure days (Romero et al. 1998)

Oxidation: photooxidation $t_{1/2} = 3.8$ –37.8 h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: stable aqueous hydrolysis rate at pH 5, 7, pH 9; measured hydroxy radical rate constant for mecoprop $k = 9.0 \times 10^{12} \text{ M}^{-1} \text{ h}^{-1}$ (Armbrust 2000)

Biodegradation: aqueous aerobic $t_{1/2} = 168$ –240 h, based on aerobic soil grab sample data (Kirkland & Fryer 1972; Smith & Hayden 1981; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ –4320 h, based on anaerobic digest or sludge data (Battersby & Wilson 1989; quoted, Howard et al. 1991); aerobic rate constant, $k = 2.89 \times 10^{-3} \text{ h}^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 3.8$ –37.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 168$ –240 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 336$ –4320 h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)
reported $t_{1/2} = 8$ d (Bottoni & Funari 1992).

Sediment:

Soil: $t_{1/2} = 168$ –240 h, based on aerobic soil grab sample data (Kirkland & Fryer 1972; Smith & Hayden 1981; quoted, Howard et al. 1991);

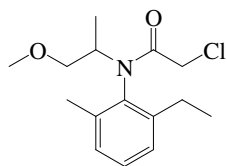
reported $t_{1/2} = 8$ d (Bottoni & Funari 1992);

$t_{1/2} = 21$ d (selected, Halfon et al. 1996)

photodegradation $t_{1/2} < 10$ –15 d on 3 Spanish natural dry soils; $t_{1/2} = 15$ –50 d on 10% peat-amended dry soils; degradation $t_{1/2} \sim 2$ –5.5 d on moist soils at field capacity and saturated soils for degradation at 0, 1 and 2 exposures days; and $t_{1/2} = 13$ –32 d on moist soils at field capacity and saturated soils for degradation at 2, 4 and 10 exposure days (Romero et al. 1998).

Biota:

17.1.1.49 Metolachlor



Common Name: Metolachlor

Synonym: Bicep, CGA 24705, Codal, Cortoran multi, Dual, Metetilachlor, Milocep, Ontrack 8E, Pennant, Primagram, Primextra

Chemical Name: 2-chloro-6'-ethyl-*N*-(2-methoxy-1-methylethyl)acet-*o*-toluidide; 2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)acetamide

Uses: pre-emergence herbicide to control most annual grasses and weeds in beans, chickpeas, corn, cotton, milo, okra, peanuts, peas, potatoes, sunflower, soybeans and some ornamentals.

CAS Registry No: 51218-45-2

Molecular Formula: C₁₅H₂₂ClNO₂

Molecular Weight: 283.795

Melting Point (°C): liquid

Boiling Point (°C):

100 (at 0.001 mmHg, Herbicide Handbook 1989; Budavari 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Density (g/cm³ at 20°C):

1.12 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

1.085 (Herbicide Handbook 1989)

Molar Volume (cm³/mol):

340.0 (calculated-Le Bas method at normal boiling point)

258.0 (calculated-density)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

530 (Martin & Worthing 1977)

440 (selected, Ellgehausen et al. 1980)

520 (20°C, Ashton & Crafts 1981; Spencer 1982)

530 (shake flask-HPLC, Ellgehausen et al. 1981)

530 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Budavari 1989; Montgomery 1993)

530 (Hartley & Graham-Bryce 1980; Beste & Humburg 1983)

530 (20°C, Worthing & Walker 1987, Worthing & Hance 1991; Majewski & Capel 1995; Milne 1995)

488 (Tomlin 1994)

530 (20–25°C, selected, Hornsby et al. 1996)

531, 505 (supercooled liquid S_L: literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00170 (20°C, Hartley & Graham-Bryce 1980)

0.00173 (20°C, Ashton & Crafts 1981)

0.00173 (20°C, volatilization rate, Burkhard & Guth 1981)

0.00170 (20°C, Hartley & Kidd 1987)

0.00170 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)

0.00173 (20°C, Herbicide Handbook 1989; Budavari 1989; Montgomery 1993)

4.20 × 10⁻³, 6.60 × 10⁻², 0.70, 5.40, 33.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

log (P_L/Pa) = 13.115 – 4619.7/(T/K); measured range 32.5–140°C (gas saturation-GC, Rordorf 1989)

0.00420 (Tomlin 1994)

- 0.0023 (liquid P_L , GC-RT correlation; Donovan 1996)
 0.00418 (selected, Halfon et al. 1996)
 0.00418 (20–25°C, selected, Hornsby et al. 1996)
 0.00239, 0.0024 (supercooled liquid P_L : literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.00092 (Hartley & Graham-Bryce 1980)
 0.00093 (20°C, volatilization rate, Burkhard & Guth 1981)
 0.00091 (20°C, calculated-P/C as per Worthing & Walker 1987)
 0.00093 (20°C, calculated-P/C, Montgomery 1993)
 0.00082 (20°C, calculated-P/C, Majewski & Capel 1995)
 0.00244 (calculated-P/C, Otto et al. 1997)
 0.00782 (20°C, distilled water, wetted wall column-GC, Rice et al. 1997b)
 0.00110 (calculated-P/C, this work)
 0.00238* (20°C, gas stripping-GC/MS, measured range 283.05–299.45 K, Feigenbrugel et al. 2004)
 $H'/(M \text{ atm}^{-1}) = (3.0 \pm 0.4) \times 10^{-11} \exp[(10200 \pm 1000)/(T/K)]$; temp range 283–310 K (Arrhenius eq., gas stripping-GC/MS, Feigenbrugel et al. 2004)
 0.0014, 0.0014 (literature derived value LDV, final adjust value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.13 (shake flask-HPLC, Ellgehausen et al. 1980; Geyer et al. 1991)
 3.28 (shake flask-HPLC, Ellgehausen et al. 1981)
 3.45 (Worthing & Hance 1991)
 2.93, 3.45 (Montgomery 1993)
 3.13, 3.28 (quoted, Sangster et al. 1993)
 2.90 (Tomlin 1994)
 3.45 (Milne 1995)
 3.31, 2.95 (selected, calculated-f const., Pinsuwan et al. 1995)
 3.13 (recommended, Hansch et al. 1995)
 2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
 3.10 (literature derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 9.37 (final adjust value FAV, Muir et al. 2004)

Bioconcentration Factor, $\log BCF$:

- 1.813 (log BF-bioaccumulation of algae, Ellgehausen et al. 1980)
 0.733 (log BF-bioaccumulation of daphnids, Ellgehausen et al. 1980; quoted, Geyer et al. 1991)
 0.851 (log BF-bioaccumulation of catfish, Ellgehausen et al. 1980)
 1.26 (calculated-S, Kenaga 1980)
 1.15 (catfish *Ictalurus melas*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.15 (soil, calculated-S, Kenaga 1980)
 2.26 (soil, screening model calculations, Jury et al. 1987b)
 2.00, 2.15, 2.28, 2.30 (soil, quoted values, Bottoni & Funari 1992)
 2.46, 2.46 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 2.30 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.08–2.49 (Montgomery 1993; Tomlin 1994)
 2.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.43 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 2.28, 2.19, 2.69 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: under optimum exposure conditions to natural sunlight, $t_{1/2} \sim 8$ d (Herbicide Handbook 1989).

Oxidation ; $k_{OH} = 5.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K in gas phase with atmospheric lifetime of 0.9 h but reduced to 0.4 h at 283 K; $\log k_{OH}(aq.) = 1.2 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ in aqueous phase (Feigenbrugel et al. 2004)

Hydrolysis: $t_{1/2} > 200$ d at 20°C and $1 \leq \text{pH} \leq 9$ (Montgomery 1993);

$t_{1/2}(\text{calc}) > 200$ d ($2 \leq \text{pH} \leq 10$) (Tomlin 1994).

Biodegradation: overall degradation rate constant $k = 0.0154 \text{ h}^{-1}$ with $t_{1/2} = 45.0$ h in sewage sludge and rate constant $k = 0.0460 \text{ d}^{-1}$ with $t_{1/2} = 15.1$ d in garden soil (Müller & Buser 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 9.11 \text{ d}^{-1}$ (catfish, Ellgehausen et al. 1980)

$k_1 = 0.336 \text{ h}^{-1}$, $k_2 = 0.024 \text{ h}^{-1}$ (catfish *Ictalurus melas*, Wang et al. 1996)

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported $t_{1/2} = 20, 30, 42$, and $47\text{--}107$ d (Bottoni & Funari 1992)
degradation time $500\text{--}1000$ d (Tomlin 1994).

Sediment:

Soil: $t_{1/2} = 15\text{--}38$ d in clay loam soils and $t_{1/2} = 33\text{--}100$ d in sandy loam soils (Zimdahl & Clark 1982; quoted, Montgomery 1993);

$t_{1/2} = 42$ d from field $t_{1/2} = 3\text{--}4$ wk by using lysimeters (Bowman 1990);

$t_{1/2}(\text{calc}) = 80, 99$ and 142 d for the disappearance from upper 15 cm on an Ontario clay loam soil while the decline was followed for 332, 364 and 370 d, respectively, in 1987, 1988 and 1989 (Frank et al. 1991);

$t_{1/2} \sim 6$ d in soil (Worthing & Hance 1991; quoted, Montgomery 1993);

reported $t_{1/2} = 20, 30, 42, 47\text{--}107$ d (Bottoni & Funari 1992)

field $t_{1/2} = 90$ d at $20\text{--}25^\circ\text{C}$ (selected, Wauchope et al. 1992; quoted, Richards & Baker 1993; Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2} = 40$ d (Pait et al. 1992);

soil $t_{1/2} = 28\text{--}46$ d (Di Guardo et al. 1994);

$t_{1/2} \sim 30$ d (Tomlin 1994);

degradation $t_{1/2} = 15.1$ d in garden soil (Müller & Buser 1995);

$t_{1/2} \sim 28.3$ d under conventional tillage, $t_{1/2} \sim 25.61$ d under ridge tillage and $t_{1/2} \sim 8.63$ d with no tillage (Otto et al. 1997).

Biota: $t_{1/2} = 1.15$ d in catfish (Ellgehausen et al. 1980);

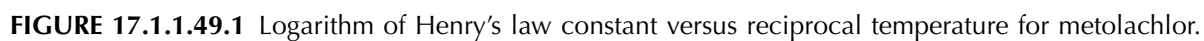
biochemical $t_{1/2} = 42$ d from screening model calculations (Jury et al. 1987b).

TABLE 17.1.1.49.1

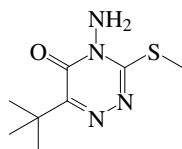
Reported Henry's law constants of metolachlor at various temperatures

Feigenbrugel et al. 2004

gas stripping-GC/MS			
$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$	$t/^\circ\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
283.05	5.39×10^{-4}	293.25	2.262×10^{-3}
283.15	6.34×10^{-4}	297.55	3.099×10^{-3}
283.25	8.126×10^{-4}	298.05	4.053×10^{-3}
283.65	8.465×10^{-4}	298.15	4.757×10^{-3}
285.55	8.01×10^{-4}	298.15	4.312×10^{-3}
287.55	1.088×10^{-3}	299.45	4.170×10^{-3}
289.45	1.193×10^{-3}		
291.55	1.419×10^{-3}	$\ln H' = A - B/(T/K)$	
293.05	2.702×10^{-3}		$H'/(M/\text{atm})$
293.05	2.471×10^{-3}	A	-24.2298
293.15	2.282×10^{-3}	B	10200
293.15	2.227×10^{-3}		



17.1.1.50 Metribuzin



Common Name: Metribuzin

Synonym: Metribuzine, Lexone, Preview, Sencor, Sencoral, Sencorer, Sencorex

Chemical Name: 4-amino-6-(t-butyl)-3-(methylthio)-1,2,4-triazin-5-(4*H*)-one

CAS Registry No: 21087-64-9

Uses: herbicide

Molecular Formula: C₈H₁₄N₄OS

Molecular Weight: 214.288

Melting Point (°C):

126 (Lide 2003)

Boiling Point (°C): 132.2 Pa (Tomlin 1994)

Density (g/cm³ at 20°C):

1.31 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

1.28 (Herbicide Handbook 1989)

Dissociation Constant pK_b:

13.0 (Wauchope et al. 1992; Hornsby et al. 1996)

1.0 (pK_a, Montgomery 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.102 (mp at 126°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

1220 (Kenaga & Goring 1980; Kenaga 1980b; Verschueren 1983)

1200 (20°C, Spencer 1982; Worthing & Walker 1983, 1987; Hartley & Kidd 1987)

1220 (Herbicide Handbook 1989)

1050 (20°C, Montgomery 1993; Tomlin 1994)

1220 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1065 (20–25°C, reported as 4.97E + 01 mol/m³, Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):

< 1.3 × 10⁻³ (20°C, Worthing 1983, 1987; Hartley & Kidd 1987; Tomlin 1994)

< 1.3 × 10⁻³; 2.67 × 10⁻² (20°C; 60°C, Herbicide Handbook 1989)

5.8 × 10⁻⁵ (20°C, Montgomery 1993)

< 1.3 × 10⁻³ (20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)

5.89 × 10⁻⁴ (20–25°C, Majewski & Capel 1995)

Henry's Law Constant (Pa·m³/mol at 25°C):

< 1.3 × 10⁻³ (Spencer 1982; Worthing 1987; Hartley & Kidd 1987)

1.21 × 10⁻⁵ (calculated-P/C, Montgomery 1993)

1.18 × 10⁻⁵ (calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{ow}:

1.60, 1.70 (quoted, Montgomery 1993)

1.58 (pH 5.6, Tomlin 1994)

1.70 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 2.46, 1.48, < 1.30 (algae, activated sludge, fish in 3-d testing, Korte et al. 1978)
- 1.77, 1.75 (*Chlorella*, calculated-solubility, Geyer et al. 1981)
- 1.77, 1.48, 1.04 (algae, activated sludge, *Golden orfe*, Geyer et al. 1982)
- 1.04, 0.602 (calculated-solubility, calculated- K_{OW} , Kenaga 1980a)
- 1.48, 1.78, 1.0 (activated sludge, algae, *Golden ide*, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.98 (soil, Kenaga & Goring 1980)
- 1.98; 1.94 (quoted, calculated- K_{OW} , Kenaga 1980b)
- 0.954–2.72 (soil, literature range, Wauchope et al. 1992)
- 1.80 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.94–1.98, 2.18 (soil, Bottoni & Funari 1992)
- 1.80–2.72 (soil, Montgomery 1993)
- 1.78 (soil, Senseman et al. 1997)
- 1.71 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 1.71; 1.68, 1.33 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.05, 2.06, 2.04 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodecomposition in water is very rapid with $t_{1/2} < 1$ d; on soil surface under natural sunlight conditions, $t_{1/2} = 14$ –25 d (Tomlin 1994).

Oxidation:

Hydrolysis: $t_{1/2} \sim 1$ wk in pond water (Hartley & Kidd 1987; Montgomery 1993).

Biodegradation: under goes microbial degradation in moist soil (Worthing 1987)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} \sim 1$ wk in pond water (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994); stable to dilute acids and alkalis, $t_{1/2} = 6.7$ h at pH 1.2 and 37°C; $t_{1/2} = 569$ h at pH 4, $t_{1/2} = 47$ d at pH 7 and $t_{1/2} = 191$ h at pH 9 for 70°C (Tomlin 1994).

Ground water: reported half-life or persistence $t_{1/2} = 4$ –25, 17–301 and 56 d (Bottoni & Funari 1992).

Sediment:

Soil: undergoes microbial degradation in moist soil (Worthing 1983, 1987);

half-life varies with soil types, $t_{1/2} \sim 90$ –115 d for Red River, Almasippi, and Stockton soils the 3 times this period for Newdale soil for normal application rates (Verschuere 1983);

$t_{1/2} \sim 1$ –2 months in soil (Hartley & Kidd 1987; Tomlin 1994);

$t_{1/2} \sim 30$ –60 d in various soil types varies greatly with climatic conditions, during the growing season (Herbicide Handbook 1989);

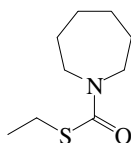
$t_{1/2} = 9$ –12 d irrespective of the number of previous treatments in the field; $t_{1/2} = 25$ –40 d irrespective of the pretreatment history of the soil at 20°C in the laboratory (Walker & Welch 1992)

reported $t_{1/2} = 23$ –120 d and the recommended field $t_{1/2} = 40$ d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Senseman et al. 1997);

half-lives of in two surface soil microcosms under nitrate, $t_{1/2} = 157$ d and non-nitrate, $t_{1/2} = 187$ and 349 d in reducing culture conditions at 16.4°C (Pavel et al. 1999).

Biota: in mammals, following oral administration, 90% elimination within 96 h (Hartley & Kidd 1987).

17.1.1.51 Molinate



Common Name: Molinate

Synonym: Felan, Higalnat, Hydram, Jalan, Molmate, Ordram, Stauffer R 4572, Sakkimok, Yalan, Yulan

Chemical Name: 1*H*-azepine-1-carbothioic acid, hexahydro, *S*-ethyl ester; ethyl 1-hexa-methyleneiminocarbothioate

Uses: selective herbicide to control the germination of annual grasses and broadleaf weeds in rice crops.

CAS Registry No: 2212-67-1

Molecular Formula: C₉H₁₇NOS

Molecular Weight: 187.302

Melting Point (°C): < 25 (Montgomery 1993)

Boiling Point (°C):

202 (at 10 mmHg, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Milne 1995)

117 (at 10 mmHg, Montgomery 1993)

Density (g/cm³ at 20°C):

1.064 (Hartley & Kidd 1987)

1.0643 (Herbicide Handbook 1989; Montgomery 1993)

1.063 (Worthing & Hance 1991; Milne 1995)

Molar Volume (cm³/mol):

220.6 (calculated-Le Bas method at normal boiling point)

176.1 (calculated-density)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

880 (20°C, Weber 1972; Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991)

800 (Martin & Worthing 1977)

800–912 (Weber et al. 1980)

912 (21°C, Spencer 1982)

800 (20°C, Herbicide Handbook 1983, 1989)

870 (Kanazawa 1989)

970 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996; Armbrust 2000)

880 (20°C, Montgomery 1993; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

0.748 (20°C, Weber 1972; Worthing & Walker 1987)

0.746 (20°C, Khan 1980)

0.185 (20°C, GC-RT correlation, Kim 1985)

0.413 (Seiber et al. 1986, 1989)

0.746 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

0.746 (Herbicide Handbook 1989; Worthing & Hance 1991)

0.746 (20–25°C, selected, Wauchope et al. 1992)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.097 (calculated-P/C, Seiber et al. 1986, 1989)

0.314 (20°C, calculated-P/C, Suntio et al. 1988)

0.159 (20°C, calculated-P/C as per Worthing & Walker 1987;)

0.159 (20°C, calculated-P/C, Muir 1991)

0.095	(20°C, calculated-P/C, Sagebiel et al. 1992)
0.460	(20°C, gas-stripping method, Sagebiel et al. 1992)
0.390	(20°C, headspace-GC method, Sagebiel et al. 1992)
0.162	(calculated-P/C, Montgomery 1993)
0.145	(calculated-P/C, this work)
0.132	(quoted lit., Armbrust 2000)
0.397	(20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
$\log K_{AW} = 6.527 - 3024/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)	

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.21	(shake flask-GC, Kanazawa 1981)
2.88	(Worthing & Hance 1991; Tomlin 1994)
2.88	(Montgomery 1993)
3.13	(RP-HPLC-RT correlation, Saito et al. 1993)
3.26	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
3.21	(recommended, Sangster 1993)
2.88	(Milne 1995)
3.21	(recommended, Hansch et al. 1995)
3.25	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log BCF$:

1.15	(calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
1.41	(<i>Peudorashbora parva</i> , Kanazawa 1981)

Sorption Partition Coefficient, $\log K_{OC}$:

2.04	(soil, calculated-S, Kenaga 1980)
1.92	(average of 2 soils, Kanazawa 1989)
1.92, 2.04	(soil, quoted values, Bottoni & Funari 1992)
1.92, 2.46	(soil, quoted exptl., calculated-MCI χ and fragments contribution, Meylan et al. 1992)
2.28	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.93–1.97	(Montgomery 1993)
2.28	(selected, Lohninger 1994)
1.92	(soil, calculated-MCI χ , Sabljic et al. 1995)
2.07	(soil, quoted lit., Armbrust 2000)
1.92; 2.31, 1.86 (soil, quoted exptl.; estimated-class specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)	

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: $k = 0.0150 \text{ h}^{-1}$ (average of 2 runs, Seiber et al. 1986); 1.1 kg ha^{-1} (1st 4 day) from flooded rice fields (Seiber et al. 1986; Seiber & McChesney 1987);
estimated $t_{1/2} = 43 \text{ d}$ from 1 m depth of water at 20°C (Muir 1991).
- Photolysis: $t_{1/2} = 7\text{--}10 \text{ d}$ for $8\text{--}10 \mu\text{g mL}^{-1}$ to degrade in distilled water under $> 290 \text{ nm}$ light (Soderquist et al. 1977; quoted, Cessna & Muir 1991);
 $t_{1/2} = 96 \text{ h}$ for $< 5\%$ of $0.2 \mu\text{g mL}^{-1}$ to degrade in distilled water under sunlight (Deuel et al. 1978; quoted, Cessna & Muir 1991);
 $t_{1/2} = 245 \text{ h}$ for $2\text{--}54\%$ of $10 \mu\text{g mL}^{-1}$ to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Muir 1991).
- Oxidation: calculated life-time of 6 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992);
measured rate constant for reaction with hydroxyl radical, $k(\text{aq.}) = 0.85 \times 10^9 \text{ M}^{-1}\cdot\text{s}^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996);
measured hydroxy radical reaction rate constant for molinate $k = 7.7 \times 10^{12} \text{ M}^{-1} \text{ h}^{-1}$ (Armbrust 2000).
- Hydrolysis: $t_{1/2} > 10 \text{ d}$ in aqueous buffer at pH 5–9 in the dark (Soderquist et al. 1977; quoted, Muir 1991); stable aqueous hydrolysis rate at pH 5, 7, 9 (Armbrust 2000).

Biodegradation: $t_{1/2} \sim 16$ d for $0.2 \mu\text{g mL}^{-1}$ to biodegrade in flooded soils (Deuel et al. 1978; quoted, Muir 1991);
 $t_{1/2} = 10$ wk for $4.2 \mu\text{g mL}^{-1}$ to biodegrade in flooded soil and $t_{1/2} < 2$ wk in water both at $21\text{--}26^\circ\text{C}$ (Thomas & Holt 1980; quoted, Muir 1991);
aerobic rate constant, $k = 2.22 \times 10^{-3} \text{ h}^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated lifetime of 6 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Surface water: $t_{1/2} = 84$ h from dissipation from flooded rice fields (Seiber & McChesney 1987; quoted, Seiber et al. 1989).

Ground water: reported half-lives or persistence, $t_{1/2} = 3\text{--}14$, $8\text{--}25$ and $40\text{--}160$ d (Bottoni & Funari 1992)

Sediment:

Soil: persistence of 2 months in soil (Wauchope 1978);

$t_{1/2} \sim 3$ wk in moist loam soils at $21\text{--}27^\circ\text{C}$ (Herbicide Handbook 1989);

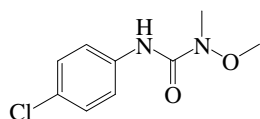
selected field $t_{1/2} = 21$ d (Wauchope et al. 1992; quoted, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2} = 21$ d (Pait et al. 1992);

reported $t_{1/2} = 3\text{--}14$ d, $8\text{--}25$ d and $40\text{--}160$ d (Bottoni & Funari 1992).

Biota:

17.1.1.52 Monolinuron



Common Name: Monolinuron

Synonym: Afesin, Aresin, Arresin, Hoe 02747

Chemical Name: 3-(4-chlorophenyl)-1-methoxy-1-methylurea; *N'*-(4-chlorophenyl)-*N*-methoxy-*N*-methylurea

Uses: herbicide for pre- or post-emergence control of annual broadleaf weeds and annual grasses in asparagus, berry fruit, cereals, maize, field beans, vines, leeks, onions, potatoes, herbs, lucerne, flowers, ornamental shrubs and trees, etc.

CAS Registry No: 1746-81-2

Molecular Formula: $C_9H_{11}ClN_2O_2$

Molecular Weight: 214.648

Melting Point ($^{\circ}C$):

77 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

224.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.309 (mp at $77^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

735 ($20^{\circ}C$, Melnikov 1971)

735 (Spencer 1973, 1982)

580 (Martin & Worthing 1977; Khan 1980)

735 (Worthing & Walker 1983, 1987, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

735 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.02 ($22^{\circ}C$, Khan 1980; Hartley & Kidd 1987)

0.0015 ($20^{\circ}C$, Spencer 1982)

6.40 ($65^{\circ}C$, Worthing & Hance 1991)

0.02 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

0.0013, 0.10 ($20^{\circ}C$, $50^{\circ}C$, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0058 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.60 (Briggs 1969)

2.30 (shake flask-UV, Briggs 1981)

1.60 (selected, Dao et al. 1983)

1.99 (RP-HPLC- k' correlation, Braumann et al. 1983)

2.22 (shake flask, Mitsutake et al. 1986)

2.20 (Worthing & Hance 1991; Tomlin 1994)

2.16 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)

2.30 (recommended, Sangster 1993)

2.30 (recommended, Hansch et al. 1995)

2.31 (Pomona-database, Müller & Kördel 1996)

2.16 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.23; 1.00 (calculated-S, calculated- K_{OC} , Kenaga 1980)
- 1.85 (activated sludge, Freitag et al. 1982, 1984, 1985)
- 1.52, < 1.0 (algae, golden orfe, Freitag et al. 1982)
- 1.60, 1.30 (algae, golden ide, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC} :

- 2.30 (soil, Hamaker & Thompson 1972)
- 2.11 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 1.60 (reported as log K_{OM} , Briggs 1981)
- 2.36, 2.08, 1.21 (estimated-S, calculated-S and mp, calculated- K_{OW} , Karickhoff 1981)
- 2.40–2.70 (soil, Worthing & Hance 1991)
- 2.26–2.30, 2.40–2.70 (soil, quoted values, Bottoni & Funari 1992)
- 1.78 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995b)
- 2.30 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 2.10 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.78; 2.33 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.44, 1.50, 1.71, 1.754, 2.45 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.05, 1.72, 1.695, 1.825, 2.407 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 2.050, 1.721, 1.695, 1.825, 2.407 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask-batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
- 2.10; 2.04, 2.31 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 1.88, 1.88 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Photolysis: $t_{1/2} = 23$ h for 66% of 286 $\mu\text{g/mL}$ to degrade in distilled water under > 300 nm light (Kotzias et al. 1974; quoted, Cessna & Muir 1991).

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported half-lives or persistence, $t_{1/2} = 45\text{--}60$ d (Bottoni & Funari 1992)

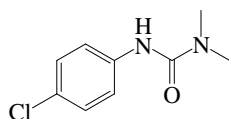
Sediment:

Soil: reported $t_{1/2} = 45\text{--}60$ d (Worthing & Hance 1991);

estimated field $t_{1/2} = 60$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

17.1.1.53 Monuron



Common Name: Monuron

Synonym: Chlorfenidim, CMU, Karmex, Lirobetarex, Monurex, Monurox, Rosuran, Telvar, Urox

Chemical Name: *N'*-(4-chlorophenyl)-*N,N*-dimethylurea; 1,1-dimethyl-3-(*p*-chlorophenyl)urea

Uses: herbicide; also as sugar cane flowering suppressant.

CAS Registry No: 150-68-5

Molecular Formula: C₉H₁₁ClN₂O

Molecular Weight: 198.648

Melting Point (°C):

170.5 (Kühne et al. 1995; Lide 2003)

Boiling Point (°C):

185–200 (decomposes, Montgomery 1993)

Density (g/cm³ at 20°C):

1.27 (Spencer 1982; Hartley & Kidd 1987; Montgomery 1993)

Molar Volume (cm³/mol):

202.9 (calculated-Le Bas method at normal boiling point)

173.0 (modified Le Bas method, Spurlock & Biggar 1994a)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0374 (mp at 170.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

203 (Freed 1966)

230 (Günther et al. 1968; Sanborn et al. 1977; Khan 1980; Ashton & Crafts 1981)

262 (shake flask-UV, Hurle & Freed 1972)

230 (20°C, Weber 1972; Worthing & Walker 1987)

230 (Martin & Worthing 1977; Hartley & Kidd 1987)

200 (shake flask-HPLC, Ellgehausen et al. 1981)

200 (20°C, selected, Suntio et al. 1988)

275 (Spurlock 1992; Spurlock & Biggar 1994b)

230 (at pH 6.26, Montgomery 1993)

230 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7.60×10^{-5} , 1.2×10^{-5} (25, 27°C, Nex & Swezey 1954)

6.67×10^{-5} (Bailey & White 1965)

6.72×10^{-5} (20°C, Weber 1972; Worthing & Walker 1987)

6.67×10^{-5} (Ashton & Crafts 1973, 1981; Khan 1980)

5.33×10^{-5} * (30.35°C, Knudsen effusion, measured range 303.5–379.1 K, Wiedemann 1972)

$\log(P/\text{mmHg}) = 13.3052 - 5988.39/(T/K)$; temp range 303.5–379.1 K (Antoine eq., effusion, Wiedemann 1972)

6.70×10^{-5} (OECD 1981)

2.30×10^{-5} (calculated, Jury et al. 1983)

6.00×10^{-5} (Hartley & Kidd 1987)

6.67×10^{-5} (Budavari 1989)

2.30×10^{-5} (selected, Taylor & Spencer 1990)

6.00×10^{-5} (20°C, Montgomery 1993)

6.67×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 5.80×10^{-5} (20°C , volatilization rate, Burkhard & Guth 1981)
- 1.88×10^{-5} (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
- 3.00×10^{-3} (20°C , calculated-P/C, Suntio et al. 1988)
- 1.91×10^{-5} (calculated-P/C, Taylor & Glotfelty 1988)
- 5.60×10^{-5} (20°C , calculated-P/C, Muir 1991)
- 3.00×10^{-3} (20°C , calculated-P/C, Montgomery 1993)
- 6.60×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

- 1.46 (Briggs 1969)
- 1.66 (calculated-fragment const., Rekker 1977)
- 1.80 (shake flask-UV, Erckell & Walum 1979)
- 2.08 (selected, Ellgehausen et al. 1980; Geyer et al. 1991)
- 2.12 (Rao & Davidson 1980)
- 1.98 (shake flask-UV, Briggs 1981)
- 2.08 (shake flask, Ellgehausen et al. 1980)
- 1.66 (shake flask, Ellgehausen et al. 1981)
- 1.86 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 1.91 (RP-HPLC- k' correlation Braumann et al. 1983)
- 1.80 (selected, Suntio et al. 1988)
- 2.12 (shake flask-HPLC, Spurlock 1992; Spurlock & Biggar 1994b)
- 1.46, 2.12 (Montgomery 1993)
- 1.86 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 1.94 (recommended, Sangster 1993)
- 1.89; 1.88 (shake flask-UV; RP-HPLC- k' correlation, Liu & Qian 1995)
- 1.94 (recommended, Hansch et al. 1995)
- 1.99 (Pomona-database, Müller & Kördel 1996)
- 1.86 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.786 ($\log \text{BF}$ bioaccumulation factor for algae, Ellgehausen et al. 1980)
- 0.32 ($\log \text{BF}$ bioaccumulation factor for daphnids, Ellgehausen et al. 1980)
- 0.245 ($\log \text{BF}$ bioaccumulation factor for daphnids, Ellgehausen et al. 1980)
- 1.46 (calculated-S, Kenaga 1980)
- 0.699 (calculated- K_{OC} , Kenaga 1980)
- 0.0 (*Trialenodes tardus*, Belluck & Felsot 1981)
- 1.58, 1.67 (cuticle/water: tomato, pepper; Evelyne et al. 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.00 (soil, Hamaker & Thompson 1972)
- 2.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.26 (av. of 18 soils, Rao & Davidson 1980)
- 1.70 (soil, converted from reported K_{OM} , multiplied by 1,724, Briggs 1981)
- 2.58, 1.51 (estimated-S, calculated-S and mp, Karickhoff 1981)
- 1.07, 1.73 2.58 (estimated- K_{OW} , Karickhoff 1981)
- 2.03, 1.85; 2.17, 1.52 (estimated- K_{OW} s; solubilities, Madhun et al. 1986)
- 1.99; 2.12 (quoted; calculated-MCI χ , Gerstl & Helling 1987)
- 2.26 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
- 1.99, 2.33 (Montgomery 1993)
- 2.18 (20 – 25°C , estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 1.99 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
- 2.29 (calculated- K_{OW} , Liu & Qian 1995)
- 1.95 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

- 1.99; 1.92 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.58, 1.77, 1.85, 1.77, 2.41 (first generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.14, 2.018, 1.79, 1.764, 2.243 (second generation Eurosoils ES-1, ES2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 2.141, 2.018, 1.793, 1.764, 2.243 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)
- 1.95; 1.96, 2.13 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 1.80, 1.80 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

- Photolysis: $t_{1/2}$ = 14 d for 6% of 200 $\mu\text{g mL}^{-1}$ to degrade in distilled water under sunlight (Crosby & Tang 1969; quoted, Cessna & Muir 1991);
- $t_{1/2}$ = 2.25 h for 44% of 200 $\mu\text{g mL}^{-1}$ to degrade in distilled water under 300 nm light (Tanaka et al. 1977; quoted, Cessna & Muir 1991);
- $t_{1/2}$ = 2.25 s for 75% of 100 $\mu\text{g mL}^{-1}$ to degrade in 0.2% Triton X-100 aqueous solution under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991);
- $t_{1/2}$ = 2.25 h for > 70% of 200 $\mu\text{g mL}^{-1}$ to degrade in aqueous solutions of nonionic surfactants at concns. in excess of critical micelle concn. under 300 nm light (Tanaka et al. 1979; quoted, Cessna & Muir 1991);
- $t_{1/2}$ = 45 h for 69% of 165 $\mu\text{g mL}^{-1}$ to degrade in distilled water under > 280 nm light (Tanaka et al. 1982; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: $t_{1/2}$ > 4 months for 3974 $\mu\text{g mL}^{-1}$ to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991).

Biodegradation: aerobic $t_{1/2}$ ~ 7 d for 0.01 $\mu\text{g mL}^{-1}$ to biodegrade in river water (Eichelberger & Lichtenberg 1971; quoted, Muir 1991);

$t_{1/2}$ = 166 d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989);

aerobic $t_{1/2}$ ~ 10–15 d for 0.0005–10 $\mu\text{g mL}^{-1}$ to biodegrade in filtered sewage water at 20°C (Wang et al. 1985; quoted, Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_2 = 21.05 d^{-1} (catfish, Ellgehausen et al. 1980)

Half-Lives in the Environment:

Air:

Surface water: persistence of up to 8 wk in river water (Eichelberger & Lichtenberg 1971).

Ground water:

Sediment:

Soil: $t_{1/2}$ = 5.0 months at 15°C and 4.1 months at 30°C in soils (Freed & Haque 1973);

reported $t_{1/2}$ = 166 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989; quoted, Montgomery 1993);

estimated field $t_{1/2}$ = 170 d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota: $t_{1/2}$ = 0.45 d in catfish (Ellgehausen et al. 1980);

biochemical $t_{1/2}$ = 166 d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

TABLE 17.1.1.53.1
Reported vapor pressures of monuron at various temperatures

Wiedemann 1972			
Knudsen effusion			
T/K	P/Pa	T/K	P/Pa
303.5	5.33×10^{-5}	358.7	0.0536
316.0	2.44×10^{-4}	360.2	0.0561
329.8	2.16×10^{-3}	379.1	0.399
330.6	1.53×10^{-3}		
330.6	2.22×10^{-3}	$\log P = A - B/(T/K)$	
338.8	7.05×10^{-3}		P/mmHg
341.4	9.45×10^{-3}	A	13.3952
345.7	0.0105	B	5988.39
349.5	0.0204		
357.0	0.0529	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 114.6$	

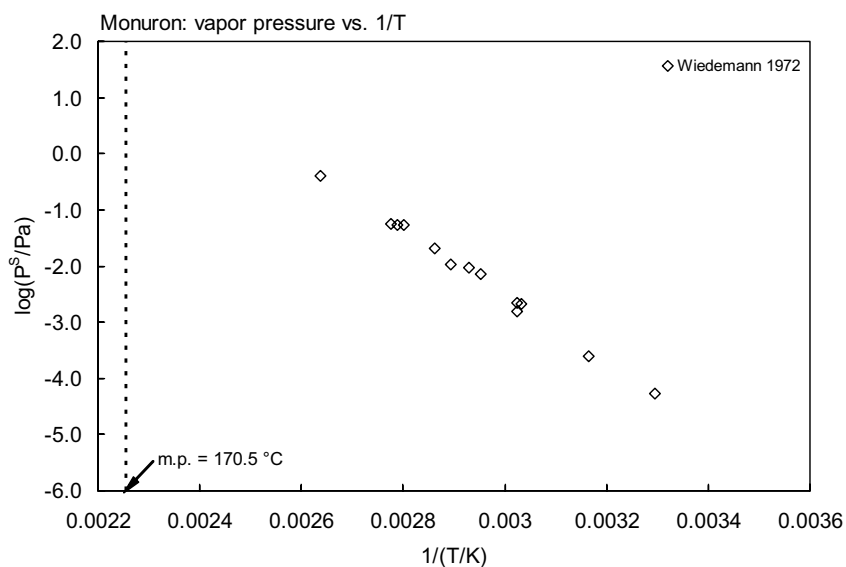
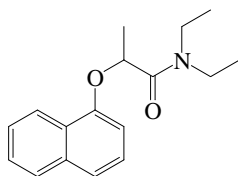


FIGURE 17.1.1.53.1 Logarithm of vapor pressure versus reciprocal temperature for monuron.

17.1.1.54 Napropamide



Common Name: Napropamide

Synonym: Devrinol

Chemical Name: 2-(α -naphthloxy)-*N,N*-diethylpropionamide

CAS Registry No: 15299-99-7

Uses: herbicide

Molecular Formula: $C_{17}H_{21}NO_2$

Molecular Weight: 271.355

Melting Point ($^{\circ}C$):

75 (Worthing & Walker 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

2.93 (Woodburn et al. 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.323 (mp at $75^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

69 (shake flask-LSC or GC, Gerstl & Mingelgrin 1984)

73 ($20^{\circ}C$, Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Herbicide Handbook 1989; Montgomery 1993; Tomlin 1994)

74 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

2.67×10^{-4} (Spencer 1982)

5.3×10^{-4} (Herbicide Handbook 1989)

5.3×10^{-4} (Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

2.27×10^{-5} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.67×10^{-3} (20 – $25^{\circ}C$, Majewski & Capel 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.00294 (calculated-P/C, Montgomery 1993)

0.00197 (20 – $25^{\circ}C$, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.08 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)

3.36 (Montgomery 1993)

3.30 (Tomlin 1994)

3.36 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

2.04–3.09 (various soils, Mingelgrin & Gestl 1983)

2.82, 3.56 (soil: quoted, calculated-MCI χ , Gerstl & Helling 1987)

- 2.62 (soil, average of log K_{OC} values, Gerstl 1990)
 3.52–4.29; 3.72 at pH 2, 3.35 at pH 6 (Dead sea sediment, Gestl & Kilger 1990)
 2.62–3.54; 3.54 at pH 2, 3.40 at pH 6 (Kinnert F sediment, Gestl & Kilger 1990)
 2.71–3.62; 3.62 at pH 2, 3.27 at pH 6 (Kinnert G sediment, Gestl & Kilger 1990)
 2.40–3.31; 3.31 at pH 2, 3.20 at pH 5 (Oxford soil, Gestl & Kilger 1990)
 2.39–3.15; 3.15 at pH 2, 2.88 at pH 6 (Malkiya soil, Gestl & Kilger 1990)
 2.28–3.29; 3.29 at pH 2, 3.09 at pH 5 (Neve Ya'ar soil, Gestl & Kilger 1990)
 2.85 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
 2.29–3.99 (soil/sediment, literature range, Montgomery 1993)
 2.83 (soil, Montgomery 1993)
 2.62 (soil, calculated-MCI χ , Sabljic et al. 1995)
 2.58, 2.58, 2.61 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
 2.80 (sediment: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: very little loss occurred by volatilization from soil surface (Herbicide Handbook 1989).

Photolysis: under condition of high sunlight intensity in the summer, $t_{1/2} \sim 4$ d on the soil surface (Herbicide Handbook 1989);

decomposed by sunlight, $t_{1/2} = 25.7$ min. (Tomlin 1994).

Oxidation:

Hydrolysis: stable to hydrolysis between pH 4 and 10 at 40°C (Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).

Biodegradation: slowly broken down by microorganisms in soil, in pure culture, a soil fungus metabolizes rapidly with $t_{1/2} = 2$ wk (Herbicide Handbook 1989).

Biotransformation: rapidly metabolized in plants to water-soluble metabolites (Tomlin 1994).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water: decomposed by sunlight, $t_{1/2} = 25.7$ min. (Montgomery 1993; Tomlin 1994).

Sediment:

Soil: $t_{1/2} \sim 55$ d in the plots treated for the first time whereas $t_{1/2} = 6$ –12 d in pre-treated plots that had previously been sprayed with napropamide in the field; $t_{1/2} = 25$ –40 d irrespective of the pre-treatment history of the soil in the laboratory at 20°C (Walker & Welch 1992)

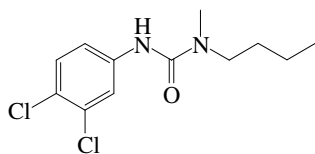
$t_{1/2} \sim 8$ –12 wk (Hartley & Kidd 1987; Tomlin 1994);

field $t_{1/2} = 70$ d (Wauchope et al. 1992; Hornsby et al. 1996);

moist loam or sandy-loam soils at 79–90°C, $t_{1/2} = 8$ –12 wk (Montgomery 1993).

Biota: rapidly metabolized in plants to water-soluble metabolites (Tomlin 1994).

17.1.1.55 Neburon



Common Name: Neburon

Synonym: Kloben, Neburea, Neburex

Chemical Name: 1-butyl-3-(3,4-dichlorophenyl)-1-methylurea; *N*-butyl-*N'*-(3,4-dichloro-phenyl)-*N*-methylurea

Uses: pre-emergence herbicide to control grasses and broadleaf weeds in peas, beans, lucerne, garlic, beets, cereals, strawberries, ornamentals and forestry.

CAS Registry No: 555-37-3

Molecular Formula: $C_{12}H_{16}Cl_2N_2O$

Molecular Weight: 275.174

Melting Point ($^{\circ}C$):

102–103 (Khan 1980; Spencer 1982; Worthing & Hance 1991; Tomlin 1994)

101.5–103 (Montgomery 1993)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

236.0 (modified Le Bas method at normal boiling point, Spurlock & Biggar 1994a)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

96.91 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

29.71 (DSC method, Plato & Glasgow 1969)

26.9 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.8 ($24^{\circ}C$, Bailey & White 1965; Melnikov 1971)

4.8 (Martin & Worthing 1977)

4.8 ($28^{\circ}C$, Khan 1980)

5.0 (Hartley & Kidd 1987; Tomlin 1994)

4.8 ($24^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991; Montgomery 1993)

5.2 (Spurlock 1992; Spurlock & Biggar 1994b)

5.0 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; selected, Hornsby et al. 1996)

4.67, 9.99 (quoted, calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

6.30×10^{-6} , 4.10×10^{-4} , 0.015, 0.33, 4.90 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 18.272 - 6999.1/(T/K)$; measured range 50 – $103^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 13.285 - 5062.2/(T/K)$; measured range 105 – $140^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.59 (selected, Dao et al. 1983; Gerstl & Helling 1987)

4.31 (RP-HPLC- k' correlation, Braumann et al. 1983)

4.22 (Spurlock 1992; Spurlock & Biggar 1994b)

3.80 (selected, Sangster 1993)

3.80 (calculated, Montgomery 1993)

- 4.10 (shake flask-UV, Liu & Qian 1995)
- 3.99 (RP-HPLC- k' correlation, Liu & Qian 1995)
- 3.80 (recommended, Hansch et al. 1995)
- 3.40, 4.02, 4.13 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 2.41 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- 1.85, 2.18 (calculated-S, K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

- 3.36 (soil, Hamaker & Thompson 1972)
- 3.26, 2.72 (soil, calculated-S, Kenaga 1980)
- 3.49 (average of soils/sediments, Rao & Davidson 1980)
- 3.36, 3.23 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
- 2.95 (soil, calculated- χ and fragment contribution, Meylan et al. 1992)
- 3.49 (Montgomery 1993)
- 3.40 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 3.40 (selected, Lohninger 1994)
- 3.60 (calculated- K_{OW} , Liu & Qian 1995)
- 3.140 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.40; 2.86, 2.69 (soil, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

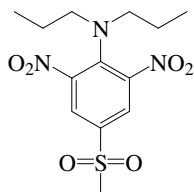
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Hydrolysis: $t_{1/2} > 4$ months for 5500 $\mu\text{g/mL}$ to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-dib & Aly 1976; quoted, Muir 1991).

Half-Lives in the Environment:

- Soil: residual activity in soil is limited to approximately 3–4 months (Hartley & Kidd 1987; quoted, Montgomery 1993);
- selected field $t_{1/2} = 120$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.56 Nitralin



Common Name: Nitralin

Synonym: Planavin

Chemical Name: 4-(methylsulfonyl)-2,6-dinitro-*N,N*-dipropylbenzamine

CAS Registry No: 4726-14-1

Uses: herbicide

Molecular Formula: $C_{13}H_{19}N_3O_6S$

Molecular Weight: 345.371

Melting Point ($^{\circ}C$):

150 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.39 (Hartley & Kidd 1987)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0594 (mp at $150^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.60 (Melnikov 1971; Kenaga & Goring 1980; Kenaga 1980b; Isensee 1991)

0.60 (Ashton & Crafts 1981; Hartley & Kidd 1987; Worthing & Walker 1987)

Vapor Pressure (Pa at $25^{\circ}C$):

0.240 (Ashton & Crafts 1981)

2.0×10^{-5} (Hartley & Kidd 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.73 (calculated-MCI χ , Patil 1994)

2.81 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.90, 1.76 (calculated-solubility, K_{ow} , Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{oc}$:

2.98 (Kenaga & Goring 1980)

3.76 (calculated, Kenaga 1980a)

2.92 (soil, calculated-MCI χ , Sabljic et al. 1995)

2.92; 3.28 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Biotransformation: Degradation by abiotic reductive transformations:

$k = 3.44 M^{-1} s^{-1}$ in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 0.44 \times 10^{-3} \text{ h}^{-1}$ at pH 6.5, $k = 0.68 \times 10^{-2} \text{ h}^{-1}$ at pH 7.0, $k = 0.133 \text{ h}^{-1}$ at pH 7.4, and $k = 1.96 \text{ h}^{-1}$ at pH 7.8 for aqueous ferrous ion system;

$k = 0.580 \text{ h}^{-1}$ at pH 6.5, $k = 1.15 \text{ h}^{-1}$ at pH 6.7, $k = 6.06 \text{ h}^{-1}$ at pH 7.0, and $k = 20.9 \text{ h}^{-1}$ at pH 7.3 for Fe(II)/goethite system;

$k = 2.54 \times 10^{-3} \text{ h}^{-1}$ at pH 6.5, $k = 1.83 \times 10^{-3} \text{ h}^{-1}$ at pH 7.0, $k = 4.13 \times 10^{-3} \text{ h}^{-1}$ at pH 7.4 and $k = 7.70 \times 10^{-3} \text{ h}^{-1}$ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

Half-Lives in the Environment:

Air:

Surface water:

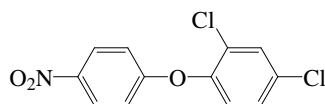
Ground water:

Sediment:

Soil: $t_{1/2} \sim 30\text{--}54 \text{ d}$ in dry soil (Hartley & Kidd 1987)

Biota: in mammals, following oral administration, degradation and elimination occur within a few days (Hartley & Kidd 1987).

17.1.1.57 Nitrofen



Common Name: Nitrofen

Synonym: nitrophen Tok, Tokkron

Chemical Name: 2,4-dichloro-1-(4-nitrophenoxy)benzene

CAS Registry No: 1836-75-5

Uses: herbicide

Molecular Formula: $C_{12}H_7Cl_2NO_3$

Molecular Weight: 284.095

Melting Point ($^{\circ}C$):

70 (Lide 2003)

Boiling Point ($^{\circ}C$):

180–190/0.25 mmHg (Hartley & Kidd 1987)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

93.66 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.7 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.362 (mp at $70^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.0 (Kenaga 1980b)

~1.0 (Spencer 1982)

0.7–1.2 ($22^{\circ}C$, Worthing 1987)

~1 (room temp., Hartley & Kidd 1987)

1.0 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations.):

1.07×10^{-3} ($40^{\circ}C$, Spencer 1982)

1.06×10^{-3} ($40^{\circ}C$, Worthing 1987; Hartley & Kidd 1987)

1.30×10^{-4} , 4.50×10^{-3} , 0.091, 1.20, 12.0 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 15.867 - 5886.5/(T/K)$; measured range 50 – $70.2^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 13.022 - 4892.8/(T/K)$; measured range 72.7 – $140^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

1.33×10^{-5} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.09 (Rao & Davidson 1980)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.79 (fish, Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{OC}$:

3.64 (soil, calculated, Kenaga 1980b)

3.01, 3.64, 4.18, 4.05 (quoted literature values, Augustijn-Beckers et al. 1994)

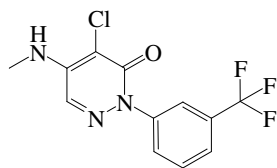
4.0 (soil, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: reported field $t_{1/2} = 3$ to 25 d and the recommended field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

17.1.1.58 Norflurazon



Common Name: Norflurazon

Synonym: Zorial, Solicam, Evital, Telok

Chemical Name: 4-chloro-5-(methylamino)-2[3-(trifluoromethyl)phenyl]-3-(2*H*)-pyridazinone

CAS Registry No: 27314-13-2

Uses: herbicide

Molecular Formula: C₁₂H₉ClF₃N₃O

Molecular Weight: 303.666

Melting Point (°C):

184 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0275 (mp at 184°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

- 28 (Kenaga & Goring 1980; Kenaga 1980b; Gerstl & Helling 1987; Isensee 1991)
- 28 (Ashton & Crafts 1981; Worthing & Walker 1987; Herbicide Handbook 1989; Tomlin 1994)
- 40 (Spencer 1982)
- 28 (23°C, Hartley & Kidd 1987)
- 28 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996; quoted, Senseman et al. 1997)

Vapor Pressure (Pa at 25°C or as indicated):

- 2.7 × 10⁻⁶ (20°C, Ashton & Crafts 1981; Spencer 1982)
- 2.8 × 10⁻⁶ (20°C, Worthing & Walker 1987; Tomlin 1994)
- 2.7 × 10⁻⁶, 3.3 × 10⁻⁵, 3.3 × 10⁻⁴, 1.6 × 10⁻³, 1.3 × 10⁻² (20, 40, 60, 80, 100°C, Herbicide Handbook 1989)
- 9.24 × 10⁻⁵ (20–25°C, Majewski & Capel 1995)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 3.04 × 10⁻⁵ (20–25°C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{ow}:

- 2.30 (22°C, shake flask-UV, Braumann & Grimme 1981)
- 2.52 (shake flask, Takahashi et al. 1993)
- 2.45 (pH 6.5, Tomlin 1994)
- 2.30 (recommended, Hansch et al. 1995)
- 2.30 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
- 2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_B:

- 1.97 (fish, calculated-solubility, Kenaga 1980b; Isensee 1991)

Sorption Partition Coefficient, $\log K_{oc}$:

- 3.28 (soil, Kenaga & Goring 1980)
- 2.85 (calculated-solubility, Kenaga 1980b)
- 3.28, 3.07 (soil: quoted, calculated-MCI χ , Gerstl & Helling 1987)
- 2.85 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.02, 2.64, 3.02, 2.46 2.59 (sandy loam, Mississippi loam, Mississippi sediment, Keaton sandy loam, Biggs clay, Tomlin 1994)
- 3.75 (calculated-MCI χ , Meylan et al. 1992)
- 3.28 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 2.78 (soil, Senseman et al. 1997)

Environmental Fate Rate Constants, or Half-Lives, $t_{1/2}$:

Volatilization: dissipated in soil by photodegradation and volatilization, $t_{1/2} = 45\text{--}180$ d (Tomlin 1994)

Photolysis: rapidly degraded by sunlight (Worthing 1987; Tomlin 1994)

dissipated in soil by photodegradation and volatilization, $t_{1/2} = 45\text{--}180$ d (Tomlin 1994)

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 3.4$ and 1.9 d reported in the absence and presence of 20 ppm H_2O_2 (quoted, Massad et al. 2004)

Ground water:

Sediment:

Soil: the average $t_{1/2} = 45\text{--}130$ d residues in soil from the Delta and Southeast depending on clay and organic content (Herbicide Handbook 1989)

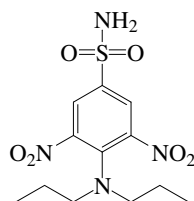
field $t_{1/2} \sim 30$ d (estimated, Wauchope et al. 1992; Hornsby et al. 1996)

dissipated in soil by photodegradation and volatilization, $t_{1/2} = 45\text{--}180$ d (Tomlin 1994)

soil $t_{1/2} = 90$ d (Senseman et al. 1997)

Biota:

17.1.1.59 Oryzalin



Common Name: Oryzalin

Synonym: Dirimal, EL 119, Rycelan, Ryzelon, Ryzelan, Surflan

Chemical Name: 4-(dipropylamino)-3,5-dinitrobenzene-sulfonamide; 3,5-dinitro-*N*^d, *N*^d-dipropylsulfanilamide

Uses: herbicide for pre-emergence control of many annual grasses and broadleaf weeds in cotton, fruit trees, vines, nut trees, soybeans, groundnuts, oilseed rape, sunflowers, lucerne, peas, sweet potatoes, mint, ornamentals and also used in noncrop areas.

CAS Registry No: 19044-88-3

Molecular Formula: C₁₂H₁₈N₄O₆S

Molecular Weight: 346.359

Melting Point (°C):

141 (Lide 2003)

Boiling Point (°C): 265 (dec. Tomlin 1994)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

351.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

9.40 (Worthing & Hance 1991; Tomlin 1994)

8.60 (Wauchope et al. 1992; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0728 (mp at 141°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

- 2.4 (Martin & Worthing 1977; Spencer 1982; Ashton & Crafts 1981)
- 2.6 (Weber et al. 1980)
- 2.5 (Hartley & Kidd 1987; Budavari 1989; Milne 1995)
- 2.4 (Worthing & Walker 1987, Worthing & Hance 1991)
- 2.6 (Herbicide Handbook 1989; Tomlin 1994)
- 2.5 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.5 (calculated-group contribution fragmentation method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated):

- < 1.33 × 10⁻⁵ (30°C, Ashton & Crafts 1981)
- < 1.30 × 10⁻⁵ (30°C, Hartley & Kidd 1987)
- < 1.33 × 10⁻⁶ (Herbicide Handbook 1989; Tomlin 1994)
- < 1.33 × 10⁻⁵ (30°C, Budavari 1989)
- < 1.30 × 10⁻⁶ (Worthing & Hance 1991)
- < 1.30 × 10⁻⁶ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.000188 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow}:

- 4.13 (selected, Dao et al. 1983)
- 3.73 (Worthing & Hance 1991)

- 3.72 (pH 7, Tomlin 1994)
- 3.73 (Milne 1995)
- 3.73 (selected, Hansch et al. 1995)
- 2.79 (MedChem master file or ClogP program, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

- 2.58 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

- 3.43 (soil, calculated-S, Kenaga 1980)
- 2.78 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.78 (estimated-chemical structure, Lohninger 1994)
- 2.85–3.04 (Tomlin 1994)
- 3.40 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 3.40; 3.18 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

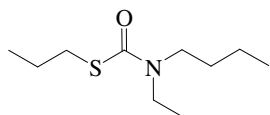
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: in soil, microbial degradation occurs rapidly, $t_{1/2}$ = 2.1 months for aerobic and $t_{1/2}$ = 10 d for anaerobic metabolism (Tomlin 1994).

Half-Lives in the Environment:

Soil: selected field $t_{1/2}$ = 20 d (Wauchope et al. 1992; Hornsby et al. 1996);
 $t_{1/2}$ = 2.1 months for aerobic degradation and $t_{1/2}$ = 10 d for anaerobic degradation (Tomlin 1994).

17.1.1.60 Pebulate



Common Name: Pebulate

Synonym: PEBC, R-2061, Stauffer 2061, Tillam, Timmam-6-E

Chemical Name: *S*-propyl butylethyl(thiocarbamate); *S*-propyl butylethylcarbamothioate

Uses: selective pre-emergence herbicide to control annual grasses and broadleaf weeds in tomatoes, sugar beet, and tobacco.

CAS Registry No: 1114-71-2

Molecular Formula: $C_{10}H_{21}NOS$

Molecular Weight: 203.345

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

142 (at 20 mmHg, Hartley & Kidd 1987; Budavari 1989; Montgomery 1993; Milne 1995)

142 (at 21 mmHg, Herbicide Handbook 1989)

Density (g/cm^3 at $20^{\circ}C$):

0.956 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

0.9555 (Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

258.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

92 ($21^{\circ}C$, Woodford & Evans 1963)

92 ($21^{\circ}C$, Spencer 1973, 1982)

60 (Herbicide Handbook 1978, 1989; quoted, Kenaga 1980; Kenaga & Goring 1980)

60 (Ashton & Crafts 1973, 1981)

60 ($20^{\circ}C$, Khan 1980; Hartley & Kidd 1987; Tomlin 1994; Montgomery 1993; Milne 1995)

60 ($20^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991)

100 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

4.67 (Ashton & Crafts 1973, 1981; Herbicide Handbook 1989)

3.60 ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

9.06 ($30^{\circ}C$, Khan 1980)

0.216 ($20^{\circ}C$, GC-RT correlation, Kim 1985)

9.00 ($30^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

3.50 ($20^{\circ}C$, selected, Suntio et al. 1988)

4.70 (Worthing & Hance 1991; Tomlin 1994)

1.186 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

9.064 ($20^{\circ}C$, Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

11.67 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

11.65 ($20^{\circ}C$, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.78 (selected, Magee 1991)

3.84 (Worthing & Hance 1991; Montgomery 1993; Milne 1995)

- 3.83 (Tomlin 1994)
- 3.84 (selected, Hansch et al. 1995)
- 4.19, 3.74, 3.27 (RP-HPLC, CLOGP, calculated-S, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.79 (calculated-S, Kenaga 1980)
- 1.54 (calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

- 2.80 (soil, Hamaker & Thompson 1972)
- 2.66 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.80 (reported as log K_{OM} , Magee 1991)
- 2.65 (estimated as log K_{OM} , Magee 1991)
- 2.63 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.80 (Montgomery 1993)
- 2.63 (selected, Lohninger 1994)
- 2.80 (quoted or calculated-QSAR MCI χ , Sabljic et al. 1995)
- 2.48, 2.10 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: in soil, microbial degradation $t_{1/2} = 2\text{--}3$ wk (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 11$ d, at pH 4 and pH 10, $t_{1/2} = 12$ d at pH 7 (40°C, Tomlin 1994).

Ground water:

Sediment:

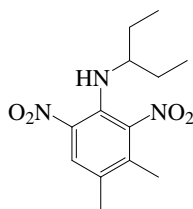
Soil: $t_{1/2} \sim 2$ wk in moist loam soil at 21–27°C (Herbicide Handbook 1989; Montgomery 1993);

selected field $t_{1/2} = 14$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 2\text{--}3$ wk (Tomlin 1994);.

Biota:

17.1.1.61 Pendimethalin



Common Name: Pendimethalin

Synonym: penoxalin

Chemical Name: *N*-(1-ethylpropyl-3,4-dimethyl-2,6-dinitrobenzenamine

CAS Registry No: 40487-42-1

Uses: herbicide

Molecular Formula: C₁₃H₁₉N₃O₄

Molecular Weight: 281.308

Melting Point (°C):

56 (Lide 2003)

Boiling Point (°C):

330 (Ashton & Crafts 1981; Herbicide Handbook 1989)

decomposes on heating (Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm³ at 25°C):

1.19 (Ashton & Crafts 1981; Montgomery 19993; Tomlin 1994)

1.12 (Hartley & Kidd 1987)

1.17 (Herbicide Handbook 1989)

Molar Volume (cm³/mol):

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.496 (mp at 56°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.50 (23°C, Ashton & Crafts 1981)

0.30 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

0.275 (Herbicide Handbook 1989)

0.275 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.61 (20–25°C, Majewski & Capel 1995)

Vapor Pressure (Pa at 25°C or as indicated):

0.004 (Ashton & Crafts 1981; Herbicide Handbook 1989)

0.004 (Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)

1.25 × 10⁻³ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.004 (Montgomery 1993)

8.16 × 10⁻³ (20–25°C, Majewski & Capel 1995)

0.00123; 0.00776 (liquid P_L, GC-RT correlation; quoted lit., Donovan 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.0867 (Montgomery 1993)

3.75 (20–25, calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{ow}:

5.18 (Montgomery 1993)

5.18 (Tomlin 1994)

5.24 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

2.95	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
4.20	(soil, Bottoni & Funari 1992)
4.14, 4.47	(loam, pH 7, pH 6.5, quoted, Montgomery 1993)
3.81	(sand, pH 7.6, Montgomery 1993)
4.07, 4.14	(sandy loam pH 6.4, silty loam, pH 7.0, Montgomery 1993)
1.48–2.93	(soil, Montgomery 1993)
3.70	(soil, Senseman et al. 1997)
3.14	(soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: slowly decomposed by light (Hartley & Kidd 1987; Tomlin 1994).

Oxidation:

Hydrolysis: $t_{1/2} < 21$ d (Montgomery 1993).

Biodegradation: observed $t_{1/2} = 33$ d, 45 d, 52 d and 67 d in flooded and nonflooded conditions in nonsterile and sterile soils, respectively, in the study of degradation of pendimethalin under the influence of soil moisture and microbial activity in a sandy loam soil, in both nonsterile nonflooded and flooded soil, degradation followed first-order kinetics. (Kulshrestha & Singh 1992; quoted, Montgomery 1993).

Biotransformation: Degradation by abiotic reductive transformations:

$k = 1.25 \text{ M}^{-1} \text{ s}^{-1}$ in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 0.50 \times 10^{-3} \text{ h}^{-1}$ at pH 6.5, $k = 0.27 \times 10^{-2} \text{ h}^{-1}$ at pH 7.0, $k = 0.093 \text{ h}^{-1}$ at pH 7.4, and $k = 0.81 \text{ h}^{-1}$ at pH 7.8 for aqueous ferrous ion system;

$k = 0.216 \text{ h}^{-1}$ at pH 6.5, $k = 0.274 \text{ h}^{-1}$ at pH 6.7, $k = 0.918 \text{ h}^{-1}$ at pH 7.0, and $k = 2.10 \text{ h}^{-1}$ at pH 7.3 for Fe(II)/goethite system;

$k = 3.81 \times 10^{-3} \text{ h}^{-1}$ at pH 6.5, $k = 2.66 \times 10^{-3} \text{ h}^{-1}$ at pH 7.0, $k = 1.13 \times 10^{-2} \text{ h}^{-1}$ at pH 7.4 and $k = 1.74 \times 10^{-2} \text{ h}^{-1}$ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} < 21$ d in water (Tomlin 1994).

Ground water: reported $t_{1/2} = 30$ –90 d (Bottoni & Funari 1992)

Sediment:

Soil: $t_{1/2} = 98$ and 409 d at 30 and 10°C in a sandy loam soil with 75% moisture (Walker & Bond 1977)

$t_{1/2} = 4$ d on Bosket silt loam, $t_{1/2} = 6$ d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with $t_{1/2} = 18$ d on Bosket silt loam, $t_{1/2} = 27$ d on Sharkey clay (Savage & Jordon 1980)

$t_{1/2} = 58$ –63 d in IARI sandy loam soil under Indian tropical climate (Kulshrestha & Yaduraju 1987)

$t_{1/2} = 30$ –90 d or persistence (Bottoni & Funari 1992)

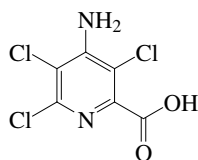
$t_{1/2} = 66.9$ d in sterile, $t_{1/2} = 52.2$ d in nonsterile non-flooded sandy loam soil; $t_{1/2} = 44.9$ d in sterile and 33.4 d in nonsterile flooded sandy loam soil in the study of degradation under the influence of soil moisture and microbial activity (Kulshrestha & Singh 1992; quoted, Montgomery 1993)

reported field $t_{1/2} = 8$ –480 d, recommended $t_{1/2} = 90$ d (Wauchope et al 1992; Hornsby et al. 1996);

soil $t_{1/2} = 90$ d (Senseman et al. 1997).

Biota: $t_{1/2} = 3$ –4 months (quoted, Hartley & Kidd 1987; Tomlin 1994)

17.1.1.62 Picloram



Common Name: Picloram

Synonym: Amdon, ATCP, Borolin, Grazon, K-Pin, Tordon

Chemical Name: 4-amino-3,5,6-trichloropicolinic acid; 4-amino-3,5,6-trichloro-2-pyridinecarboxylic acid

Uses: systemic herbicide to control most broadleaf weeds on grassland and noncropland.

CAS Registry No: 1918-02-1

Molecular Formula: $C_6H_3Cl_3N_2O_2$

Molecular Weight: 241.459

Melting Point ($^{\circ}C$):

218.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

204.2 (calculated-Le Bas method at normal boiling point, Suntio et al. 1988)

Dissociation Constant pK_a :

3.43, 3.42, 3.39, 3.36 (10, 20, 30, $40^{\circ}C$, Cheung & Biggar 1974)

1.90 (Weber et al. 1980; Willis & McDowell 1982)

3.60 (Windholz 1983; quoted, Howard 1991; Yao & Haag 1991; Haag & Yao 1992; Montgomery 1993)

2.3 ($22^{\circ}C$, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

1.94 (Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0126 (mp at $218.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

430 (Bailey & White 1965; Freed 1966; Khan 1980; Weber et al. 1980; Ashton & Crafts 1981; Spencer 1982)

546* ($20^{\circ}C$, shake flask-IR, measured range $10-40^{\circ}C$, pH 2.8, distilled water, Cheung & Biggar 1974)

73.65* ($20^{\circ}C$, shake flask-IR, measured range $10-40^{\circ}C$ at pH 0.2, Cheung & Biggar 1974)

62.7* ($20^{\circ}C$, shake flask-IR, measured range $10-40^{\circ}C$ at pH 1.1, Cheung & Biggar 1974)

137* ($20^{\circ}C$, shake flask-IR, measured range $10-40^{\circ}C$ at pH 2.0, Cheung & Biggar 1974)

19560* ($20^{\circ}C$, shake flask-IR, measured range $10-40^{\circ}C$ at pH 4.2, Cheung & Biggar 1974)

74593* ($20^{\circ}C$, shake flask-IR, measured range $10-40^{\circ}C$ at pH 4.7, Cheung & Biggar 1974)

430 (Martin & Worthing 1977, Worthing & Hance 1991; quoted, Kenaga 1980; Kenaga & Goring 1980; Isensee 1991; Howard 1991)

430 (Hartley & Graham-Bryce 1980; Taylor & Glotfelty 1988)

430 (Hartley & Kidd 1987; Herbicide Handbook 1989; Tomlin 1994; Milne 1995)

400-430 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

7.30×10^{-7} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

8.20×10^{-5} ($35^{\circ}C$, Khan 1980; Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989)

8.26×10^{-5} ($20-25^{\circ}C$, Weber et al. 1980; Willis & McDowell 1982)

9.70×10^{-9} (Dobbs & Cull 1982; quoted, Howard 1991)

7.30×10^{-6} ($20^{\circ}C$, quoted from Hartley & Graham-Bryce 1980, Dobbs et al. 1984)

6.00×10^{-5} ($20^{\circ}C$, selected, Suntio et al. 1988)

1.40×10^{-4} ($45^{\circ}C$, Herbicide Handbook 1989)

- 4.50×10^{-8} (quoted, Nash 1989)
- 7.40×10^{-7} (20°C, selected, Taylor & Spencer 1990)
- 8.20×10^{-5} (35°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

- 3.40×10^{-5} (20°C, calculated-P/C, Suntio et al. 1988; quoted, Mabury & Crosby 1996)
- 4.20×10^{-7} (calculated-P/C, Taylor & Glotfelty 1988)
- 2.50×10^{-5} (calculated-P/C, Nash 1989)
- 4.10×10^{-6} (calculated-P/C, Howard 1991)
- 3.40×10^{-5} (20–35°C, calculated-P/C, Montgomery 1993)
- 3.17×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 0.30 (Kenaga 1975)
- 0.63 (selected, Dao et al. 1983)
- 0.30 (Hansch & Leo 1985; Hansch et al. 1995;)
- −3.47 (selected, Gerstl & Helling 1987)
- 1.166 (calculated as per Broto et al. 1984, Karcher & Devillers 1990)
- 0.26, 0.30 (quoted, Sangster 1993)
- 1.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, $\log BCF$:

- −1.70 (fish in static water, quoted from Dow Chemical data, Kenaga & Goring 1980)
- 1.30 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
- −0.222 (calculated- K_{oc} , Kenaga 1980)
- 0.0 (estimated- K_{ow} , Lyman et al. 1982; quoted, Howard 1991)
- 1.49 (fish in flowing water, Garten & Trabalka 1983; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{oc}$:

- 1.23 (soil, Hamaker & Thompson 1972)
- 1.10 (average in soil, Hamaker & Thompson 1972)
- 1.10 (average in soil, Reinhold et al. 1979)
- 1.23 (Kenaga & Goring 1980; quoted, Bahnick & Doucette 1988)
- 2.20 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 1.41 (av. of 26 soils, Rao & Davidson 1980)
- 1.40 (soil, Rao & Davidson 1982)
- 1.31, 1.05, 1.34, 1.0, 1.26, 1.10, 1.05 (Catlin soil, Commerce soil, Fargo soil, Holdredge soil, Norfolk soil, Kawkawlin soil, Walla-Walla soil, McCall & Agin 1985; quoted, Brusseau & Rao 1989)
- 2.11 (calculated-MCI χ , Gerstl & Helling 1987)
- 1.68 (screening model calculations, Jury et al. 1987b)
- 1.47 (calculated-MCI χ , Bahnick & Doucette 1988)
- 1.88 (Nash 1989)
- 1.23 (reported as $\log K_{OM}$, Magee 1991)
- 1.20 (organic carbon, Wauchope et al. 1991)
- 1.11, 1.41, 1.68 (soil, quoted values, Bottoni & Funari 1992)
- 1.41 (Montgomery 1993)
- 1.30 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 1.55, 1.39, 2.38 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH 2.0–10.5, average, Delle Site 2001)
- 3.07, 2.96, 3.30 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH ≤ 2.0 undissociated, average, Delle Site 2001)
- 1.80, 1.76 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, pH 4.2–5.9, average, Delle Site 2001)
- 1.12, 2.02, 1.93 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, pH ≥ 6.0 , dissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 200$ h for 40% of 4,840 $\mu\text{g/mL}$ to degrade in dilute NaOH solution under sunlight (Hall et al. 1968; quoted, Cessna & Muir 1991);

$t_{1/2} = 2.3$ d to 9.58 d direct photolysis by sunlight under various conditions, at depths of 2.54 cm–3.65 m at various times of the year; one result at 3.65 m during Sept.–Oct. gave $t_{1/2} = 41.3$ d; distilled water and canal water gave essentially the same results in one set of experiments (Hedlund & Youngson 1972; quoted, Cessna & Muir 1991; Howard 1991);

$t_{1/2} = 72$ h for 99% of 548 $\mu\text{g mL}^{-1}$ to degrade in Na salt solution under 300–380 nm light (Mosier & Guenzi 1973; quoted, Cessna & Muir 1991);

$t_{1/2} = 0.5$ h for 38% of 265 $\mu\text{g mL}^{-1}$ to degrade in distilled water under 254 nm light (Glass 1975; quoted, Cessna & Muir 1991);

$t_{1/2} = 2.2$ d for < 2.4 $\mu\text{g mL}^{-1}$ L to degrade in distilled water under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991);

$t_{1/2} = 16$ h in surface water estimated from direct midday sunlight photolysis in mid-summer at 40°N (Zepp 1991).

Oxidation:

photooxidation: $t_{1/2} = 12.21$ d in air, based on estimated rate constant for the reaction with photochemically produced hydroxyl radical in the atmosphere (GEMS 1986; quoted, Howard 1991)

$k = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 2.1–3.7 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k(\text{aq.}) = (50\text{--}150) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.5–4.9 and $21 \pm 1^\circ\text{C}$, with $t_{1/2} = 4.0$ min at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = (3.4 \pm 0.3) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radicals in aqueous solutions at pH 2.1–3.7 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992)

$k(\text{aq.}) = 1.3 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with hydroxyl radical, in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

Hydrolysis:

Biodegradation: $t_{1/2} = 128\text{--}144$ h in mixture of 5 g soil and 1–4 mL water, $t_{1/2} = 90\text{--}1000$ h in mixture of 1 mL water with 0.25–10 g soil, (Hance 1969; quoted, Howard 1991);

$t_{1/2} > 15$ months for 0.07, 0.72 and 10 $\mu\text{g mL}^{-1}$ to biodegrade in groundwater (Weidner 1974; quoted, Muir 1991);

$k = 0.0073 \text{ d}^{-1}$ by soil incubation die-away test studies (Rao & Davidson 1980; quoted, Scow 1982);

biochemical $t_{1/2} = 100$ d from screening model calculations (Jury et al. 1987b);

$t_{1/2} = 30\text{--}300$ d, degraded slowly by soil microorganisms (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 12.21$ d, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (GEMS 1986; quoted, Howard 1991).

Surface water: $t_{1/2} = 2.6$ d decomposed by UV irradiation (Tomlin 1994);

measured rate constant $k = (50 - 150) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.5–4.9 and 21°C , with $t_{1/2} = 4.0$ min at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} > 15$ months for 0.07, 0.72 and 10 $\mu\text{g/mL}$ to biodegrade in ground water (Weidner 1974; quoted, Muir 1991);

measured rate constant $k \leq 0.005 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C , with $t_{1/2} \geq 80$ d at pH 7 (Yao & Haag 1991)

reported $t_{1/2} = 30\text{--}330, 138, 180$ and 206 d (Bottoni & Funari 1992).

Sediment:

Soil: estimated persistence of 18 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987b);

persistent in soils with $t_{1/2} > 5$ yr (Alexander 1973; quoted, Howard 1991);

estimated first-order $t_{1/2} = 95$ d in soil from biodegradation rate constant $k = 0.0073 \text{ d}^{-1}$ by soil incubation die-away test studies (Rao & Davidson 1980; quoted, Scow 1982);

persistent in soil with $t_{1/2} > 100$ d (Willis & McDowell 1982);
 $t_{1/2} = 100$ d from screening model calculations (Jury et al. 1987b);
 selected $t_{1/2} = 90$ d (Wauchope et al. 1991; quoted, Dowd et al. 1993);
 reported $t_{1/2} = 30$ –330 d, 18 d, 180 d and 206 d (Bottoni & Funari 1992);
 $t_{1/2} = 3$ –330 d (Tomlin 1994).

Biota: biochemical $t_{1/2} = 100$ d from screening model calculations (Jury et al. 1987b);
 average $t_{1/2} = 60$ d in the forest (USDA 1989; quoted, Neary et al. 1993).

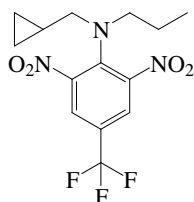
TABLE 17.1.1.62.1

Reported aqueous solubilities of picloram at various temperatures

Cheung & Biggar 1974

shake flask-IR spec.						
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$
	pH 0.20	pH 1.10	pH 2.0	pH 2.8	pH 4.2	pH 4.7
10	43.95	39.12	89.11	475	22240	84446
20	73.65	62.78	136.92	545.74	19560	74953
30	119.5	108.9	205.3	683.4	21395	82248
40	214.9	199	316.3	704.5	21371	78240
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1})$	38.49	38.91	31.38	12.97	0	0

17.1.1.63 Profluralin



Common Name: Profluralin

Synonym: CGA 10832, Pregard, Tolban

Chemical Name: *N*-(cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzenamine; *N*-(cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl) benzenamine

Uses: herbicide for pre-planting by soil incorporation to control annual and perennial broadleaf and grass weeds in cotton, soybeans, brassicas, capsicums, tomatoes and other crops.

CAS Registry No: 26399-36-0

Molecular Formula: $C_{14}H_{16}F_3N_3O_4$

Molecular Weight: 347.290

Melting Point ($^{\circ}C$):

34 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.45 ($25^{\circ}C$, Ashton & Crafts 1981)

1.38 (Hartley & Kidd 1987; Worthing & Hance 1991)

Molar Volume (cm^3/mol):

304.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.816 (mp at $34^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.10 ($20^{\circ}C$, Weber 1972)

0.10 (Spencer 1973, 1982; Wauchope 1978; Kenaga 1980)

0.10 ($27^{\circ}C$, Ashton & Crafts 1973, 1981)

0.10 (shake flask-HPLC, Ellgehausen et al. 1981)

0.10 ($20^{\circ}C$, Hartley & Kidd 1987; Milne 1995)

0.10 ($20^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991)

0.10 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0092 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

0.0092 ($20^{\circ}C$, Ashton & Crafts 1973, 1981)

0.0084 ($20^{\circ}C$, Hartley & Kidd 1987)

0.0084 ($20^{\circ}C$, Worthing & Hance 1991)

0.0084 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

39.07 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

31.91 ($20^{\circ}C$, calculated-P/C, Muir 1991)

Octanol/Water Partition Coefficient, log K_{ow} :

5.16 (selected, Dao et al. 1983)

6.34 (shake flask-HPLC/UV, Ellgehausen et al. 1981)

6.34 (recommended, Sangster 1993)

- 4.46 (calculated-fragment const., Pinsuwan et al. 1995)
 6.34 (recommended, Hansch et al. 1995)
 5.08 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

- 3.35 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 2.83 (calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

- 3.93 (soil, exptl., Kenaga 1980)
 4.19 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 3.83 (estimated as log K_{OM} , Magee 1991)
 3.93 (soil, quoted exptl., Meylan et al. 1992)
 4.26 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 4.00 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 4.16 (selected, Lohninger 1994)
 4.01 (soil, calculated-QSAR MCI χ , Sabljic et al. 1995)
 3.87 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 1.2$ d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} = 12$ d for 0.5 $\mu\text{g mL}^{-1}$ to biodegrade in flooded soils at 20–42°C (Savage 1978; quoted, Muir 1991);

Degradation $t_{1/2} < 1$ month in three soils, Goldsborol loamy sand, Cecil loamy sand Drummer clay loam treated with 1 ppm profluralin) for 4 month under aerobic conditions, no degradation in sterile controls. (shake flask-TLC, Camper et al. 1980)

$t_{1/2} < 1$ month for 1 $\mu\text{g/mL}$ to biodegrade in flooded soils at 25°C (derived from results of Camper et al. 1980, Muir 1991);

biodegradation $t_{1/2} < 20$ d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: biodegradation $t_{1/2} < 20$ d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).

Ground water:

Sediment: biodegradation $t_{1/2} < 20$ d in water and sediment with flooded soils and terrestrial-aquatic model ecosystems (Muir 1991).

Soil: $t_{1/2} = 12$ d for 0.5 $\mu\text{g mL}^{-1}$ to biodegrade in flooded soils at 20–42°C (Savage 1978, Muir 1991) persistence of 12 months in soil (Wauchope 1978);

aerobic and anaerobic degradation $t_{1/2} < 1$ month in 3 flooded soils at 25°C (Camper et al. 1980);

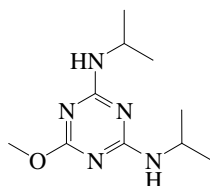
field studies, $t_{1/2} = 10.9$ wk - 1978 first study; $t_{1/2} = 10.1$ wk -1978 second study; $t_{1/2} = 11.5$ wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)

laboratory studies: $t_{1/2} = 19.9$ wk at 4°C, $t_{1/2} = 6.7$ wk at 25°C for soil of field capacity moisture (27% w/w for Crowley silt loam), $t_{1/2} = 20.4$ wk at 4°C, $t_{1/2} = 4.8$ wk at 25°C for flooded soils, Crowley silt loam; and $t_{1/2} = 25.8$ wk at 4°C, $t_{1/2} = 8.6$ wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay), $t_{1/2} = 21.3$ wk at 4°C and $t_{1/2} = 6.2$ wk at 25°C for flooded soils, Sharkey silty clay (Brewer et al. 1982);

selected field $t_{1/2} = 110$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

17.1.1.64 Prometon



Common Name: Prometon

Synonym: G 31435, Gesafram, Gesagram, Methoxypropazine, Ontracac 800, Ontrack, Pramitol, Prometone

Chemical Name: 6-methoxy-*N,N'*-bis(methylethyl)-1,3,5-triazine-2,4-diamine; 2,4-bis(isopropylamino)-6-methoxy-1,3,5-triazine

Uses: nonselective pre-emergence and post-emergence herbicide to control most annual and broadleaf weeds, grasses, and brush weeds on noncropland.

CAS Registry No: 1610-18-0

Molecular Formula: C₁₀H₁₉N₅O

Molecular Weight: 225.291

Melting Point (°C):

91.5 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.088 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm³/mol):

280.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

4.28 (pK_a, Weber 1970; quoted, Bintein & Devillers 1994)

4.30 (pK_a, 21°C, Worthing & Hance 1991; Montgomery 1993)

9.73 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)

9.7 (21°C, pK_b, Tomlin 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

90.77 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.175 (DSC method, Plato & Glasgow 1969)

21.6 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.223 (mp at 91.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

750 (20°C, Bailey & White 1965; Ashton & Crafts 1981; Herbicide Handbook 1989)

1000, 678, 669 (26°C, pH 3.0, 7.0, 10.0, shake flask-UV, Ward & Weber 1968)

750 (Martin & Worthing 1977; Herbicide Handbook 1978)

677 (Weber et al. 1980)

620 (20°C, Spencer 1982)

750 (20°C, Verschueren 1983)

750 (20°C, Hartley & Kidd 1987; Montgomery 1993)

620 (20°C, Worthing & Walker 1987, 1991; Tomlin 1994)

720 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

3.07 × 10⁻⁴ (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stambach 1964) (See figure at the end of this section.)

log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stambach 1964)

0.00030 (20°C, Khan 1980)
 0.00031 (20°C, Ashton & Crafts 1981; Worthing & Hance 1991)
 0.00083 (Jury et al. 1984; selected, Spencer et al. 1988; Spencer & Cliath 1990; Taylor & Spencer 1990)
 0.00031 (20°C, Hartley & Kidd 1987)
 0.00031, 0.00105 (20°C, 30°C, Herbicide Handbook 1989)
 1.0×10^{-3} , 3.30×10^{-2} , 0.65, 8.60, 82 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
 $\log (P_g/P_a) = 16.525 - 5817.4/(T/K)$; measured range 32.1–89.3°C (gas saturation-GC, Rordorf 1989)
 $\log (P_L/P_a) = 13.617 - 4741.7/(T/K)$; measured range 92.3–140°C (gas saturation-GC, Rordorf 1989)
 0.00103 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.00031 (20°C, Montgomery 1993)
 0.000306 (20°C, Tomlin 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

2.50×10^{-4} (calculated-P/C, Jury et al. 1984; Spencer et al. 1988; Spencer & Cliath 1990)
 9.02×10^{-5} (20°C, calculated-P/C, Montgomery 1993)
 9.01×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.94 (selected, Dao et al. 1983)
 1.94 (Gerstl & Helling 1987)
 2.99 (RP-HPLC-RT correlation, Finizio et al. 1991; quoted, Sangster 1993)
 2.85 (selected, Magee 1991)
 2.55 (shake flask-UV, Liu & Qian 1995)
 2.69, 2.99 (Montgomery 1993)
 2.99 (recommended, Hansch et al. 1995)
 2.82 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

1.18 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 1.28 (calculated- K_{oc} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

2.54 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
 2.04 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 2.61 (Jury et al. 1984; quoted, Spencer & Cliath 1990)
 2.40 (calculated-MCI χ , Gerstl & Helling)
 2.48 (Spencer et al. 1988)
 2.35 (estimated as $\log K_{om}$, Magee 1991)
 2.20 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 2.18 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 1.92–2.24 (Montgomery 1993)
 2.77 (selected, Lohninger 1994)
 2.39 (calculated- K_{ow} , Liu & Qian 1995)
 2.50 (soil, calculated-MCI χ , Sabljic et al. 1995)
 2.60; 2.70, 2.68 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 2.47, 2.50 (soils: organic carbon $\text{OC} \geq 0.1\%$, $\text{OC} \geq 0.5\%$, pH 4.3–7.1, average, Delle Site 2001)
 2.81, 2.65, 2.53 (soils with organic carbon $\text{OC} \geq 0.5\%$ at: pH 4.3–4.9, pH 5.0–5.9, pH- 6.0, average, Delle Site 2001)

Environmental Fate Rate Constants, or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 100$ d (Spencer & Cliath 1990).

Photolysis: $t_{1/2} = 2.25$ h for 1% of $100 \mu\text{g mL}^{-1}$ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: selected field $t_{1/2} = 500$ d (Wauchope et al. 1992; Hornsby et al. 1996).

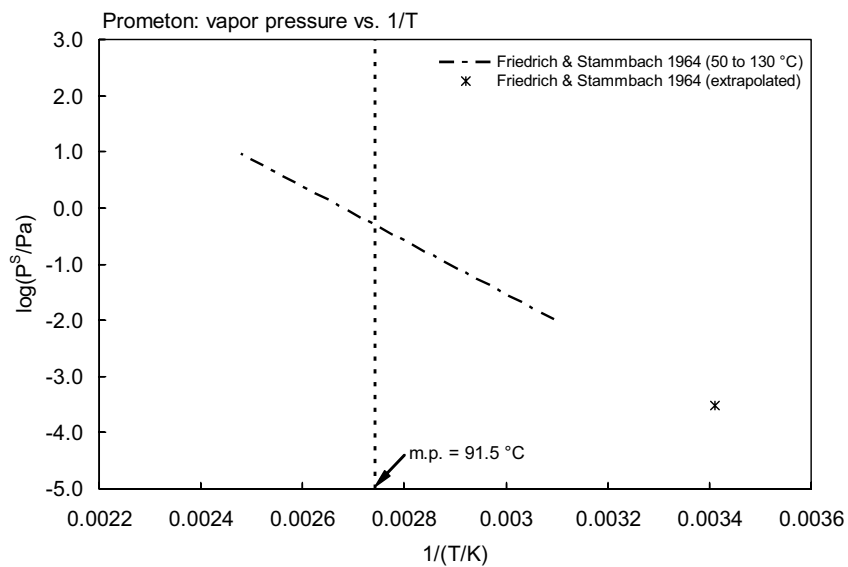
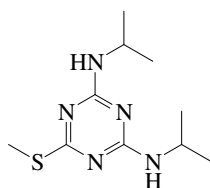


FIGURE 17.1.1.64.1 Logarithm of vapor pressure versus reciprocal temperature for prometon.

17.1.1.65 Prometryn



Common Name: Prometryn

Synonym: Caparol, Cotton-Pro, Gesagard, G-34161, Mercasin, Mercazin, Polisin, Primatol, Prometrex, Prometrin, Selectin, Sesagard, Uvon

Chemical Name: *N,N'*-bis(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine; 2,4-bis(isopropylamino)-6-(methylthio)-1,3,5-triazine

Uses: selective herbicide to control many annual grass and broadleaf weeds in celery, cotton and peas.

CAS Registry No: 7287-19-6

Molecular Formula: C₁₀H₁₉N₅S

Molecular Weight: 241.357

Melting Point (°C):

119 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.157 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Molar Volume (cm³/mol):

299.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

4.05 (pK_a, Weber 1970; Pacakova et al. 1988; Somasundaram et al. 1991; Bintein & Devillers 1994)

4.10 (pK_a, 21°C, Weber et al. 1980; Willis & McDowell 1982; Worthing & Hance 1991)

9.95 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)

4.05 (pK_a, 21°C, Montgomery 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

96.43 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

26.36 (DSC method, Plato & Glasgow 1969)

25.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.120 (mp at 119°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

48 (20°C, Woodford & Evans 1963)

48 (20°C, Bailey & White 1965; Ashton & Crafts 1973, 1981; Khan 1980)

206, 40.3, 41.8 (26°C, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

48 (Martin & Worthing 1977; Herbicide Handbook 1978)

40 (Weber et al. 1980)

48 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Milne 1995)

33 (20°C, Worthing & Walker 1987, Worthing & Hance 1991)

33 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

33 (Tomlin 1994; selected, Lohninger 1994)

241 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

1.33 × 10⁻⁴ (20°C, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50–130°C, Friedrich & Stambach 1964) (See figure at the end of this section.)

log (P/mmHg) = 11.911 – 4933/(T/K), temp range 50–130°C (gas saturation-GC, data presented in Antoine eq., Friedrich & Stambach 1964)

0.00028 (from Friedrich & Stambach 1964; Jury et al. 1983; 1984; Spencer & Cliath 1990)
 0.00013 (20°C, Ashton & Crafts 1973, 1981)
 0.00013 (20–25°C, Weber et al. 1980)
 0.00028 (quoted, Jury et al. 1984; Spencer & Cliath 1990)
 0.00013 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
 0.00010 (20°C, selected, Suntio et al. 1988)
 0.00013, 0.00053 (20, 30°C, Herbicide Handbook 1989)
 1.60×10^{-4} , 6.70×10^{-3} , 0.16, 2.50, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
 $\log (P_g/P_a) = 17.063 - 6215.6/(T/K)$; measured range 32.4–117°C (gas saturation-GC, Rordorf 1989)
 $\log (P_L/P_a) = 14.013 - 5037.2/(T/K)$; measured range 129–140°C (gas saturation-GC, Rordorf 1989)
 0.00017 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.000169 (Tomlin 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.00139 (calculated-P/C, Jury et al. 1984; quoted, Spencer & Cliath 1990)
 0.00139 (calculated-P/C, Jury et al. 1987a,b; Jury & Ghodrati 1989)
 0.00050 (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
 0.00050 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.99 (selected, Dao et al. 1983)
 1.91 (RP-HPLC- k' correlation, Braumann et al. 1983)
 3.46 (selected, Yoshioka et al. 1986)
 3.51 (shake flask, Mitsutake et al. 1986)
 2.99 (Gerstl & Helling 1987)
 3.34 (RP-HPLC-RT correlation, Finizio et al. 1991)
 3.43 (selected, Magee 1991)
 3.34 (Worthing & Hance 1991; Milne 1995)
 3.34, 3.46 (Montgomery 1993)
 3.51 (recommended, Sangster 1993)
 2.93 (RP-HPLC- k' correlation, Liu & Qian 1995)
 3.51 (recommended, Hansch et al. 1995)
 3.35 (Pomona-database, Müller & Kördel 1996)
 3.25 (RP-HPLC-RT correlation, Finizio et al. 1997)
 2.99 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$:

1.85, 1.67 (calculated-S, K_{oc} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

2.91 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
 2.72 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 2.79 (Rao & Davidson 1980)
 3.17 (calculated-MCI χ , Gerstl & Helling)
 2.78 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
 2.75 (estimated as $\log K_{om}$, Magee 1991)
 2.72–2.91, 2.79, 2.83 (soil, quoted values, Bottoni & Funari 1992)
 2.60 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.38 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
 2.28–2.79 (Montgomery 1993)
 3.15 (estimated-chemical structure, Lohninger 1994)
 2.60 (soil, Tomlin 1994)
 2.63 (calculated- K_{ow} , Liu & Qian 1995)
 2.85 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

2.38; 2.84 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.54, 1.595, 1.968, 1.77, 2.67 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 3.24, 2.16, 2.86, 2.59, 2.53 (calculated- K_{OW} ; HPLC-screening method with different LC-columns, Szabo et al. 1999)
 2.544, 2.635, 2.484, 1.816, 2.933 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
 2.85, 2.89 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 60$ d (Jury et al. 1984).

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 22$ d in 0.1 N hydrochloric acid solution, $t_{1/2} = 500$ yr at pH 7 in distilled water and $t_{1/2} = 30$ yr in 0.01 sodium hydroxide solution all at 25°C (Montgomery 1993).

Biodegradation: $t_{1/2} = 60$ d (Wauchope 1978);

$t_{1/2} = 60$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1987a,b; Jury & Ghodrati 1989);
 soil microbial degradation $t_{1/2} = 70$ d (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: completely decomposed when exposed to UV light for 3 h (Montgomery 1993).

Ground water: reported half-lives or persistence, $t_{1/2} = 40$ –70, 60 and 94 d (Bottoni & Funari 1992)

Sediment:

Soil: estimated persistence of 3 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a,b; Jury & Ghodrati 1989);

$t_{1/2} \sim 6$ months to biodegrade in flooded soils (Plimmer et al. 1970; quoted, Muir 1991);

persistence of 2 months in soil (Wauchope 1978);

reported $t_{1/2} = 40$ –70 d, 60 d and 94 d (Bottoni & Funari 1992);

selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 70$ d for microbial degradation in soil (Tomlin 1994).

Biota: biochemical $t_{1/2} = 60$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

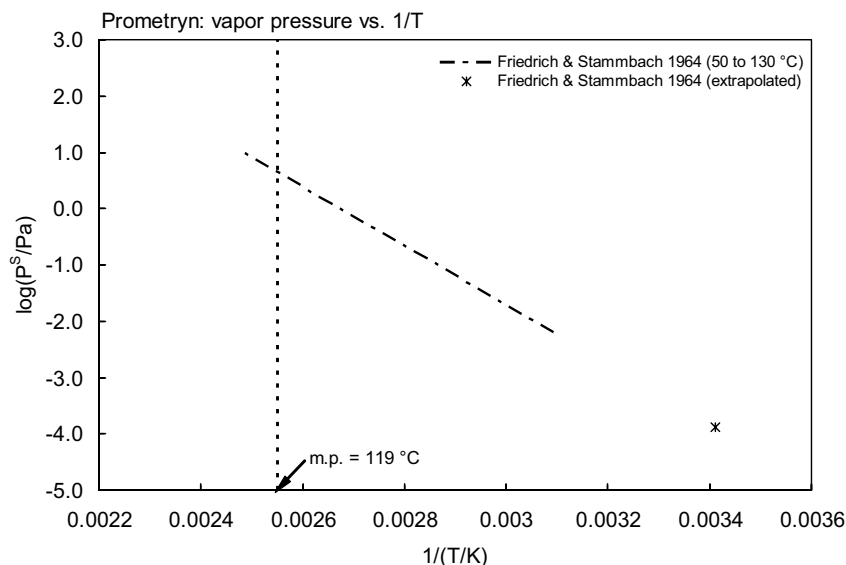
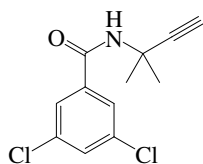


FIGURE 17.1.1.65.1 Logarithm of vapor pressure versus reciprocal temperature for prometryn.

17.1.1.66 Pronamide



Common Name: Pronamide

Synonym: Kerb, Promamide, Propyzamide, RH-315

Chemical Name: 3,5-dichloro-N-(1,1-dimethylpropynyl)benzamide

Uses: herbicide.

CAS Registry No: 23950-58-5

Molecular Formula: $C_{12}H_{11}Cl_2NO$

Molecular Weight: 256.127

Melting Point ($^{\circ}C$):

155 (Lide 2003)

Boiling Point ($^{\circ}C$): 321

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

270.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0530 (mp at $155^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

15 (Martin & Worthing 1977; Herbicide Handbook 1978, 1983; Worthing & Walker 1987)
 15 ($15^{\circ}C$, Khan 1980)
 15 (Ashton & Crafts 1981)
 15 ($24^{\circ}C$, Herbicide Handbook 1989)
 15 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 15 (Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0113 (Khan 1980)
 0.0113 (Ashton & Crafts 1981; Herbicide Handbook 1989)
 0.0536 (Dixon & Rissman 1985; quoted, Howard 1991)
 0.227 (Worthing & Walker 1987)
 0.0113 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.000058 (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.912 (Dixon & Rissman 1985)
 0.193 (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
 0.188 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.26 (estimated, Lyman et al. 1982; quoted, Howard 1991)
 3.36 (selected, Magee 1991)
 3.26 (selected, Dao et al. 1983)
 2.95 (estimated-QSAR and SPARC, Kollig et al. 1993)
 3.09–3.28 (Tomlin 1994; Milne 1995)
 3.87 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, log BCF:

2.13	(calculated-S, Kenaga 1980)
1.00	(calculated- K_{OC} , Kenaga 1980)
2.25	(estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1991)
2.13	(estimated-S, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC} :

2.30	(soil, Leistra et al. 1974; Carlson et al.)
2.30	(measured for single soil, Kenaga 1980)
3.00	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
2.99	(soil, estimated-S, Lyman et al. 1982; quoted, Howard 1991)
2.30; 2.42	(reported as log K_{OM} , estimated as log K_{OM} , Magee 1991)
2.30; 3.20	(soil, quoted; calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.90	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.63	(estimated-QSAR and SPARC, Kollig 1993)
2.54	(selected, Lohninger 1994)
2.31	(soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: based on a Henry's law constant of 0.9118 Pa·m³/mol, $t_{1/2}$ ~ 6.6 d from a river 1-m deep flowing 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982; quoted, Howard 1991).

Photolysis: degraded photolytically on soil thin films, $t_{1/2}$ = 13–57 d in artificial sunlight (Tomlin 1994).

Oxidation: photooxidation $t_{1/2}$ = 4.2 h in air, based on an estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Hydrolysis: neutral hydrolysis rate constant $k < 1.5 \times 10^{-5} \text{ h}^{-1}$ with a calculated $t_{1/2} > 700 \text{ d}$ in neutral solution and with faster hydrolysis rates in acidic and basic solutions to be expected (Ellington et al. 1987, 1988; quoted, Howard 1991).

Biodegradation: depending on soil and climatic conditions, the degradation $t_{1/2}$ = 10 to 112 d, but a $t_{1/2}$ = 40 d may be more common under field conditions (Walker 1976, 1978; Zandvoort et al. 1979; quoted, Howard 1991).

Biotransformation: second-order rate constant $k = 5 \times 10^{-14} \text{ L/organisms} \cdot \text{h}$ with an estimated $t_{1/2}$ ~ 580 d for microbial degradation in natural water (Steen & Collette 1989; quoted, Howard 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 4.2 h, based on an estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radicals in the atmosphere (Atkinson 1985; quoted, Howard 1991).

Surface water:

Ground water:

Sediment:

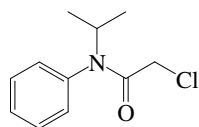
Soil: depending on soil and climatic conditions, the degradation $t_{1/2}$ = 10 to 112 d, but a $t_{1/2}$ = 40 d may be more common under field conditions (Walker 1976, 1978; Zandvoort et al. 1979; quoted, Howard 1991);

selected field $t_{1/2}$ = 60 d (Wauchope et al. 1992; Hornsby et al. 1996);

degraded photolytically on soil thin films, $t_{1/2}$ = 13–57 d in artificial sunlight (Tomlin 1994).

Biota:

17.1.1.67 Propachlor



Common Name: Propachlor

Synonym: Albrass, Bexton, CIPA, CP 31393, Niticid, Propachlore, Prolex, Ramrod, Satecid

Chemical Name: 2-chloro-*N*-(1-methylethyl)-*N*-phenylacetamide; 2-chloro-*N*-isopropyl-acetanilide

Uses: selective pre-emergence herbicide to control most annual grasses and some broadleaf weeds in brassicas, corn, cotton, flax, leeks, maize, milo, onions, peas, roses, ornamental trees and shrubs, soybeans, and sugar cane.

CAS Registry No: 1918-16-7

Molecular Formula: $C_{11}H_{14}ClNO$

Molecular Weight: 211.688

Melting Point ($^{\circ}C$):

77 (Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

110 (at 0.03 mmHg, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.13 ($25^{\circ}C$, Ashton & Crafts 1981)

1.242 ($25^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

1.134 ($25^{\circ}C$, Herbicide Handbook 1989)

Molar Volume (cm^3/mol):

231.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.614 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.309 (mp at $77^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

700 (Melnikov 1971; Khan 1980)

614 ($20^{\circ}C$, Weber 1972)

693 (Spencer 1973, 1982)

580 ($20^{\circ}C$, Ashton & Crafts 1973)

580 (Martin & Worthing 1977; Herbicide Handbook 1978)

839 (generator column-HPLC-RI, Swann et al. 1983)

2300 (HPLC-RT correlation, Swann et al. 1983)

613 (Hartley & Kidd 1987; Worthing & Walker 1987, Herbicide Handbook 1989 Worthing & Hance 1991; Tomlin 1994; Milne 1995)

613 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

613–700 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.032 (20 – $25^{\circ}C$, Weber et al. 1980)

0.0307 ($24^{\circ}C$, Beestman & Demming 1974)

0.0307 (Ashton & Crafts 1981; Herbicide Handbook 1989)

0.03 (Hartley & Kidd 1987)

0.03 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.0306 (Worthing & Hance 1991; Tomlin 1994)

0.0307 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.03 (Montgomery 1993)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.011 (20°C, calculated-P/C, Suntio et al. 1988)
 0.011 (20°C, calculated-P/C, Muir 1991)
 0.011 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{ow}:

2.75 (Leo et al. 1971)
 1.61 (Rao & Davidson 1980)
 2.80 (selected, Gerstl & Helling 1987)
 2.18 (shake flask, Log P Database, Hansch & Leo 1987)
 2.18 (selected, Magee 1991)
 1.61 (Montgomery 1993)
 2.18 (recommended, Sangster 1993)
 1.62–2.30 (Tomlin 1994)
 2.18 (recommended, Hansch et al. 1995)
 2.36 (RP-HPLC-RT correlation, Finizio et al. 1997)
 2.88 ± 0.17, 2.86 ± 0.12 (isocratic RP-HPLC-k' correlation, gradient RP-HPLC-k' correlation, Paschke et al. 2004)

Bioconcentration Factor, log BCF:

1.23 (calculated-S, Kenaga 1980)
 1.15 (calculated-K_{oc}, Kenaga 1980)

Sorption Partition Coefficient, log K_{oc}:

2.42 (soil, Beestman & Demming 1976; Kenaga 1980; Kenaga & Goring 1980)
 2.11 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 2.43 (calculated-MCI χ , Gerstl & Helling 1987)
 2.62 (screening model calculations, Jury et al. 1987b)
 2.31 (estimated as log K_{om}, Magee 1991)
 2.45 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 1.90 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.07–2.11 (Montgomery 1993)
 2.62 (estimated-chemical structure, Lohninger 1994)
 2.42 (quoted or calculated-QSAR MCI χ , Sabljic et al. 1995)
 2.18 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization: estimated t_{1/2} = 671 d from 1 m depth of water at 20°C (Muir 1991).

Photolysis: t_{1/2} = 2.25 h in distilled water (Tanaka et al. 1981; quoted, Cessna & Muir 1991);

1 ppb contaminated water in the presence of TiO₂ and H₂O₂ completely photodegraded after 3 h by solar irradiation (Muszkat et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation: t_{1/2} μ 10–14 d for 0.001–1.0 μ g/mL to biodegrade in sewage effluent lake water (Novick & Alexander 1985; quoted, Muir 1991);

biochemical t_{1/2} = 7 d from screening model calculations (Jury et al. 1987b).

Biotransformation: second-order microbial rate constant k = 1.1 × 10⁻⁹ L·organisms⁻¹ h⁻¹ (Steen & Collette 1989).

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: t_{1/2} ~ 10–14 d for 0.001–1.0 μ g/mL to biodegrade in sewage effluent lake water (Novick & Alexander 1985; quoted, Muir 1991).

Ground water:

Sediment:

Soil: persistence of 2 months (Wauchope 1978);

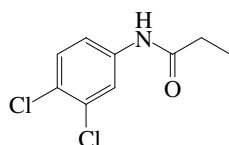
$t_{1/2} = 7$ d from screening model calculations Jury et al. 1987b);

persists in soil for 28–42 d (Worthing & Hance 1991);

selected field $t_{1/2} = 6.3$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical $t_{1/2} = 7$ d from screening model calculations (Jury et al. 1987b).

17.1.1.68 Propanil



Common Name: Propanils

Synonym: Bay 30130, Chem rice, Crystal Propanil-4, DCPA, Dipram, DPA, DPA, Erban, Erbanil, Farmco propanil, FW-734, Grascide, Herbax technical, Prop-Job, Propanex, Propanid, Riselect, Rogue, Rosanil, S 10165, Stam F-34, Stampede, Stam Supernox, Strel, Supernox, Surcopur, Surpur, STAM, Synpran N, Vertac, Wham EZ

Chemical Name: *N*-(3,4-dichlorophenyl)propionamide; *N*-(3,4-dichlorophenyl)propanamide

Uses: selective emergence and post-emergence herbicide to control many grasses and broadleaf weeds in potatoes, rice and wheat.

CAS Registry No: 709-98-8

Molecular Formula: $C_9H_9Cl_2NO$

Molecular Weight: 218.079

Melting Point ($^{\circ}C$):

92 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.25 ($25^{\circ}C$, Ashton & Crafts 1981; Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993; Milne 1995)

1.41 ($22^{\circ}C$, Tomlin 1994)

Molar Volume (cm^3/mol):

220.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

95.1 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.08 (DSC method, Plato & Glasgow 1969)

15.3 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.220 (mp at $92^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

225 (Woodford & Evans 1963; Khan 1980)

500 (Bailey & White 1965; Ashton & Crafts 1973; Herbicide Handbook 1989)

268 (Freed 1966)

225 (Martin & Worthing 1977; Worthing & Walker 1987; Herbicide Handbook 1983)

268–500 (Weber et al. 1980)

130 ($20^{\circ}C$, Spencer 1982)

225 (Hartley & Kidd 1987; Milne 1995)

130 ($20^{\circ}C$, Worthing & Hance 1991)

200 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

130, 225 ($20^{\circ}C$, $25^{\circ}C$, Montgomery 1993)

130 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.012 ($60^{\circ}C$, Khan 1980)

0.012 ($60^{\circ}C$, Verschueren 1983)

0.012 ($60^{\circ}C$, Hartley & Kidd 1987)

0.005 ($20^{\circ}C$, selected, Suntio et al. 1988)

2.50×10^{-4} , 7.20×10^{-3} , 0.130, 1.50, 13.0 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log (P_s/P_a) = 15.201 - 5604.1/(T/K)$; measured range 36.4–92.6°C (gas saturation-GC, Rordorf 1989)
 $\log (P_L/P_a) = 13.192 - 4863.1/(T/K)$; measured range 95.1–160°C (gas saturation-GC, Rordorf 1989)
 2.60×10^{-5} (20°C, Worthing & Hance 1991)
 0.00533 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.67×10^{-5} (20°C, Montgomery 1993)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.0036 (20°C, calculated-P/C, Suntio et al. 1988)
 0.0036 (20°C, calculated-P/C, Montgomery 1993)
 0.00545 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.02 (Rao & Davidson 1980)
 2.80 ($20 \pm 2^\circ\text{C}$, shake flask-UV, Briggs 1981)
 3.12 (selected, Dao et al. 1983)
 3.07 (shake flask, Log P Database, Hansch & Leo 1987)
 2.99 (selected, Gerstl & Helling 1987)
 2.29 (Worthing & Hance 1991; Milne 1995)
 2.34 (quoted from Kenaga 1980, Bottoni & Funari 1992)
 2.73 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
 2.03, 2.29 (Montgomery 1993)
 3.07 (recommended, Sangster 1993)
 2.80 (RP-HPLC-RT correlation, Saito et al. 1993)
 3.30 (Tomlin 1999)
 3.07 (selected, Hansch et al. 1995)
 2.73 (RP-HPLC-RT correlation, Finizio et al. 1997)
 3.21 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$:

1.46 (calculated-S, Kenaga 1980)
 1.34 (calculated, Pait et al. 1992)

Sorption Partition Coefficient, $\log K_{oc}$:

2.34 (calculated-S, Kenaga 1980)
 2.23 (calculated-MCI χ , Gerstl & Helling 1987)
 2.33 (selected, Trevisan et al. 1991)
 2.19 (Montgomery 1993)
 2.17 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.38–2.90 (Tomlin 1994)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 34$ d for 82% of 200 $\mu\text{g/mL}$ to degrade in distilled water under sunlight (Moilanen & Crosby 1972; quoted, Cessna & Grover 1991);

$t_{1/2} = 2.25$ h for 37–51% of 100 $\mu\text{g mL}^{-1}$ to degrade in distilled water under > 300 nm light (Tanaka et al. 1981; quoted, Cessna & Grover 1991);

$t_{1/2} = 245$ h for 14–81% of 15 $\mu\text{g mL}^{-1}$ to degrade in distilled water under sunlight (Draper & Crosby 1984; quoted, Cessna & Grover 1991);

photolysis $t_{1/2} = 12$ –13 h in water (Tomlin 1994).

Oxidation: measured rate constant for reaction with hydroxyl radical, $k(\text{aq.}) = 1.60 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies (Mabury & Crosby 1996).

Hydrolysis: $t_{1/2} > 4$ months for 4360 $\mu\text{g mL}^{-1}$ to hydrolyze in phosphate buffers pH 5–9 at 20°C (El-dib & Aly 1976; quoted, Muir 1991);

hydrolysis $t_{1/2} \gg 1$ yr at pH 4, 7, 9 at 22°C (Tomlin 1994).

Biodegradation: $t_{1/2} = 1-2$ d for $30 \mu\text{g mL}^{-1}$ to biodegrade in flooded soil at 30°C (Kuwatsuka 1972; quoted, Muir 1991);

$t_{1/2} \sim 10$ d for $40 \mu\text{g mL}^{-1}$ to biodegrade in pond sediment (Stepp et al. 1985; quoted, Muir 1991).

Biotransformation: second-order microbial degradation rate constant $k = 5 \times 10^{-10} \text{ L} \cdot \text{organisms}^{-1} \text{ h}^{-1}$ (Steen & Collette 1989).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} \gg 1$ yr (pH 4, 7, 9) at 22°C and photolysis $t_{1/2} = 12-13$ h in aqueous solution (Tomlin 1994).

Groundwater: reported $t_{1/2} < 5$ d (Bottoni & Funari 1992)

Sediment: $t_{1/2} \sim 10$ d for $40 \mu\text{g mL}^{-1}$ to biodegrade in pond sediment (Stepp et al. 1985; quoted, Muir 1991).

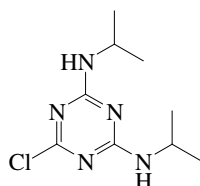
Soil: $t_{1/2} = 1-2$ d for $30 \mu\text{g mL}^{-1}$ to biodegrade in flooded soil at 30°C (Kuwatsuka 1972; quoted, Muir 1991);
selected field $t_{1/2} = 1.0$ d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Halfon et al. 1996);

soil $t_{1/2} = 15$ d (Pait et al. 1992);

$t_{1/2} < 5$ d (Bottoni & Funari 1992).

Biota:

17.1.1.69 Propazine



Common Name: Propazine

Synonym: G-30028, Geigy 30028, Gesamil, Maax, Milogard, Plantulin, Primatol P, Propasin, Prozinex

Chemical Name: 6-chloro-*N,N'*-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine; 2-chloro-4,6-bis(isopropylamino)-1,3,5-triazine

Uses: selective pre-emergence herbicide to control annual grasses and broadleaf weeds in milo and sweet sorghum.

CAS Registry No: 139-40-2

Molecular Formula: $C_9H_{16}ClN_5$

Molecular Weight: 229.710

Melting Point ($^{\circ}C$):

213 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.162 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

272.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

1.85 (pK_a , Weber 1970; quoted, Bintein & Devillers 1994)

1.80 (pK_a , Weber et al. 1980; Willis & McDowell 1982)

1.85 (pK_a , Herbicide Handbook 1989)

1.70 (pK_a , $21^{\circ}C$, Worthing & Hance 1991)

12.15 (pK_b , Wauchope et al. 1992)

1.85 (pK_a , $22^{\circ}C$, Montgomery 1993)

12.3 (pK_b , $21^{\circ}C$, Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

41.84 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0143 (mp at $213^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

10 (Gysin 1962)

8.6 (20 – $22^{\circ}C$, Bailey & White 1965; Spencer 1973; Quellette & King 1977)

4.82, 4.60, 5.05 ($26^{\circ}C$, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

8.60 (Martin & Worthing 1977)

4.8–8.6 (Weber et al. 1980)

5.0 ($20^{\circ}C$, Spencer 1982)

8.60 ($20^{\circ}C$, Hartley & Kidd 1987; Herbicide Handbook 1989)

5.0 ($20^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

8.60 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

8.50 ($20^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3.87×10^{-6} ($20^{\circ}C$, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50 – $130^{\circ}C$, Friedrich & Stambach 1964) (See figure at the end of this section.)

$\log (P/mmHg) = 11.911 - 4933/(T/K)$, temp range 50 – $130^{\circ}C$ (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stambach 1964)

3.90×10^{-6} ($20^{\circ}C$, Quellette & King 1977)

- 4.00×10^{-6} (20–25°C, Weber et al. 1980)
- 3.90×10^{-6} (20°C, Ashton & Crafts 1981; Herbicide Handbook 1989)
- 4.00×10^{-6} (20°C, Hartley & Kidd 1987)
- 2.10×10^{-5} (30°C, Herbicide Handbook 1989)
- 3.90×10^{-6} (20°C, Worthing & Hance 1991; Montgomery 1993)
- 1.75×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 1.00×10^{-4} (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)
- 1.00×10^{-3} (20°C, calculated-P/C, Montgomery 1993)
- 1.04×10^{-3} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

- 2.89 (Kenaga & Goring 1980; Yoshioka et al. 1986)
- 2.94 (shake flask-GC or UV, Brown & Flagg 1981)
- 2.59 (RP-HPLC- k' correlation, Braumann et al. 1983)
- 2.93 (shake flask, Biagi et al. 1991)
- 2.91 (RP-HPLC-RT correlation, Finizio et al. 1991)
- 2.91, 2.94 (Montgomery 1993)
- 2.77 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.93 (recommended, Sangster 1993; Hansch et al. 1995)
- 2.89 (shake flask-UV, Liu & Qian 1995)
- 3.13 (Pomona-database, Müller & Kördel 1996)
- 2.77 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 2.26 (calculated-S, Kenaga 1980)
- 0.903 (calculated- K_{oc} , Kenaga 1980)

Sorption Partition Coefficient, log K_{oc} :

- 2.20 (soil, Hamaker & Thompson 1972; Brown 1978; Kenaga 1980; Kenaga & Goring 1980; Sabljic 1987)
- 3.11 (soil, calculated-S per Kenaga & Goring 1980; Kenaga 1980)
- 2.56 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
- 2.78 (calculated-MCI χ , Gerstl & Helling 1987)
- 2.34 (estimated as log K_{OM} , Magee 1991)
- 2.18 (soil, quoted, Bottoni & Funari 1992)
- 2.19 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.94 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
- 1.69–2.56 (Montgomery 1993)
- 2.44 (selected, Lohninger 1994)
- 1.90, 2.0 (Tomlin 1994)
- 2.57 (calculated- K_{ow} , Liu & Qian 1995)
- 2.40 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 1.94; 2.55 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.59, 1.93, 2.08, 1.95, 2.70 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 2.18, 2.148, 2.10, 1.98, 2.58 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 2.818, 2.148, 2.100, 1.977, 2.579 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
- 2.40; 2.43, 2.84 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
- 2.15, 2.17 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, pH 3.2–7.4, average, Delle Site 2001)

2.29, 2.21, 2.03 (soil with organic carbon $OC \geq 0.5\%$ at: pH 4.3–5.0, pH 5.1–5.0, pH ≥ 6.0 , average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: 1 ppb contaminated water in presence of TiO_2 and H_2O_2 completely photodegraded after 3.5 h by solar irradiation (Muszkat et al. 1992).

Oxidation:

Hydrolysis: calculated rate constant $k = 9.70 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 83 \text{ d}$ at 20°C in a buffer at pH 5 (Burkhard & Guth 1981).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water: reported half-lives or persistence, $t_{1/2} = 80\text{--}100 \text{ d}$ (Bottoni & Funari 1992)

Sediment:

Soil: persistence of 18 months (Edwards 1973; quoted, Morrill et al. 1982);

persistence of 12 months in soil (Wauchope 1978);

$t_{1/2} = 62 \text{ d}$ and 127 d in a Hatzenbühl soil at pH 4.8 and Neuhoefen soil at pH 6.5 respectively at 22°C under laboratory conditions (Burkhard & Guth 1981; quoted, Montgomery 1993);

reported $t_{1/2} = 80\text{--}100 \text{ d}$ (Bottoni & Funari 1992);

selected field $t_{1/2} = 135 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

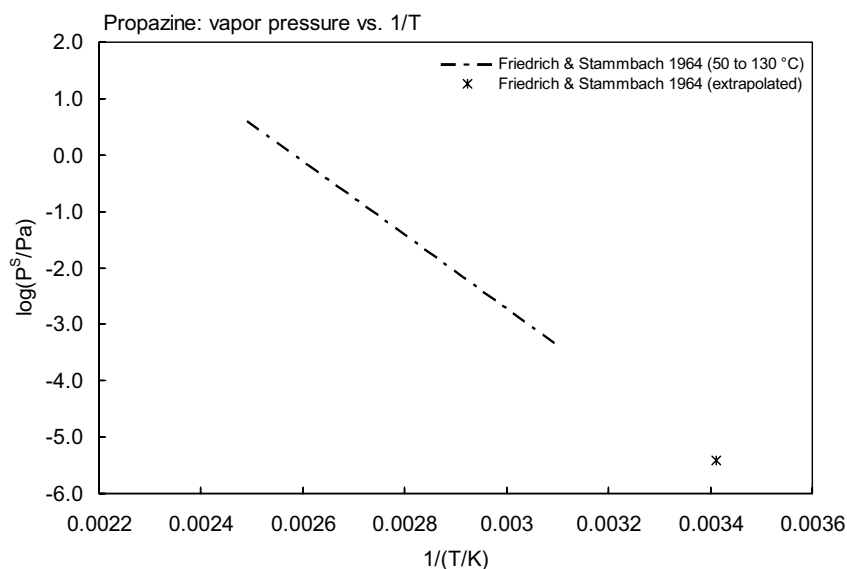
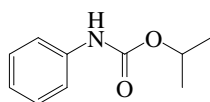


FIGURE 17.1.1.69.1 Logarithm of vapor pressure versus reciprocal temperature for propazine.

17.1.1.70 Propham



Common Name: Propham

Synonym: Agermin, Ban-Hoe, Beet-Kleen, Birgin, Chem-Hoe, Collavin, IFC, IFK, INPC, IPC

Chemical Name: carbanilate acid isopropyl ester; isopropyl carbanilate; isopropyl-N-phenyl carbamate; 1-methylethyl phenylcarbamate

Uses: pre-emergence and post-emergence herbicide to control annual grass weeds in peas, beans, sugar beet, lettuce, lucerne, clover, flax, sunflowers and lentils.

CAS Registry No: 122-42-9

Molecular Formula: $C_{10}H_{13}NO_2$

Molecular Weight: 179.2 16

Melting Point ($^{\circ}C$):

90 (Lide 2003)

Boiling Point ($^{\circ}C$):

> 150 (sublimes but decomposes, Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

1.09 (Spencer 1982; Tomlin 1994; Hartley & Kidd 1987; Milne 1995)

1.09 ($30^{\circ}C$, Ashton & Crafts 1981; Herbicide Handbook 1989; Montgomery 1993)

Molar Volume (cm^3/mol):

213.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.230 (mp at $90^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

100 (Freed 1953)

250 (Nex & Swezey 1954; Ashton & Crafts 1981)

22.5–32 (Bailey & White 1965)

250 ($20^{\circ}C$, Spencer 1973, 1982)

250 (Martin & Worthing 1977; Herbicide Handbook 1978, 1983, 1989; Hartley & Kidd 1987)

250–254 (Weber et al. 1980)

127 (selected, Gerstl & Helling 1987)

32–250 (20 – $25^{\circ}C$, Worthing & Hance 1991; Montgomery 1993)

250 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

250 ($20^{\circ}C$, Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

sublimes (rm. temp., Herbicide Handbook 1989)

sublimes (rm. temp., Montgomery 1993; Tomlin 1994)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.60 ($20 \pm 2^{\circ}C$, shake flask-UV, Briggs 1981)

2.16 (selected, Dao et al. 1983; Gerstl & Helling 1987)

2.27 (shake flask, Mitsutake et al. 1986)

2.60 (recommended, Sangster 1993)

Bioconcentration Factor, log BCF:

1.43	(calculated-S, Kenaga 1980)
0.301	(calculated- K_{OC} , Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

1.71	(Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.32	(soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
1.71	(20 \pm 2°C, reported as log K_{OM} , Briggs 1981)
1.93	(calculated-MCI χ , Gerstl & Helling 1987)
2.30	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.71	(Montgomery 1993)
2.30	(estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct $t_{1/2}$ = 254 d in clear water body near the surface for a mid-summer day at latitude 40° (Wolfe et al. 1978)

direct $t_{1/2}$ = 254 d in distilled water assuming for a mid-summer day at latitude 40°; $t_{1/2}$ = 2.25 h for 1% of 100 $\mu\text{g/mL}$ to degrade in distilled water under 300 nm light (Tanaka et al. 1981; quoted, Cessna & Muir 1991).

Oxidation:

Hydrolysis: $t_{1/2}$ > 4 months for 3550 $\mu\text{g/mL}$ to hydrolyze in phosphate buffer at pH 5–9 and 20°C (El-Dib & Aly 1976; quoted, Muir 1991)

$k(\text{alkaline}) = 7.6 \times 10^{-6} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C, $k = 5.6 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ at 50°C, $k = 2.6 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ at 70°C; with $t_{1/2} > 1 \times 10^4$ d at pH 5, 7 and 9 (Wolfe et al. 1978)

Biodegradation: $t_{1/2}$ = 190 d by 1 mg/L fungus *Asperillus fumigatus*, $t_{1/2}$ = 3.2 d by bacteria (Wolfe et al. 1978)

$k = 1.5 \times 10^{-4} \text{ L (mg M)}^{-1} \text{ h}^{-1}$ with $t_{1/2}$ = 190 d for 2–25 $\mu\text{g/mL}$ fungus *Aspergillus fumigatus*; $k = 9 \times 10^{-2} \text{ L (mg M)}^{-1} \text{ h}^{-1}$ with $t_{1/2}$ = 3.2 d for bacteria *Pseudomonas striata* to biodegrade in stream water at pH 7 and 28°C (Muir 1991)

$t_{1/2} \sim 30\text{--}40$ d for 1–0.0004 $\mu\text{g/mL}$ to biodegrade in filtered sewage water at 20–22°C and $t_{1/2} \sim 20$ to 50 d at 29°C in filtered lake water (Wang et al. 1984; quoted, Muir 1991)

$t_{1/2}(\text{aerobic}) > 4$ months for 6–7 $\mu\text{g/mL}$ to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} > 1 \times 10^4$ d based on neutral and alkaline hydrolysis assuming pseudo-first order kinetics; direct photolysis $t_{1/2}$ = 254 d assuming a mid-summer day at altitude 40°, and biolysis $t_{1/2}$ = 190 d for 1 mg/L of fungus and $t_{1/2}$ = 3.2 d for bacteria at 28°C (Wolfe et al. 1978);

$t_{1/2} \sim 30\text{--}40$ d for 1–0.0004 $\mu\text{g/mL}$ to biodegrade in filtered sewage water at 20–22°C and $t_{1/2} \sim 20$ to 50 d at 29°C in filtered lake water (Wang et al. 1984; quoted, Muir 1991);

aerobic $t_{1/2} > 4$ months for 6–7 $\mu\text{g/mL}$ to biodegrade in river water at 25°C (Stepp et al. 1985; quoted, Muir 1991).

Ground water:

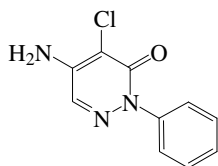
Sediment:

Soil: $t_{1/2} \sim 15$ d in soil and $t_{1/2}$ = 5 d at 16 and 29°C (Hartley & Kidd 1987; Herbicide Handbook 1989; quoted, Montgomery 1993; Tomlin 1994);

selected field $t_{1/2}$ = 10 d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

17.1.1.71 Pyrazon



Common Name: Pyrazon

Synonym: chloridazon, chloridazone, Blurex, Burex, Dazon, Phenosane, Piramin, Pyramin

Chemical Name: 5-amino-4-chloro-2-phenylpyridazin-3(2H)-one

Uses: as pre- and post-emergence herbicide to control of annual broadleaf weeds in sugar-beet, fodder beet and beet root; and also used in combination with other herbicides, etc.

CAS Registry No: 1698-60-8

Molecular Formula: $C_{10}H_8ClN_3O$

Molecular Weight: 221.643

Melting Point ($^{\circ}C$):

205 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.54 (Tomlin 1994)

Molar Volume (cm^3/mol):

205.7 (calculated-Le Bas method at normal boiling point)

143.9 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

26.59 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0171 (mp at $205^{\circ}C$)

0.013 ($20^{\circ}C$, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

400 ($20^{\circ}C$, Ashton & Crafts 1973, 1981)

300 ($20^{\circ}C$, Khan 1980)

400 ($20^{\circ}C$, Spencer 1982)

400 ($20^{\circ}C$, Worthing & Walker 1987; Hartley & Kidd 1987; Milne 1995)

360 ($20^{\circ}C$, selected, Suntio et al. 1988)

400 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

340 ($20^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

9.86 ($40^{\circ}C$, Ashton & Craft 1973; Spencer 1982)

< 0.00001 ($20^{\circ}C$, Worthing & Walker 1987; Hartley & Kidd 1987; Tomlin 1994)

7.0 ($20^{\circ}C$, estimated, Suntio et al. 1988)

6.67 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

4.31 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.14 ($22^{\circ}C$, shake flask-AS, Braumann & Grimme 1981; quoted, Sangster 1993)

1.50 (selected, Gerstl & Helling 1987)

1.12 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)

1.19 (pH 7, Tomlin 1994)

- 2.20 (Milne 1995)
- 1.14 (recommended, Hansch et al. 1995)
- 1.12 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.32 (calculated-S per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{oc} :

- 2.12, 2.18 (selected, calculated-MCI χ , Gerstl & Helling 1987)
- 2.74 (soil, calculated-MCI and fragments contribution method, Meylan et al. 1992)
- 2.08 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.95–2.53 (soil, Tomlin 1994)

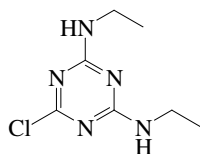
Environmental Fate Rate Constants, or Half-Lives:

Photolysis: $t_{1/2} = 150$ h at pH 7 in simulated sunlight and $t_{1/2} = 47.7$ h by 80000 lux, xenon lamp (Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2} = 21$ d (Wauchope et al. 1992; Hornsby et al. 1996)

17.1.1.72 Simazine



Common Name: Simazine

Synonym: A 2079, Aktinit S, Amizine, Aquazine, Batazina, Bitemol, Cekusan, CAT, CET, DCT, Framed, G 27692, Gesapun, Gesaran, Gesatop, Herbazin, Herbex, Herboxy, Premazine, Primatol, Primcep, Princep, Printop, Radocon, Radokor, Simadex, Simanex, Sim-Trol, Tafazine, Weedex, Zeapur

Chemical Name: 6-chloro-*N,N'*-diethyl-1,3,5-triazine-2,4-diamine; 2-chloro-4,6-bis(ethyl-amino)-1,3,5-triazine

Uses: selective pre-emergence systemic herbicide to control many broadleaf weeds and annual grasses in deep-rooted fruit and vegetable crops.

CAS Registry No: 122-34-9

Molecular Formula: $C_7H_{12}ClN_5$

Molecular Weight: 201.657

Melting Point ($^{\circ}C$):

226 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.302 (Hartley & Kidd 1987; Milne 1995)

1.203 (Montgomery 1993)

Molar Volume (cm^3/mol):

228.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

1.65 (pK_a , Weber 1970; quoted, Bintein & Devillers 1994)

1.60 (pK_a , Weber et al. 1980; Willis & McDowell 1982)

1.70 (pK_a , $21^{\circ}C$, Worthing & Hance 1991; Montgomery 1993)

2.00 (pK_a , Yao & Haag 1991; Haag & Yao 1992)

12.35 (pK_b , Wauchope et al. 1992; Hornsby et al. 1996)

12.3 (pK_b , Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

43.932 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0107 (mp at $226^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

5.0 (Bailey & White 1965 Freed 1976; Wauchope 1978)

5.8, 5.0, 5.0 ($26^{\circ}C$, shake flask-UV at pH 3.0, 7.0, 10.0, Ward & Weber 1968)

15.1 ($26^{\circ}C$, Getzen & Ward 1971)

5.0 ($20^{\circ}C$, Weber 1972; Spencer 1973; Khan 1980)

5.0 ($20^{\circ}C$, Martin & Worthing 1977; Worthing & Walker 1987; Worthing & Hance 1991; Milne 1995)

3.5 (Herbicide Handbook 1978, 1989)

3.5 ($20^{\circ}C$, Ashton & Crafts 1981; Hartley & Kidd 1987)

5.0, 3.50, 7.4 ($20^{\circ}C$, quoted, exptl., calculated-Parachor & mp, Briggs 1981)

6.2 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

3.5–5.0 ($20^{\circ}C$), Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence):

8.13×10^{-7} ($20^{\circ}C$, extrapolated-Antoine eq. from gas saturation-GC measurements, measured range 50 – $130^{\circ}C$, Friedrich & Stambach 1964) (See figure at the end of this section.)

$\log (P/mmHg) = 11.911 - 4933/(T/K)$, temp range 50 – $130^{\circ}C$ (gas saturation-GC, data presented in graph and Antoine eq., Friedrich & Stambach 1964)

- 8.10 × 10⁻⁷ (20°C, Weber 1972; Khan 1980; Ashton & Crafts 1981; Herbicide Handbook 1989)
- 2.00 × 10⁻⁶ (gas saturation, Spencer & Cliath 1974)
- 8.00 × 10⁻⁷ (20–25°C, Weber et al. 1980; Willis & McDowell 1982)
- 8.10 × 10⁻⁷ (20°C, Hartley & Kidd 1987; Worthing & Walker 1987; Worthing & Hance 1991; Montgomery 1993)
- 8.50 × 10⁻⁶ (20°C, selected, Suntio et al. 1988)
- 4.80 × 10⁻⁶ (30°C, Herbicide Handbook 1989)
- 2.95 × 10⁻⁶ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.94 × 10⁻⁶ (OECD 104, Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 8.40 × 10⁻⁵ (calculated-P/C, Jury et al. 1983, 1984, 1987a; Jury & Ghodrati 1989)
- 3.40 × 10⁻⁴ (20°C, calculated-P/C, Suntio et al. 1988)
- 8.40 × 10⁻⁵ (calculated-P/C, Taylor & Glotfelty 1988)
- 3.30 × 10⁻⁵ (20°C, calculated-P/C, Muir 1991)
- 3.40 × 10⁻⁴ (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW}:

- 2.19 (Kenaga & Goring 1980)
- 1.94 (Rao & Davidson 1980)
- 1.51 (shake flask-UV, Lord et al. 1980)
- 1.51 (20 ± 2°C, shake flask-UV, Briggs 1981)
- 2.16 (shake flask, Brown & Flagg 1981)
- 1.96, 2.06 (RP-HPLC-k' correlation, McDuffie et al. 1981)
- 2.27 (selected, Dao et al. 1983; Gerstl & Helling 1987)
- 2.14 (shake flask, Mitsutake et al. 1986)
- 1.50 (Nicholls 1988)
- 2.18 (shake flask, Biagi et al. 1991)
- 2.26, 2.20 (RP-HPLC-RT correlation, calculated, Finizio et al. 1991)
- 1.96 (Worthing & Hance 1991; Milne 1995)
- 2.00 (shake flask, pH 7, Baker et al. 1992)
- 1.94–2.26 (Montgomery 1993)
- 2.07 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.18 (recommended, Sangster 1993)
- 2.10 (Tomlin 1994)
- 2.18 (shake flask-UV, Liu & Qian 1995)
- 2.18 (recommended, Hansch et al. 1995)
- 2.51 (Pomona-database, Müller & Kördel 1996)
- 2.07 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 1.83 (RP-HPLC-RT correlation, Nakamura et al. 2001)
- 1.49 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 2.48 (calculated-S, Kenaga 1980)
- 0.778 (calculated-K_{OC}, Kenaga 1980)
- 2.16 (earthworms, Lord et al. 1980)
- 0.699 (calculated-K_{OW}, Briggs 1981)

Sorption Partition Coefficient, log K_{OC}:

- 2.13 (soil, Hamaker & Thompson 1972; Brown 1978; Kenaga 1980; Kenaga & Goring 1980)
- 3.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 2.15 (av. soils/sediments, Rao & Davidson 1980)
- 1.68 (20 ± 2°C, K_{OM} multiplied by 1.724, Briggs 1981)
- 2.33 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)
- 3.66, 2.53, 1.77 (estimated-S, calculated-S and mp, estimated-K_{OW}, Karickhoff 1981)
- 2.14 (soil average, Jury et al. 1983)

- 2.20, 2.15 (selected, calculated-MCI χ , Gerstl & Helling 1987)
 2.15 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
 1.60–2.20 (Carsel 1989)
 1.92 (estimated as $\log K_{OM}$, Magee 1991)
 2.13–3.34, 2.15, 2.45, 2.70 (soil, quoted values, Bottoni & Funari 1992)
 2.11 (soil, 20–25°C, selected, Wauchope et al. 1991, Hornsby et al. 1996)
 3.02 (average of 12 soils, calculated-linearize Freundlich Isotherm, Sukop & Cogger 1992)
 2.14 (Montgomery 1993)
 1.78 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
 2.37 (selected, Lohninger 1994)
 2.01–2.58 (Tomlin 1994)
 2.18 (calculated- K_{OW} , Liu & Qian 1995)
 2.10 (soil, calculated-MCI χ , Sabljic et al. 1995)
 1.79; 2.17 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.07, 1.65, 1.68, 1.61, 2.48 (soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
 2.625, 1.90, 1.69, 1.66, 2.382 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
 2.625, 1.901, 1.689, 1.656, 2.382 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
 2.10; 2.10, 2.47 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 2.29, 2.29, 2.29 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, pH 3.2–8.0, average, Delle Site 2001)
 2.50, 2.34, 2.10 (soils with organic carbon $OC \geq 0.5\%$ at: pH 3.2–5.0, pH 5.1–5.9, pH ≥ 6.0 , average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 276$ d (Jury et al. 1983; quoted, Grover 1991); measured rate constant $k = 600$ d⁻¹ and estimated rate constant $k = 1000$ d⁻¹ (Glottfelty et al. 1989).

Photolysis:

Oxidation:

$k(aq.) = 5.9 \times 10^9$ M⁻¹ s⁻¹ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) = (4.8 \pm 0.2)$ M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 4.3 and 23°C , with $t_{1/2} = 1.9$ h at pH 7 (Yao & Haag 1991).

$k(aq.) = (2.8 \pm 0.2) \times 10^9$ M⁻¹ s⁻¹ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992).

Hydrolysis: calculated rate constant $k = 8.32 \times 10^{-6}$ s⁻¹ with $t_{1/2} = 96$ d at 20°C in a buffer at pH 5 (Burkhard & Guth 1981).

Biodegradation: rate constant $k = 0.014$ d⁻¹ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 8$ –27 d for $3 \mu\text{g mL}^{-1}$ to biodegrade in pond sediment/water and $t_{1/2} > 32$ d in pond water both at 25°C (Tucker & Boyd 1981; quoted, Muir 1991);

$t_{1/2} = 75$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989; Grover 1991);
 microbial degradation $t_{1/2} = 70$ –11 d in soil (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} > 32$ d for $3 \mu\text{g mL}^{-1}$ to biodegrade in pond water at 25°C (Tucker & Boyd 1981; quoted, Muir 1991);

$t_{1/2} = 1$ –4 wk in estuarine systems (Jones et al. 1982; quoted, Meakins et al. 1994);

$t_{1/2} \sim 30$ d in ponds (Herbicide Handbook 1989);
 measured rate constant $k = (4.8 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 4.3 and 23°C,
 with $t_{1/2} = 1.9$ h at pH 7 (Yao & Haag 1991).
 Ground water: reported half-lives or persistence, $t_{1/2} = 15\text{--}75$, 46–174 and 56 d (Bottoni & Funari 1992)
 Sediment: $t_{1/2} = 8\text{--}27$ d for $3 \mu\text{g mL}^{-1}$ to biodegrade in pond sediment/water at 25°C (Tucker & Boyd 1981;
 quoted, Muir 1991).
 Soil: estimated persistence of 12 months (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury
 et al. 1987a);
 persistence of 12 months (Wauchope 1978);
 estimated first-order $t_{1/2} = 49.5$ d from biodegradation rate constant $k = 0.014 \text{ d}^{-1}$ by soil incubation die-away
 studies (Rao & Davidson 1980; quoted, Scow 1982);
 $t_{1/2} = 45$ d in Hatzenbühl soil at pH 4.8 and $t_{1/2} = 100$ d in Neuhausen soil at pH 6.5 both at 22°C, respectively,
 under lab. conditions (Burkhard & Guth 1981; quoted, Montgomery 1993);
 $t_{1/2} = 1\text{--}6$ months (Jones et al. 1982; quoted, Meakins et al. 1994);
 $t_{1/2} = 75$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989);
 moderately persistent in soils with $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982);
 degradation rate constant $k = (1.51 \pm 0.086) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 45.9$ d in control soil and $k = (1.76 \pm 0.177)$
 $\times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 39.4$ d in pretreated soil in the field; $k = (0.943 \pm 0.047) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 73.5$ d
 in control soil and $k = (0.864 \pm 0.048) \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 80.2$ d in pretreated soil once only in the
 laboratory (Walker & Welch 1991);
 reported $t_{1/2} = 15\text{--}75$ d, 46–174 d and 56 d; 29 d at 5°C and $t_{1/2} = 209$ d at 30°C (Bottoni & Funari 1992);
 selected field $t_{1/2} = 60$ d (Wauchope et al. 1991, 1992; quoted, Dowd et al. 1993; Richards & Baker 1993;
 quoted, Halfon et al. 1996; Hornsby et al. 1996);
 soil $t_{1/2} = 75$ d (Pait et al. 1992);
 degradation by microorganism in biometer systems: $t_{1/2} = 58$ d in silty sand standard laboratory conditions,
 $t_{1/2} = 87$ d for corrected standard conditions and $t_{1/2} = 91$ d in simulated outdoor conditions; $t_{1/2} = 51$ d in
 silty loam standard laboratory conditions, $t_{1/2} = 77$ d corrected standard conditions, $t_{1/2} = 63$ d in simulated
 outdoor conditions at constant soil moisture and 20°C. Degradation by microorganism in outdoor exper-
 iments in small lysimeter systems: $t_{1/2} = 32$ d outdoor fallow, $t_{1/2} = 35$ d outdoor barley in silty sand, and
 $t_{1/2} = 49$ d outdoor fallow, $t_{1/2} = 53$ d outdoor barley in silty loam (Rüdel et al. 1993)
 $t_{1/2} = 49\text{--}50$ d in 0–40 cm soil cores taken from: cultivated field; from meadow $t_{1/2} = 32\text{--}39$ d and from gravel
 track $t_{1/2} = 62\text{--}51$ d (Hassink et al. 1994);
 degradation $t_{1/2} = 70\text{--}110$ d (Tomlin 1994).
 Biota: biochemical $t_{1/2} = 75$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

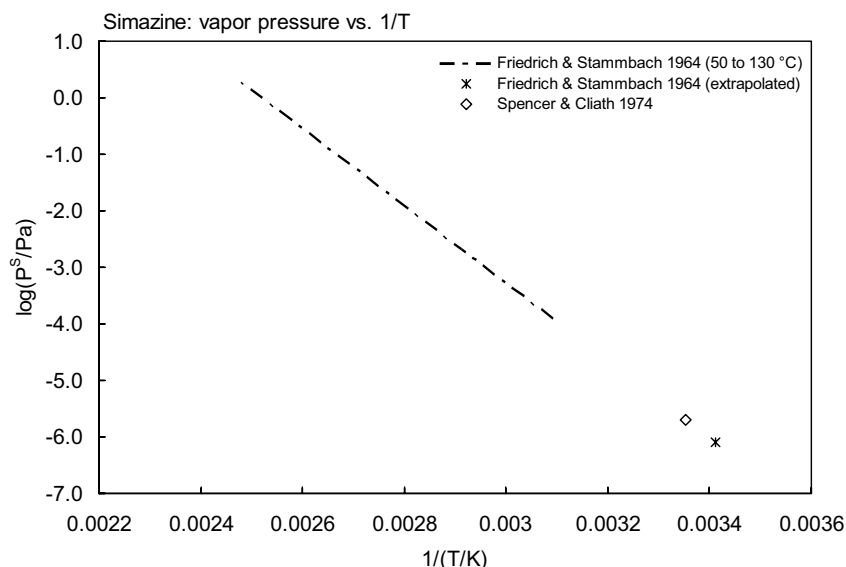
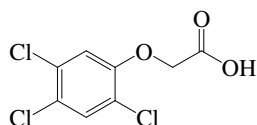


FIGURE 17.1.1.72.1 Logarithm of vapor pressure versus reciprocal temperature for simazine.

17.1.1.73 2,4,5-T



Common Name: 2,4,5-T

Synonym: Amine 2,4,5-T for rice, BCF-bushkiller, Brush rhap, Brush-Khap, Brushtox, Dacamine, Ded-Weed, Dinoxol, Envert-T, Estercide T-2 & T-245, Esterone 245, Fence rider, Forron, Fortex, Fruitone A, Gesatop, Inverton 245, Line rider, Phortox, Reddon, Reddox, Spontox, Super D Weedone, Tippon, Tormona, Transamine, Tributon, Trinoxol, Trioxone, Veon, Weddar, Weedone

Chemical Name: 2,4,5-trichlorophenoxyacetic acid

Uses: herbicide to control undesirable brush and woody plants; also used as plant hormone, defoliant.

CAS Registry No: 93-76-5

Molecular Formula: $C_8H_5Cl_3O_3$

Molecular Weight: 255.483

Melting Point ($^{\circ}C$):

153 (Lide 2003)

Boiling Point ($^{\circ}C$):

> 200 (dec., Howard 1991)

Density (g/cm^3 at $20^{\circ}C$):

1.80 (Ashton & Crafts 1981; Hartley & Kidd 1987; Montgomery 1993)

1.80 ($25^{\circ}C$, Que Hee et al. 1981)

1.80 (Spencer 1982; Budavari 1989; Milne 1995)

Molar Volume (cm^3/mol):

226.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

2.88 (potentiometric titration, Nelson & Faust 1969)

2.85 (Cessna & Grover 1978; Somasundaram et al. 1991; Augustijn-Beckers et al. 1994)

2.70 (Haag & Yao 1992)

2.80–2.88 (Montgomery 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

107.8 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

34.936 (DSC method, Plato & Glasgow 1969)

34.2 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0555 (mp at $153^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

268 (shake flask-UV, Leopold et al. 1960)

238 ($20^{\circ}C$, Loos 1975)

238 (Martin & Worthing 1977)

238–280 (Weber et al. 1980)

238 ($30^{\circ}C$, Ashton & Crafts 1981; Budavari 1989)

278 (Spencer 1982; Verschueren 1983)

278 ($20^{\circ}C$, Hartley & Kidd 1987)

280 (selected, Gerstl & Helling 1987)

150 (Worthing & Walker 1987, Worthing & Hance 1991)

220 ($20^{\circ}C$, Montgomery 1993)

278 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994)

238 ($20^{\circ}C$, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

- 0.0063 (effusion method, Hamaker & Kerlinger 1971)
- $< 1.0 \times 10^{-6}$ (20°C, Hartley & Kidd 1983)
- 0.005 (20°C, selected, Suntio et al. 1988; Riederer 1990)
- $< 1.0 \times 10^{-5}$ (20°C, Hartley & Kidd 1983; 1987)
- 2.30×10^{-6} , 1.90×10^{-4} , 8.50×10^{-3} , 0.230, 4.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
- $\log (P_s/\text{Pa}) = 19.238 - 7418.9/(T/K)$; measured range 80.4–145°C (solid, gas saturation-GC, Rordorf 1989)
- $\log (P_L/\text{Pa}) = 15.058 - 5632.4/(T/K)$; measured range 80.4–145°C (liquid, gas saturation-GC, Rordorf 1989)
- 7.00×10^{-7} (Worthing & Hance 1991)
- 0.0040 (20°C, Montgomery 1993)
- 0.0 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 8.79×10^{-4} (Hine & Mookerjee 1975)
- 0.0058 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.0049 (20°C, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.13 (electrometric titration, Freese et al. 1979)
- 0.60 (pH dependent quoted from Dow Chemical data, Kenaga & Goring 1980)
- 0.85 (Rao & Davidson 1980)
- 2.99 (RP-HPLC- k' correlation, Braumann et al. 1983)
- 3.13 (Hansch & Leo 1985)
- 3.40 (OECD 81 method, Kerler & Schönherr 1988)
- 3.36 (selected, Travis & Arms 1988)
- 3.31 (shake flask-HPLC/UV, Jafvert et al. 1990)
- 0.60–3.40 (Montgomery 1993)
- 3.13 (countercurrent LC, Ilchmann et al. 1993)
- 3.13 (selected, Sangster 1993)
- 3.13 (recommended, Hansch et al. 1995)
- 3.31 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, $\log BCF$:

- 4.55 (milk biotransfer factor $\log B_m$, correlated- K_{OW} , Bjerke et al. 1972)
- 1.18 (measured, Isensee 1976)
- 4.82 (beef biotransfer factor $\log B_b$, correlated- K_{OW} , Kenaga 1980)
- 1.63 (fish under flowing water conditions, Kenaga & Goring 1980)
- 1.45 (calculated-S, Kenaga 1980)
- 0.301 (calculated- K_{OC} , Kenaga 1980)
- 1.36–1.40 (fish under static ecosystem tests, Kenaga & Goring 1980; Garten & Tralbalka 1983)
- 1.41 (mosquito fish 32 d under unspecified conditions, Ang et al. 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.72 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980; Sabljic 1987)
- 2.34 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
- 1.93, 2.27, 2.31, 2.31, 2.45, 2.31 (sand soil, whole soil, fine soil, coarse clay soil, medium silt soil, coarse silt soil, Nkedi-Kizza et al. 1983)
- 2.38 (calculated-MCI χ , Gerstl & Helling 1987)
- 1.90 (soil, screening model calculations, Jury 1987b)
- 1.72 (soil, Sabljic 1987)
- 1.77; 2.63; 1.94 (Alfisol soil, Podzol soil; sediment, von Oepen et al. 1991)
- 1.72, 2.27 (Montgomery 1993)
- 1.90 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994)

- 1.72 (estimated-chemical structure, Lohninger 1994)
 1.99 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
 1.99 (1.63–2.35) (soils: organic carbon OC \geq 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 48$ h for 17–80% of 1 $\mu\text{g/mL}$ to degrade in buffered aqueous solution at pH 7.8 under sunlight (Crosby & Wong 1973; quoted, Cessna & Muir 1991);

$t_{1/2} = 15$ d for < 2.6 $\mu\text{g/mL}$ to degrade in distilled water under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991);

$t_{1/2} = 8.7$ d for < 2.6 $\mu\text{g/mL}$ to degrade in aqueous fulvic acid solution (17 mg/L) and $t_{1/2} = 3.5$ d for < 2.6 $\mu\text{g/mL}$ to degrade in aqueous fulvic acid solution (55 mg/L) under sunlight (Skurlatov et al. 1983; quoted, Cessna & Muir 1991).

Oxidation:

photooxidation $t_{1/2} = 12.2$ –122 h in air, based on an estimated rate constant for the reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard et al. 1991)

$k(\text{aq.}) = (8.9 \pm 1.3) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.7–5.0 and 26°C, with $t_{1/2} = 1.0$ h at pH 7 (Yao & Haag 1991)

$k_{\text{OH}}(\text{calc}) = 4.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with hydroxy radical in aqueous solutions (Haag & Yao 1992).

Hydrolysis: will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes (Kollig 1993).

Biodegradation:

$t_{1/2}(\text{aerobic}) = 27$ d for 50 $\mu\text{g/mL}$ in sediment-water microcosm by long lag phase degradation (Alexander 1974; quoted, Muir 1991)

$t_{1/2}(\text{aq. aerobic}) = 240$ –480 h, based on unacclimated soil grab sample data (Smith 1978, 1979; quoted, Howard et al. 1991)

$k = 0.001 \text{ d}^{-1}$ by river die-away test in aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)

$k = 0.035 \text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982)

$k = 0.01$ –0.03 d^{-1} at 9–21°C by river die-away test in slurry sediment of aquatic systems (Lee & Ryan 1979; quoted, Scow 1982)

$t_{1/2} = 33$ d from screening model calculations (Jury et al. 1987b)

$t_{1/2}(\text{aq. anaerobic}) = 672$ –4320 h, based on anaerobic digester sludge data (Battersby & Wilson 1989; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 12.2$ –122 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: estimated first-order $t_{1/2} = 693$ d from biodegradation rate constant $k = 0.001 \text{ d}^{-1}$ by river die-away test in aquatic systems (Lee & Ryan 1979; quoted, Scow 1982);

$t_{1/2} = 240$ –480 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

extremely resistant degradation in natural water with $t_{1/2} = 580$ d for static sediment-sea water to $t_{1/2} = 1400$ d for static estuarine river water (Muir 1991);

measured rate constant $k = (8.9 \pm 1.3) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 1.7–5.0 and $21 \pm 1^\circ\text{C}$, with $t_{1/2} = 3.9$ h at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 480$ –4320 h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment: estimated first-order $t_{1/2} = 23$ –69.3 d from biodegradation rate constant $k = 0.01$ –0.03 d^{-1} at 9–21°C by river die-away test in slurry sediment of aquatic systems (Lee & Ryan 1979; quoted, Scow 1982);

$t_{1/2} = 27$ d for sediment-water microcosm under aerobic conditions (quoted, Muir 1991).

Soil: degradation $t_{1/2} = 24$ d and 14 d in Quachita Highlands' forest and grassland soil, respectively, $t_{1/2} = 21$ d in Gross Timbers Forest soil, average $t_{1/2} = 17$ d in 3 soils (Altom & Stritzke 1973);

$t_{1/2} = 240\text{--}480$ h, based on unacclimated soil grab sample data (Smith 1978, 1979; quoted, Howard et al. 1991); estimated first-order $t_{1/2} = 19.8$ d from rate constant $k = 0.035\text{ d}^{-1}$ by soil incubation die-away studies (Rao & Davidson 1980; quoted, Scow 1982);

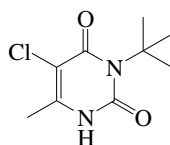
$t_{1/2} = 33$ d from screening model calculations (Jury et al. 1987b);

aerobic degradation $t_{1/2} > 25$ d at 29°C , to $t_{1/2} = 58$ d at 21°C in soil suspension from pre-incubated soil (Muir 1991);

selected field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994).

Biota: biochemical $t_{1/2} = 33$ d from screening model calculations (Jury et al. 1987b).

17.1.1.74 Terbacil



Common Name: Terbacil

Synonym: Sinbar, Turbacil

Chemical Name: 3-*tert*-butyl-5-chloro-6-methyluracil

CAS Registry No: 5902-51-2

Uses: control of most annual grasses and broadleaf weeds, and some perennial weeds in established apples, asparagus, blueberries, citrus, lucerne, mint, peaches, pecans, strawberries, and sugar cane, etc.

Molecular Formula: C₉H₁₃ClN₂O₂

Molecular Weight: 216.664

Melting Point (°C):
176 (Lide 2003)

Boiling Point (°C):
sublime(below mp, Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm³ at 20°C):
1.34 (25°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

Molar Volume (cm³/mol):
217.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:
9.0 (Wauchope et al. 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0330 (mp at 176°C)
0.027 (20°C, Suntio et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
710 (Ashton & Crafts 1973; 1981; Spencer 1982)
710 (Martin & Worthing 1977; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)
600 (20°C, selected, Suntio et al. 1988)
710 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):
6.40 × 10⁻⁵ (29.5°C, Ashton & Crafts 1973; 1981)
6.00 × 10⁻⁵ (30°C, Hartley & Kidd 1987)
5.00 × 10⁻⁵ (20°C, selected, Suntio et al. 1988)
6.00 × 10⁻⁵ (20°C, Montgomery 1993)
6.25 × 10⁻⁵ (29.5°C, Tomlin 1994)
1.91 × 10⁻³ (20–25°C, supercooled liquid value, quoted, Majewski & Capel 1995)
4.13 × 10⁻⁵ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):
1.80 × 10⁻⁵ (20°C, calculated-P/C, Suntio et al. 1988)
1.82 × 10⁻⁵ (20–25°C, calculated, Montgomery 1993)
1.53 × 10⁻⁵ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow}:
1.89 (Karickhoff et al. 1979)
1.89 (Rao & Davidson 1980)

- 1.89, 1.90 (quoted, Montgomery 1993)
- 1.89 (recommended, Sangster 1993)
- 1.91 (Tomlin 1994)
- 1.89 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 1.18 (calculated-S, Kenaga 1980)
- 1.74 (Montgomery 1993)

Sorption Partition Coefficient, log K_{OC} :

- 1.71, 2.08 (soil: exptl., calculated, Kenaga 1980; Kenaga & Goring 1980)
- 1.62, 1.98 (soil, quoted, Madhun et al. 1986)
- 1.89, 1.76; 1.82, 1.04 (estimated- K_{OW} ; solubilities, Madhun et al. 1986)
- 1.62 (soil, screening model calculations, Jury et al. 1987b)
- 1.74 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.32–2.20 (soil, quoted, Montgomery 1993)
- 1.66 (soil, calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 1.58 (1.38–1.78) (soils: organic carbon OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: $t_{1/2} = 50$ d (Jury et al. 1987b).

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil: moderately persistent in soil with $t_{1/2} = 20$ –100 d (Willis & McDowell 1982);

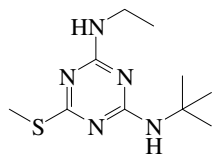
$t_{1/2} \sim 5$ –7 months (Hartley & Kidd 1987);

$t_{1/2} = 50$ d from screening model calculations (Jury et al. 1987b);

field $t_{1/2} = 50$ –175 d and the selected $t_{1/2} = 120$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical $t_{1/2} = 50$ d (Jury et al. 1987b).

17.1.1.75 Terbutryn



Common Name: Terbutryn

Synonym: Clarosan, GS 14260, Igran, Prebane, Shortstop, Terbutrex, Terbutrin, Terbutryn

Chemical Name: *N*-(1,1-dimethylethyl)-*N'*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine; 2-(*tert*-butylamino)-4-(ethylamino)-6-(methylthio)-*s*-triazine

Uses: selective herbicide to control annual broadleaf and grass weeds in wheat.

CAS Registry No: 886-50-0

Molecular Formula: C₁₀H₁₉N₅S

Molecular Weight: 241.357

Melting Point (°C):

104 (Herbicide Handbook 1989, Lide 2003)

Boiling Point (°C):

154–160 (at 0.06 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Density (g/cm³ at 20°C):

1.115 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

Molar Volume (cm³/mol):

273.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

4.30 (pK_a, Worthing & Hance 1991)

9.70 (pK_b, Wauchope et al. 1992; Hornsby et al. 1996)

4.07 (pK_a, Montgomery 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

101.4 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

59 (Rordorf 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.168 (mp at 104°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

25 (20°C, Weber 1972; Ashton & Crafts 1973, 1981)

58 (20°C, Quellette & King 1977)

25 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991; Herbicide Handbook 1978)

25 (shake flask-HPLC, Ellgehausen et al. 1981)

25 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Montgomery 1993)

22 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00013 (20°C, Weber 1972; Worthing & Walker 1987; Worthing & Hance 1991)

0.00013 (20°C, Ashton & Crafts 1973; 1981)

0.00013 (20°C, Hartley & Kidd 1987; Herbicide Handbook 1989)

2.20×10^{-4} , 9.10×10^{-3} , 0.22, 3.40, 38.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log (P_s/\text{Pa}) = 17.151 - 6201.4/(T/\text{K})$; measured range 45–100°C (solid, gas saturation-GC, Rordorf 1989)

$\log (P_L/\text{Pa}) = 14.654 - 5297.1/(T/\text{K})$; measured range 109–139°C (liquid, gas saturation-GC, Rordorf 1989)

- 0.00128 (20°C, Montgomery 1993)
 0.00028 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 0.0013 (20°C, calculated-P/C, Suntio et al. 1988)
 0.0012 (20°C, calculated-P/C, Muir 1991)
 0.0120 (20°C, calculated-P/C, Montgomery 1993)
 0.0014 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

- 3.74 (shake flask-GC, Elkell & Walum 1979)
 3.72, 3.74 (shake flask, Ellgehausen et al. 1981)
 2.56 (RP-HPLC-k' correlation, Braumann et al. 1983)
 3.34 (Worthing & Walker 1987)
 3.43 (RP-HPLC-RT correlation, Finizio et al. 1991)
 3.49 (Worthing & Hance 1991; Milne 1995)
 3.43–3.73 (Montgomery 1993)
 3.34 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
 3.74 (recommended, Sangster 1993)
 3.38, 3.36 (shake flask-UV, calculated-RP-HPLC-k' correlation, Liu & Qian 1995)
 3.74 (recommended, Hansch et al. 1995)
 3.44 (Pomona-database, Müller & Kördel 1996)
 3.34 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.17 (*Daphnia magna*, wet wt. basis, Ellgehausen et al. 1980)
 2.00, 2.00 (calculated-S, calculated-K_{OC}, Kenaga 1980)
 1.95 (catfish *Ictalurus melas*, wet wt basis, Wang et al. 1996)

Sorption Partition Coefficient, log K_{OC}:

- 2.85 (soil, Colbert et al. 1975; Gaillardon et al. 1977; Kenaga 1980; Kenaga & Goring 1980)
 2.87 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 2.85–2.87 (soil, quoted values, Bottoni & Funari 1992)
 3.30 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.68 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995b)
 3.21–4.07 (Montgomery 1993)
 3.30 (estimated-chemical structure, Lohninger 1994)
 2.84 (calculated-K_{OW}, Liu & Qian 1995)
 2.85 (soil, calculated-MCI χ , Sabljic et al. 1995)
 2.68; 2.80 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 4.62, 2.57, 2.90, 1.56, 3.55 soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 3.554, 2.878, 2.778, 2.505, 3.054 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)
 2.85; 2.82, 2.74 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 3.79 (3.28–4.30) (soil: organic carbon OC ≥ 0.5%, average, Delle Site 2001)
 2.59, 2.86 (Kishon river sediments, sorption isotherm, Chefetz et al. 2004)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis: 4 ppb contaminated water in the presence of TiO₂ and H₂O₂ completely photodegraded after 15 h by solar irradiation (Muszkat et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation: aerobic $t_{1/2} = 80\text{--}240$ d for $1\text{ }\mu\text{g/mL}$ to biodegrade in sediment-water and anaerobic $t_{1/2} > 650$ d for $1\text{ }\mu\text{g/mL}$ to biodegrade in sediment-water both at 25°C (Muir & Yarechewski 1982; quoted, Muir 1991). biological degradation rate followed a first order kinetics, with $t_{1/2} = 8.9\text{--}18.2$ d by raw water microflora from Rivere Nile, $t_{1/2} = 4.0\text{--}6.9$ d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 1.70\text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 1.9\text{--}1.5\text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 3.6\text{--}2.7\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 3.6\text{--}4.4\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

$k_2 = 0.053\text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, calculated by initial uptake data of 0–12 h, Muir et al. 1983)

$k_2 = 0.043\text{ h}^{-1}$ (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.040\text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.040\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_1 = 3.11\text{ h}^{-1}$, $k_2 = 0.0346\text{ h}^{-1}$ (catfish *Ictalurus melas*, Wang et al. 1996)

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 8.9\text{--}18.2$ d by raw water microflora from River Nile, $t_{1/2} = 4.0\text{--}6.9$ d by raw water microflora + sewage (El-Dib & Abou-Waly 1998)

Ground water: reported half-lives or persistence, $t_{1/2} = 14\text{--}28$ d (Bottoni & Funari 1992)

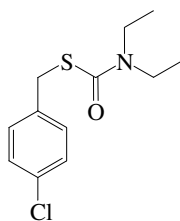
Sediment: aerobic $t_{1/2} = 80\text{--}240$ d for $1\text{ }\mu\text{g mL}^{-1}$ to biodegrade in sediment-water and anaerobic $t_{1/2} > 650$ d for $1\text{ }\mu\text{g mL}^{-1}$ to biodegrade in sediment-water both at 25°C (Muir & Yarechewski 1982; quoted, Muir 1991).

Soil: reported $t_{1/2} = 14\text{--}28$ d (Worthing & Hance 1991; Bottoni & Funari 1992);

$t_{1/2} \sim 42$ d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota: elimination $t_{1/2} = 13.1$ h in pond sediment-water, $t_{1/2} = 16.1$ h in river water, $t_{1/2} = 17.3$ h in river sediment-water, $t_{1/2} = 17.3$ in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

17.1.1.76 Thiobencarb



Common Name: Thiobencarb

Synonym: benthioncarb, Bolero, Saturn, Saturno, Siacarb

Chemical Name: *S*-(4-chlorophenyl)methyl diethylcarbamothioate

Pesticide Class: herbicide; Group: carbamate

Uses: herbicide

CAS Registry No: 28249-77-6

Molecular Formula: $C_{12}H_{16}ClNOS$

Molecular Weight: 257.779

Melting Point ($^{\circ}C$):

1.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

126–129/0.008 mmHg (Ashton & Crafts 1981)

126–128/0.008 mmHg (Spencer 1982; Hartley & Kidd 1987; Herbicide Handbook 1989)

Density (g/cm^3 at $20^{\circ}C$):

1.148–1.180 (Spencer 1982; Hartley & Kidd 1987; Herbicide Handbook 1989)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

30 (Ashton & Crafts 1981)

30 (reported as 30 g/L, Spencer 1982)

30 ($20^{\circ}C$, Hartley & Kidd 1987; Herbicide Handbook 1989)

28 (20 – $25^{\circ}C$, recommended, Wauchope et al. 1992; Hornsby et al. 1996)

17.0 (Majewski & Capel 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.96×10^{-4} ($20^{\circ}C$, Ashton & Crafts 1981)

4.21×10^{-3} ($20^{\circ}C$, GC-RT correlation, Kim 1985)

2.0×10^{-4} ($20^{\circ}C$, Hartley & Kidd 1987)

1.97×10^{-4} (Herbicide Handbook 1989)

2.93×10^{-3} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.78×10^{-3} (Majewski & Capel 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.027 (calculated-P/C, Majewski & Capel 1995)

0.0274 (quoted lit., Armbrust 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.42 ($20^{\circ}C$, shake flask-GC, Kanazawa 1981)

3.40 (shake flask-GC, Schimmel et al. 1983)

3.98 (HPLC-RT correlation, Kawamoto & Urano 1989)

3.42 (Gerstl 1990)

- 3.40 (recommended, Sangster 1993)
- 3.93 (HPLC-RT correlation, Scibaldi & Finizio 1993)
- 3.40 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)
- 3.78 (RP-HPLC-RT correlation, Yu et al. 1997)
- 4.37 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF or log K_B :

- 2.97 (Pait et al. 1992)
- 1.76, 1.77 (37.2, 18.6 $\mu\text{g/L}$ concn in water; carp, 3–5 d exposure, Wang et al. 1992)
- 1.38, 1.0 (20.0, 2.0 $\mu\text{g/L}$ concn in water; tilapia, 3–5 d exposure, Wang et al. 1992)
- 1.49, 1.13 (20.0, 2.0 $\mu\text{g/L}$ concn in water; loach, 3–5 d exposure, Wang et al. 1992)
- 0.92, 1.08 (15.0, 7.5 $\mu\text{g/L}$ concn in water; Grass carp, 3–5 d exposure, Wang et al. 1992)
- 1.20, 1.26 (10.0, 5.0 $\mu\text{g/L}$ concn in water; eel, 3–5 d exposure, Wang et al. 1992)
- 2.57, 1.94 (5.0, 1.4 $\mu\text{g/L}$ concn in water; black silver carp, 3–5 d exposure, Wang et al. 1992)
- 0.46, 0.86 (200, 20 $\mu\text{g/L}$ concn in water; freshwater clam, 3v5 d exposure, Wang et al. 1992)
- 1.82; 2.23 (*Gnathopogon aerulescens*; *Pseudorasbora parva*, flow-through condition, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC} :

- 2.83 (soil, Gerstl 1990)
- 2.49, 3.02, 2.83 (soil, Bottoni & Funari 1992)
- 2.95 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.43 (soil, calculated- χ , Meylan et al. 1992)
- 3.27 (calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 2.95 (quoted lit., Armbrust 2000)
- 3.32, 2.75 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: stable aqueous hydrolysis rates at pH 5, 7, 9; measured hydroxy radical rate constant $k = 6.8 \times 10^{12} \text{ M}^{-1}/\text{h}$ (Armbrust 2000)

Biodegradation: $t_{1/2} = 2\text{--}3$ wk in soil varies under aerobic conditions to $t_{1/2} = 6\text{--}8$ months under anaerobic conditions (Hartley & Kidd 1987; Herbicide Handbook 1989)

aerobic degradation rate constant $k = 0.057 \text{ d}^{-1}$ with $t_{1/2} = 12 \text{ d}$ by aerobic activated sludge at 20°C (Kawamoto & Urano 1990)

aerobic rate constant, $k = 1.38 \times 10^{-3} \text{ h}^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: lost from aqueous solution by volatility and photodegradation (Herbicide Handbook 1989)

biodegradation $t_{1/2} = 12 \text{ d}$ by aerobic activated sludge at 20°C (Kawamoto & Urano 1990).

Ground water: reported half-lives or persistence, $t_{1/2} = 6\text{--}7$, 23–120, and 26–40 d (Bottoni & Funari 1992)

Sediment:

Soil: laboratory studies with Stockton adobe and Crowley silty clay loam gave $t_{1/2} = 2\text{--}3$ wk under aerobic conditions to $t_{1/2} = 6\text{--}8$ months under anaerobic conditions (Hartley & Kidd 1987; Herbicide Handbook 1989);

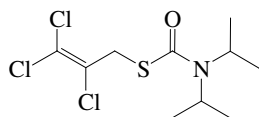
reported half-lives or persistence of 6–7 d, 23–120 d, 26–40 d (Bottoni & Funari 1992);

soil; $t_{1/2} = 18 \text{ d}$ (Pait et al. 1992);

field $t_{1/2} = 21 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

17.1.1.77 Triallate



Common Name: Triallate

Synonym: Avadex BW, Buckle, CP 23426, Dipthal, Far-Go

Chemical Name: 2,3,3-trichloro-2-propene-1-thiol diisopropylcarbamate; *S*-(2,3,3-trichloro-allyl)diisopropyl-(thio-carbamate); *S*-(2,3,3-trichloro-2-propenyl) bis(1-methylethyl)-carbamothioate

Uses: herbicide to control wild oats in lentils, barley, peas, and winter wheat.

CAS Registry No: 2303-17-5

Molecular Formula: C₁₀H₁₆Cl₃NOS

Molecular Weight: 304.664

Melting Point (°C):

29 (Lide 2003)

Boiling Point (°C):

148–149 (Khan 1980; Spencer 1982)

117 (at 40 mPa, Herbicide Handbook 1989; Montgomery 1993; Milne 1995)

Density (g/cm³ at 20°C):

1.273 (25°C, Hartley & Kidd 1987; Herbicide Handbook 1989; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm³/mol):

314.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.86 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.7 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.914 (mp at 29°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

4.0 (20°C, Weber 1972; Weber et al. 1980)

4.0 (Ashton & Crafts 1973; Spencer 1973, 1982; Khan 1980)

4.0 (Martin & Worthing 1977, Worthing & Walker 1983, 1987; Worthing & Hance 1991; Herbicide Handbook 1978, 1989)

4.0 (Hartley & Graham-Bryce 1980; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

< 1.0 (27°C, Ashton & Crafts 1981)

3.0 (20°C, selected, Suntio et al. 1988)

4.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.016 (20°C, Weber 1972; Worthing & Walker 1987)

0.016 (Ashton & Crafts 1973; Spencer 1982; quoted, Suntio et al. 1988)

0.0276* (gas saturation-GC, measured range 20–45°C, Grover et al. 1978)

log (P/mmHg) = 11.045 – 4401/(T/K); temp range 20–45°C (Antoine eq., gas saturation-GC, Grover et al. 1978)

0.0265 (29.5°C, Ashton & Crafts 1981)

0.0276 (gas saturation method, Spencer & Cliath 1983)

6.07 × 10⁻³, 4.81 × 10⁻³ (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)

0.016 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

0.010 (20°C, selected, Suntio et al. 1988; quoted, Majewski & Capel 1995)

- 0.015 (Herbicide Handbook 1989)
 0.017* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
 $\log (P_s/Pa) = 18.124 - 5932/(T/K)$; measured range 32.3–150°C (solid, gas saturation-GC, Rordorf 1989)
 $\log (P_L/Pa) = 13.395 - 4485.1/(T/K)$; measured range 32.3–150°C (liquid, gas saturation-GC, Rordorf 1989)
 0.026 (selected, Taylor & Spencer 1990)
 0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.016 (20°C, Montgomery 1993)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 1.96 (calculated-P/C, Jury et al. 1983, 1984, 1987a, 1990; Jury & Ghodrati 1989)
 1.02 (20°C, calculated-P/C, Suntio et al. 1988)
 1.983 (calculated-P/C, Taylor & Glotfelty 1988)
 1.226 (20°C, calculated-P/C, Muir 1991)
 1.013 (20–25°C, calculated-P/C, Montgomery 1993)
 0.762 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 4.29 (Montgomery 1993)
 4.53 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Bioconcentration Factor, $\log BCF$:

- 2.45 (calculated-S, Kenaga 1980; quoted, Isensee 1991)
 2.18 (calculated- K_{oc} , Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

- 3.56 (Guenzi & Beard 1974)
 3.34 (soil, Grover 1974; Beestman & Demming 1976)
 3.32 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)
 3.56 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
 3.22 (soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
 3.38 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 3.31 (calculated, Montgomery 1993)
 3.38 (selected, Lohninger 1994)
 3.35 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 3.60, 3.12 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 2.70, 2.64 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 26$ d (Jury et al. 1983; quoted, Grover 1991); half-life of 100 d (Jury et al. 1984; quoted, Spencer & Cliath 1990);
 estimated $t_{1/2} \sim 8$ d from 1 m depth of water at 20°C (Muir 1991).

Photolysis:

Oxidation: calculated lifetime of 5 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Hydrolysis: $t_{1/2} > 24$ wk for 1 $\mu\text{g/mL}$ to hydrolyze in aqueous buffer at pH 4, 7, and 9 in the dark at 25°C (Smith 1969; quoted, Muir 1991).

Biodegradation: estimated $t_{1/2} = 680$ d at pH 6.8 and $t_{1/2} = 1170$ d at pH 7.0, both at 25°C from biodegradation rate constants in aquatic systems (Smith 1969; quoted, Scow 1982);

$t_{1/2} = 100$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Jury et al. 1983, 1984, 1987a,b; 1990; Jury & Ghodrati 1989; Grover 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated life-time of 5 h for the vapor-phase reaction with OH radicals in the troposphere (Atkinson et al. 1992; Kwok et al. 1992).

Surface water: $t_{1/2} = 680$ d at pH 6.8 and $t_{1/2} = 1170$ d at pH 7.0, both at 25°C for biodegradation in aquatic systems (Smith 1969; quoted, Scow 1982).

Ground water:

Sediment:

Soil: biodegradation $t_{1/2} = 100$ d from screening model calculations (Jury et al. 1984, 1987a,b; 1990; Jury & Ghodrati 1989; quoted, Montgomery 1993);
selected field $t_{1/2} = 82$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: biochemical $t_{1/2} = 100$ d from screening model calculations (Jury et al. 1987a,b; Jury & Ghodrati 1989).

TABLE 17.1.1.77.1

Reported vapor pressures of triallate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
Grover et al. 1978		Rordorf 1989	
gas saturation method-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
20	0.0133	25	0.017
23	0.0202	50	0.59
25	0.0276	75	12.0
30	0.0446	100	170
35	0.0704	125	1700
40	0.131		for solid
45	0.267	eq. 1	P _s /Pa
		A	18.124
		B	5932
eq. 1	P/mmHg		for liquid
A	11.045		
B	4401	eq. 1	P _L /Pa
		A	13.395
mp/°C	33–33.5°C	B	4485.1

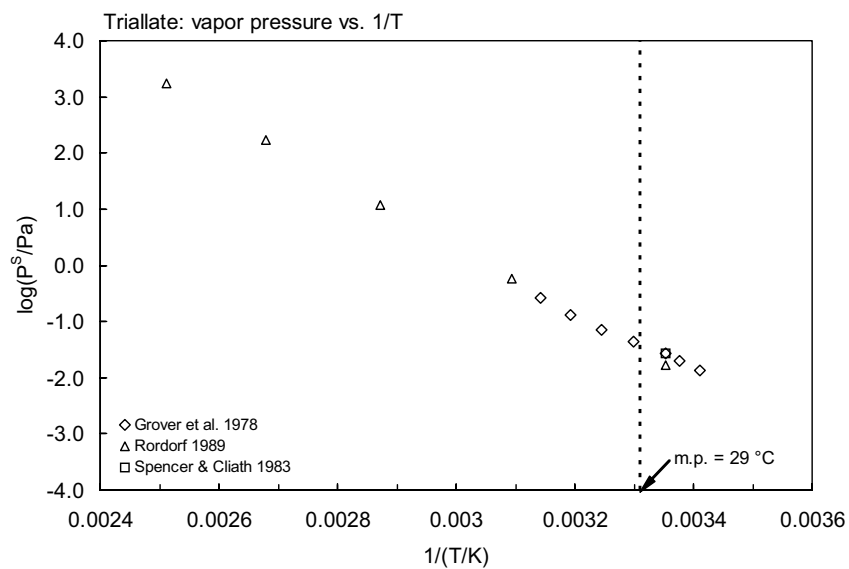
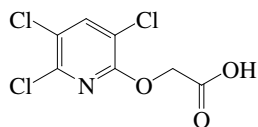


FIGURE 17.1.1.77.1 Logarithm of vapor pressure versus reciprocal temperature for triallate.

17.1.1.78 Triclopyr



Common Name: Triclopyr

Synonym: Garlon, Truflon, Crossbow

Chemical Name: 3,5,6-trichloro-2-pyridinyloxyacetic acid

CAS Registry No: 56335-06-3

Uses: herbicide

Molecular Formula: $C_7H_4Cl_3NO_3$

Molecular Weight: 256.471

Melting Point ($^{\circ}C$):

148–150 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)

150.5 (Tomlin 1994)

Boiling Point ($^{\circ}C$):

290 (dec., Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

Dissociation Constant pK_a :

2.68 (Spencer 1982; Worthing & Walker 1987)

2.93 (Woodburn et al. 1993)

3.97 (Tomlin 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

102.5 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

31.8 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

430 (Kenaga 1980a,b)

440 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)

408 ($20^{\circ}C$, Tomlin 1994)

7690, 8100, 8220 ($20^{\circ}C$, at pH 5, 7, and 9, Tomlin 1994)

7618 (20 – $25^{\circ}C$, quoted as $2.97E + 01$ mol/ m^3 , Majewski & Capel 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.6×10^{-4} (Spencer 1982)

1.68×10^{-4} (Worthing & Walker 1987; Hartley & Kidd 1987; Tomlin 1994)

1.90×10^{-5} , 1.0×10^{-3} , 0.031, 0.59, 7.80 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 17.65 - 6672.3/(T/K)$; measured range 85.4 – $145^{\circ}C$ (gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 14.445 - 5354.8/(T/K)$; measured range 150 – $186^{\circ}C$ (gas saturation-GC, Rordorf 1989)

2.0×10^{-4} (vapor pressure balance, Tomlin 1994)

2.91×10^{-3} (20 – $25^{\circ}C$, Majewski & Capel 1995)

Henry's Law Constant (Pa· m^3 /mol at $25^{\circ}C$ or as indicated):

9.79×10^{-5} (20 – $25^{\circ}C$, calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

−0.52 (Kenaga 1980a)

0.42, −0.45, −0.96 (pH 5, 7, and 9, Tomlin 1994)

1.30 (Isensee 1991)

2.53 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 1.49, -0.22 (fish: flowing water tests, static ecosystem tests, Kenaga 1980a)
- 1.30, 0 (fish: calculated-solubility, K_{OW} , Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.43 (soil, Kenaga 1980a)
- 1.43, 2.204 (soil: quoted, calculated, Kenaga 1980b)
- 1.43, 2.20 (soil, Bottoni & Funari 1992)
- 1.43 (quoted or calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

- Photolysis: photolysis $t_{1/2} < 0.4$ d in sterile, pH 5-buffered water at 40°N latitude in midday, midsummer (McCall & Gavit 1986);
- photodecomposition $t_{1/2} < 12$ h (Worthing 1987; Tomlin 1994);
- photodecomposition $t_{1/2} < 24$ h (Hartley & Kidd 1987);
- aqueous photolysis pseudo-first order $t_{1/2}(\text{average}) = 0.5$ and 1.3 d in pH 7-buffered water and natural river water, respectively, at 25°C under artificial lights and midsummer sunlight, 40°N latitude (Woodburn et al. 1993);
- aqueous photolysis rate constant, $k = 8.3 \times 10^{-2} \text{ h}^{-1}$ (Armbrust 2000).

Oxidation:

- Hydrolysis: hydrolysis $t_{1/2} > 3$ months in darkened, sterile, buffered water at pH of 5–9 and 25°C (Woodburn et al. 1993);
- stable aqueous hydrolysis rates at pH 5, 7, 9; measured hydroxy radical rate constant $k = 4.3 \times 10^{12} \text{ M}^{-1} \cdot \text{h}^{-1}$ (Armbrust 2000).

- Biodegradation: in soil, fairly rapid degradation by microbial activity, with an average $t_{1/2} = 46$ d depending on soil and climatic conditions (Spencer 1982; Tomlin 1994);
- aerobic rate constant, $k = 9.03 \times 10^{-4} \text{ h}^{-1}$ (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

- Surface water: stable to hydrolysis, but subject to photolysis with $t_{1/2} < 12$ h (Spencer 1982; Worthing 1987; Tomlin 1994);
- photolysis $t_{1/2} < 0.4$ d in sterile, pH 5 buffered water at 40°N latitude (McCall & Gavit 1986);
- $t_{1/2} \sim 3$ to 4 d in natural water during summer conditions (Solomon et al. 1988);
- pseudo-first order photolysis $t_{1/2}(\text{ave.}) = 0.5$ and 1.3 d in pH-buffered water and natural river water, respectively; the photodegradation pseudo-first-order half-lives in sterile, pH 7 water, midsummer sunlight at 40°N latitude and 25°C calculated as $k = 0.36$ (0.33–0.39) and 0.60 (0.50–0.70) d under artificial and natural sunlight, respectively; $t_{1/2} = 0.71$ (0.70–0.73) and 1.86 (1.77–1.96) d in river water under artificial and natural sunlight conditions, respectively, in midsummer sunlight and approximately 40°N latitude and 25°C (Woodburn et al. 1993);
- photodecomposition $t_{1/2} < 24$ h (Hartley & Kidd 1987).

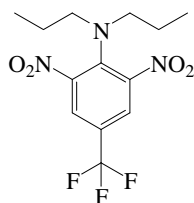
Ground water: reported half-lives or persistence, $t_{1/2} = 40$ and 46 d (Bottoni & Funari 1992).

Sediment:

- Soil: fairly rapid degradation by microbial activity, with an average $t_{1/2} = 46$ d depending on soil and climatic conditions (Spencer 1982; Tomlin 1994);

Biota:

17.1.1.79 Trifluralin



Common Name: Trifluralin

Synonym: Agreflan, Crisalin, Digermin, Elancolan, L-36352, Nitran, Nitrofor, Olitref, Treflan, Trifluoramine, Trifurex, Trikepin, Trim

Chemical Name: 2,6-dinitro-*N,N*-dipropyl-4-trifluoromethylaniline; 2,6-dinitro-*N,N*-dipropyl-4-(trifluoromethyl)-benzenamine

Uses: pre-emergence herbicide to control many grass and broadleaf weeds.

CAS Registry No: 1582-09-8

Molecular Formula: $C_{13}H_{16}F_3N_3O_4$

Molecular Weight: 335.279

Melting Point ($^{\circ}C$):

49 (Lide 2003)

Boiling Point ($^{\circ}C$):

362 (estimated, Grain 1982)

139–140 (at 4.2 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

96–97 (at 0.18 mmHg, Herbicide Handbook 1989)

Density (g/cm^3 at $20^{\circ}C$):

1.294 ($25^{\circ}C$, Montgomery 1993)

1.36 ($22^{\circ}C$, Tomlin 1994)

Molar Volume (cm^3/mol):

295.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

8754 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.85 (DSC method, Plato & Glasgow 1969)

23.5 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.581 (mp at $49^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

24 ($27^{\circ}C$, Woodford & Evans 1963; Günther et al. 1968; Spencer 1973)

40 ($29.5^{\circ}C$, Melnikov 1971)

0.35 ($20^{\circ}C$, Weber 1972; Worthing & Walker 1987)

0.1–0.5 (Probst et al. 1975)

0.60 (Herbicide Handbook 1978; Kenaga 1980; Kenaga & Goring 1980)

0.05 (Wauchope 1978; Weber et al. 1980)

< 1.0 ($20^{\circ}C$, Khan 1980)

8.11 (20 – $25^{\circ}C$, Kanazawa 1981)

0.30 (Beste & Humburg 1983; Jury et al. 1984; Taylor & Glotfelty 1988; Herbicide Handbook 1989)

0.32 (generator column-HPLC-RI, Swann et al. 1983)

0.70 (HPLC-RT correlation, Swann et al. 1983)

4.0 ($27^{\circ}C$, Verschueren 1983; Montgomery 1993)

0.75 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)

< 1.0 ($27^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

0.30 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.184, 0.221, 0.189 (at pH 5, 7, 9, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.0265 (29.5°C, Probst et al. 1967; Khan 1980)
- 0.0292 (29°C, effusion method, Hamaker & Kerlinger 1971)
- 0.0138 (20°C, Weber 1972; Worthing & Walker 1987)
- 0.0323 (30°C, from Spencer & Cliath 1973 unpublished data, Spencer et al. 1973)
- 0.0065* (20°C, gas saturation-GC, measured range 20–40°C, Spencer & Cliath 1974, Spencer 1976)
- $\log (P/\text{mmHg}) = 17.318 - 6344/(T/K)$; temp range 20–40°C (Antoine eq., Spencer 1976)
- 0.0262 (30°C, effusion method-pressure gauge, DePablo 1976)
- 0.0137 (Worthing & Walker 1979, Worthing & Hance 1991; Hartley & Kidd 1987)
- 0.0029 (20–25°C, Weber et al. 1980)
- 0.0173 (Herbicide Handbook 1983)
- 0.015 (20°C, Jury et al. 1983)
- 0.0147 (Herbicide Handbook 1989)
- 0.010* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
- $\log (P_s/\text{Pa}) = 17.46 - 5800.6/(T/K)$; measured range 48.8–124°C (solid, gas saturation-GC, Rordorf 1989)
- $\log (P_L/\text{Pa}) = 13.65 - 4573.1/(T/K)$; measured range 48.8–124°C (liquid, gas saturation-GC, Rordorf 1989)
- 0.015 (20°C, selected, Taylor & Spencer 1990)
- 0.0147 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.0147 (20°C, Montgomery 1993)
- 0.0095 (Tomlin 1994)
- 0.0363 (liquid P_L , GC-RT correlation; Donovan 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 16.61 (calculated-P/C, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989)
- 4.02 (20°C, calculated-P/C, Suntio et al. 1988)
- 16.36 (calculated-P/C, Taylor & Glotfelty 1988)
- 5.206 (fog chamber-GC/ECD, Fendinger et al. 1989)
- 5.95 (wetted-wall column-GC/ECD, Fendinger et al. 1989)
- 16.0 (calculated-P/C, Nash 1989)
- 13.27 (20°C, calculated-P/C, Muir 1991)
- 4.903 (23°C, calculated-P/C, Montgomery 1993)
- 15.2, 6.67, 4.02 (quoted literature values, Grover et al. 1997)
- 10.31, 15.06 (20°C, distilled water, salt water 33.3% NaCl, wetted wall column-GC, Rice et al. 1997b)
- $\log K_{AW} = -1546/(T/K) + 2.87$; temp range 8.3–43.5°C, (distilled water, wetted-wall column-GC, Rice et al. 1997b)
- $\log K_{AW} = -1232/(T/K) + 1.94$; temp range 8.3–43.5°C, (salt water solution, 33.3% NaCl, wetted-wall column-GC, Rice et al. 1997b)
- 11.16, 11.04; 12.50 (20°C, microlayer, subsurface natural water of salinity 17% and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
- 10.97, 10.72; 12.38 (20°C, microlayer, subsurface natural water of salinity 16% and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
- 10.40, 10.06; 11.82 (20°C, microlayer, subsurface natural water of salinity 12%, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
- 12.43, 12.70; 14.84 (20°C, microlayer, subsurface water of salinity 32%, TOC 2.2–46 ppm, ocean water from Bering/Chukchi Sea; estimated value adjusted to salinity, Rice et al. 1997b)
- 9.49, 13.14, 19.67 (8.3, 20, 43.5°C, subsurface water from Bering Sea, TOC 2.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
- 8.504, 12.80; 19.61 (8.3, 20, 43.5°C, surface microlayer water from Bering Sea, TOC 3.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
- 8.87, 12.26, 19.69 (8.3, 20, 43.5°C, subsurface water from Chukchi Sea, TOC 3.3 ppm, wetted-wall column-GC, Rice et al. 1997b)
- 7.95, 12.04; 19.40 (8.3, 20, 43.5°C, surface microlayer water from Chukchi Sea, TOC 45.5 ppm, wetted-wall column-GC, Rice et al. 1997b)

6.99, 9.94, 15.85 (8.3, 20, 43.5°C, melted surface ice from the Arctic Ocean, TOC 48.8 ppm, wetted-wall column-GC, Rice et al. 1997b)

$\log K_{AW} = -786/(T/K) + 0.307$; temp range: 8.3–43.5°C, (ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)

$\log K_{AW} = -1232/(T/K) + 1.900$; temp range: 8.3–43.5°C, (subsurface microlayer of ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)

4.026 (calculated-P/C, this work)

9.63 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 2.870 - 1546/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.34 (Kenaga & Goring 1980)

3.06 (Rao & Davidson 1980)

5.34 (shake flask-UV, Briggs 1981)

5.28 (shake flask, Brown & Flagg 1981)

3.97 (shake flask-GC, Kanazawa 1981)

4.94 (HPLC-k' correlation, McDuffie 1981)

4.86 (shake flask, Dubelman & Bremer 1983)

4.19 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)

5.07 (Herbicide Handbook 1989; Worthing & Hance 1991; Milne 1995)

5.07, 5.28, 5.34 (Montgomery 1993)

4.88 (RP-HPLC-RT correlation, Saito et al. 1993)

4.82 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)

5.34 (recommended, Sangster 1993; Hansch et al. 1995)

5.27 (pH 7.7–8.9, Tomlin 1994)

5.13 (Pomona-database, Müller & Kördel 1996)

4.82 (RP-HPLC-RT correlation, Finizio et al. 1997)

4.98 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log BCF$:

3.97, 3.66 (measured, Metcalf & Sanborn 1975)

3.51, 3.03 (fathead minnow, kinetic test, chronic exposure, Spacie & Hamelink 1979)

3.11 (mosquito fish, correlated-S, Spacie & Hamelink 1979)

3.01 (rainbow trout, correlated- K_{OW} , Spacie & Hamelink 1979)

3.26–3.76 (Spacie & Hamelink 1979)

3.66, 3.04 (quoted exptl., calculated- K_{OC} , Kenaga 1980)

2.92 (calculated-S, Kenaga 1980)

2.95 (calculated- K_{OW} , Briggs 1981)

3.50 (*Pseudorasbora parva*, Kanazawa 1981)

3.26–3.76 (selected, Schnoor & McAvoy 1981; Schnoor 1992)

2.67, 5.02 (dry leaf, wet leaf, Bacci et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

4.14 (soil, Harvey 1974; Kenaga 1980; Kenaga & Goring 1980)

3.76 (soil, calculated-S as per Kenaga & Goring 1980, Kenaga 1980)

3.64 (av. 3 soils, McCall et al. 1980)

4.49 (Georgia's Hickory Hill pond sediment, Brown & Flagg 1981)

2.70 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)

3.78 (soil, Thomas 1982)

3.87 (soil average, Jury et al. 1983)

3.63 (soil slurry method, Swann et al. 1983)

3.98 (RP-HPLC-RT correlation, Swann et al. 1983)

3.86 (screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)

5.13 (RP-HPLC-k' correlation, cyanopropyl column, Hodson & Williams 1988)

3.59 (Nash 1988)

- 2.94 (average of 2 soils, Kanazawa 1989)
 3.64–4.15, 3.76–4.14 (soil, quoted values, Bottoni & Funari 1992)
 4.71, 4.44, 4.59 (No. 1 and 2 soil, No. 3 soil and No. 4 soil; Francioso et al. 1992)
 3.90 (soil, 20–25°C, selected, Wauchope et al. 1992)
 4.37 (selected, Lohninger 1994)
 3.94 (soil, HPLC-screening method, mean value from different stationary and mobile phases, Kördel et al. 1993, 1995a,b)
 3.93 (soil, calculated-MCI χ , Sabljic et al. 1995)
 3.94; 3.99 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.86 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 3.53, 3.45, 3.96 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
 4.42 (average values for sediments with $OC \geq 0.5\%$, Delle Site 2001)

Sorption Partition Coefficient, $\log K_{OM}$:

- 3.87 (Grover et al. 1978)
 3.63 (experimental, Grover et al. 1979)
 4.14 (av. soils/sediments, Kenaga & Goring 1980)
 3.90 (sorption isotherm-GC, Briggs 1981)
 1.36, 2.08, 2.98 ($\log K_p$: with first-order rate 0.52, 0.2, $8.3 \times 10^{-3} \text{ h}^{-1}$, Karickhoff & Morris 1985)
 4.14, 3.75 (selected, estimated, Magee 1991)
 2.94–4.49 (Montgomery 1993)
 4.37 (selected, Lohninger 1994)
 3.90 (soil, 20–25°C, selected, Hornsby et al. 1996)

Adsorption Coefficient K_d (L kg^{-1}):

- 8.1 (homoionic K^+ -montmorillonite clay minerals, Haderlein et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: initial rate constant $k = 2.6 \times 10^{-2} \text{ h}^{-1}$ and predicted rate constant $k = 6.6 \times 10^{-2} \text{ h}^{-1}$ from soil with $t_{1/2} = 10.5 \text{ h}$ (Thomas 1982);

$t_{1/2} = 18 \text{ d}$ (Jury et al. 1983; quoted, Grover 1991);

measured rate constant $k = 2\text{--}6 \text{ d}^{-1}$ (Glottfelty et al. 1984; quoted, Glottfelty 1989);

estimated rate constant $k = 0.7 \text{ d}^{-1}$ (Glottfelty et al. 1989);

estimated $t_{1/2} \sim 1.6 \text{ d}$ from 1 m depth of water at 20°C (Muir 1991).

Photolysis: $t_{1/2} < 1 \text{ h}$ under acidic conditions in aqueous methanolic solution (Crosby & Leitis 1973)

$k = 2.0 \text{ d}^{-1}$ with $t_{1/2} = 22 \text{ min}$ for direct sunlight photolysis near surface water at 40°N in the summer (Zepp & Cline 1977; Zepp 1980; Zepp et al. 1984)

$t_{1/2}(\text{calc}) = 0.94 \text{ h}$ for disappearance via direct sunlight photolysis in aqueous media (Zepp & Baughman 1978; quoted, Harris 1982)

$k = 0.03 \text{ d}^{-1}$ with $t_{1/2} = 22 \text{ d}$ for direct sunlight near surface (Schnoor & McAvoy 1981)

$k = 0.028\text{--}0.012 \text{ min}^{-1}$ corresponding to $t_{1/2} = 25\text{--}60 \text{ min}$ for July, midday sunlight in an outdoor chamber (Mongar & Miller 1988)

$t_{1/2} = 0.5 \text{ h}$ estimated from photolysis reaction rate by direct sunlight of midday in mid-summer at 40°N near surface water (Zepp 1991)

$t_{1/2} \sim$ minutes to several months depending on the substrate under sunlight in all media (summary of literature data, Grover et al. 1997)

Oxidation:

Hydrolysis: $t_{1/2}(\text{calc}) > 1 \text{ yr}$ buffered at pH 4, 7, 9 and incubated at 50°C (Grover et al. 1997)

Abiotic Transformations: Degradation by abiotic reductive transformations:

$k = 1.79 \times 10^{-3} \text{ min}^{-1}$ at pH 6.5, $1.08 \times 10^{-2} \text{ min}^{-1}$ at pH 6.72–6.75, $1.64 \times 10^{-2} \text{ min}^{-1}$ at pH 6.84, $4.90 \times 10^{-2} \text{ min}^{-1}$ at pH 6.94, $7.09 \times 10^{-2} \text{ min}^{-1}$ at pH 6.97, 0.141 min^{-1} at pH 7.14, 0.390 min^{-1} at pH 7.46, 0.566 min^{-1} at pH 7.53, and 0.727 min^{-1} at pH 7.73 covering half-lives of 1–400 min., in reaction mixture of 0.5 mM Fe(II) and 100 mg/L goethite solutions (Klupinski & Chin 2003)

$k = 1.88 \text{ M}^{-1} \text{ s}^{-1}$ in H_2S with (mecapto)juglone (hydroquinone moiety, an abiotic reductant found in natural systems) solution at pH 6.65 (Wang & Arnold 2003)

Aqueous solutions with surface-bound Fe(II) species and their first-order rate constants as:

$k = 1.13 \times 10^{-3} \text{ h}^{-1}$ at pH 6.5, $k = 1.11 \times 10^{-2} \text{ h}^{-1}$ at pH 7.0, $k = 0.0251 \text{ h}^{-1}$ at pH 7.4, and $k = 3.40 \text{ h}^{-1}$ at pH 7.8 for aqueous ferrous ion system;

$k = 0.361 \text{ h}^{-1}$ at pH 6.5, $k = 0.750 \text{ h}^{-1}$ at pH 6.7, $k = 2.57 \text{ h}^{-1}$ at pH 7.0, and $k = 6.66 \text{ h}^{-1}$ at pH 7.3 for Fe(II)/goethite system; and

$k = 4.23 \times 10^{-3} \text{ h}^{-1}$ at pH 6.5, $k = 5.38 \times 10^{-3} \text{ h}^{-1}$ at pH 7.0, $k = 1.10 \times 10^{-2} \text{ h}^{-1}$ at pH 7.4 and $k = 2.36 \times 10^{-2} \text{ h}^{-1}$ at pH 7.8 for Fe(II)/clay system, all with total dissolved Fe(II) = 1 mM (Wang & Arnold 2003)

Biodegradation:

$t_{1/2} = 4\text{--}5 \text{ d}$ for 4 $\mu\text{g/mL}$ to biodegrade in flooded soils at 24.5°C and $t_{1/2} > 21 \text{ d}$ at 3.3°C (Probst et al. 1967; quoted, Means et al. 1983; Muir 1991);

$t_{1/2} > 20 \text{ d}$ for 0.33 $\mu\text{g/mL}$ to biodegrade in soil suspension at 25°C (Willis et al. 1974; quoted, Muir 1991);

$t_{1/2} = 20 \text{ d}$ for 0.5 $\mu\text{g/mL}$ to biodegrade in flooded soil with 0.5–1.0 cm of water on top of the soil at 20–42°C (Savage 1978; quoted, Muir 1991);

Degradation $t_{1/2} < 1$ month in three soils, Goldsborol loamy sand, Cecil loamy sand Drummer clay loam treated with 1 ppm trifluralin) for 4 month under aerobic conditions, no degradation in sterile controls. (shake flask-TLC, Camper et al. 1980)

$t_{1/2} < 1$ month for 1.0 $\mu\text{g/mL}$ to biodegrade in flooded soils at 25°C (derived from Camper et al. 1980; Muir 1991)

$k = 0.008 \text{ d}^{-1}$ by soil incubation die-away test and $k = 0.025 \text{ d}^{-1}$ by flooded soil incubation die-away test (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 132 \text{ d}$ for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a,b; Jury & Ghodrati 1989; Grover 1991);

$t_{1/2} = 46 \text{ wk}$ for 2.0 $\mu\text{g/mL}$ to biodegrade in flooded soils at 25°C (Brewer et al. 1982; quoted, Muir 1991);

$t_{1/2} = 20 \text{ h}$ for 0.36 $\mu\text{g/mL}$ to biodegrade in sediment-water microcosm at 20°C (Spain & Van Veld 1983; quoted, Muir 1991);

$k = -0.00504$ to -0.00730 h^{-1} in nonsterile sediment, $k = -0.00160$ to -0.00651 h^{-1} in sterile sediment by shake-tests at Range Point; $k = -0.00827$ to -0.01140 h^{-1} in nonsterile water, and $k = -0.00499$ to -0.00712 h^{-1} in sterile water by shake-tests at Range Point (Walker et al. 1988)

$k = -0.00621$, -0.0121 h^{-1} in nonsterile sediment, $k = -0.00476$, -0.00409 h^{-1} in sterile sediment by shake-tests at Davis Bayou and $k = -0.00439$, -0.00349 h^{-1} in nonsterile water, and $k = -0.00299$, -0.00598 h^{-1} in sterile water by shake-tests at Davis Bayou (Walker et al. 1988).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: mean $t_{1/2} = 42 \text{ min}$ under August conditions in California range from 21–63 min (Woodrow et al. 1978)

$t_{1/2} = 25\text{--}60 \text{ min}$ for July, midday sunlight in an outdoor chamber (Mongar & Miller 1988)

$t_{1/2} = 182\text{--}193 \text{ min}$ under fall sunlight conditions in October (Woodrow et al. 1983)

Surface water: calculated $t_{1/2} = 21 \text{ min}$ from midday direct sunlight photolysis rate constant of 2.0 h^{-1} (Zepp 1978; Zepp & Cline 1977; quoted, Zepp et al. 1984);

calculated $t_{1/2} = 0.94 \text{ h}$ for disappearance via direct sunlight photolysis in aqueous media (Zepp & Baughman 1978; quoted, Harris 1982);

$t_{1/2} < 20 \text{ d}$ for 2.5–5 cm water over flooded soils, $t_{1/2} \sim 20 \text{ h}$ in water above sediment in estuarine sediment-water microcosm (Muir 1991);

$t_{1/2} < 9 \text{ h}$ in buffered aqueous solution of pH 7 under Xenon lamp (quoted, Grover et al. 1997)

$t_{1/2} = 1\text{--}400 \text{ min}$ in reaction mixture of 0.5 mM and 100 mg/L goethite solution for pHs from 6.5 to 7.73 (Klupinski & Chin 2003).

Ground water: reported $t_{1/2} = 4\text{--}67$, 57–126, 70, 83, and 105–132 d (Bottoni & Funari 1992)

Sediment: degradation $t_{1/2} = 9 \text{ d}$ in estuarine sediment ($18^\circ/\infty$) system (Means et al. 1983).

$t_{1/2} = 18.5 \text{ d}$ in flooded sediment (quoted, Grover et al. 1997)

Soil: $t_{1/2} = 4\text{--}5 \text{ d}$ for 4 $\mu\text{g/mL}$ to biodegrade in flooded soils at 24.5°C and $t_{1/2} > 21 \text{ d}$ at 3.3°C (Probst et al. 1967; quoted, Means et al. 1983; Muir 1991);

estimated persistence of 6 months in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

degradation $t_{1/2} = 93 \text{ d}$ in soil (Parr & Smith 1973; quoted, Means et al. 1983);

- $t_{1/2} > 20$ d for $0.33 \mu\text{g mL}^{-1}$ to biodegrade in soil suspension at 25°C (Willis et al. 1974; quoted, Muir 1991);
 degradation $t_{1/2} = 1$ d (Kearney et al. 1976; quoted, Means et al. 1983); and $t_{1/2} = 54$ d in soil (Zimdahl & Gwynn 1977; quoted, Means et al. 1983);
 $t_{1/2} = 20$ d for $0.5 \mu\text{g/mL}$ to biodegrade in flooded soil with 0.5–1.0 cm of water on top of the soil at $20\text{--}42^\circ\text{C}$ (Savage 1978; quoted, Muir 1991);
 persistence of more than 6 months (Wauchope 1978);
 $t_{1/2} < 21$ d in flooded soil at $20\text{--}25^\circ\text{C}$ (Golab et al. 1979)
 biodegradation $t_{1/2} < 1$ month in 3 flooded soils at 25°C (Camper et al. 1980);
 estimated first-order $t_{1/2} \sim 86.6$ d in soil from biodegradation rate constant $k = 0.008 \text{ d}^{-1}$ by soil incubation die-away test and $t_{1/2} = 27.7$ d in anaerobic systems from rate constant $k = 0.025 \text{ d}^{-1}$ by flooded soil incubation die-away test (Rao & Davidson 1980; quoted, Scow 1982);
 $t_{1/2} = 2$ d on Bosket silt loam, $t_{1/2} = 2$ d on Sharkey clay for the first 3 to 5 days when sprayed onto soil surface, rate of loss much slower for the remainder of the 7- or 12-d sampling period with $t_{1/2} = 70$ d on Bosket silt loam, $t_{1/2} = 50$ d on Sharkey clay (Savage & Jordon 1980)
 $t_{1/2} = 30$ d flooded soil in aquatic ecosystem (Yockim et al. 1980)
 field $t_{1/2} = 0.1\text{--}0.3$ d in moist fallow soil (Glottfelty 1981; quoted, Nash 1983);
 Field studies: $t_{1/2} = 9.5$ wk - 1978 first study; $t_{1/2} = 11.8$ wk -1978 second study; $t_{1/2} = 12.2$ wk -1979, in a Crowley silt loam at Stuttgart, Arkansas (Brewer et al. 1982)
 Laboratory studies: $t_{1/2} = 19.6$ wk at 4°C , $t_{1/2} = 7.1$ wk at 25°C for soil of field capacity moisture (27% w/w for Crowley silt), $t_{1/2} = 16.2$ wk at 4°C , $t_{1/2} = 3.9$ wk at 25°C for flooded soils, Crowley silt loam; and $t_{1/2} = 27.0$ wk at 4°C , $t_{1/2} = 8.1$ wk at 25°C for soil of field capacity moisture (34% w/w for Sharkey silty clay), $t_{1/2} = 18.6$ wk at 4°C and $t_{1/2} = 5.4$ wk at 25°C for flooded soils, Sharkey silty clay (Brewer et al. 1982)
 microagroecosystem $t_{1/2} = 3\text{--}4$ d in moist fallow soil (Nash 1983);
 $t_{1/2} = 46$ wk for $2.0 \mu\text{g/mL}$ to biodegrade in flooded soils at 25°C (derived from Brewer et al. 1982, Muir 1991);
 very persistent in soils with $t_{1/2} > 100$ d (Willis & McDowell 1982);
 $t_{1/2} = 20$ h for $0.36 \mu\text{g/mL}$ to biodegrade in sediment-water microcosm at 20°C (Spain & Van Veld 1983; quoted, Muir 1991);
 measured dissipation rate $k = 0.69 \text{ d}^{-1}$ (Nash 1983; quoted, Nash 1988);
 estimated dissipation rate $k = 1.6$ and 0.24 d^{-1} (Nash 1988);
 first-order adsorption rate constants: $k = 0.52, 0.2, 8.3 \times 10^{-3} \text{ h}^{-1}$ (Karickhoff & Morris 1985; quoted, Brusseau & Rao 1989);
 $t_{1/2} \sim 22$ d in submerged soils in a model ecosystem (Muir 1991);
 reported $t_{1/2} = 4\text{--}67$ d, $57\text{--}126$ d, 70 d, 83 d, $105\text{--}132$ d (Bottoni & Funari 1992);
 selected field $t_{1/2} = 60$ d (Wauchope et al. 1992; Hornsby et al. 1996; quoted, Halfon et al. 1996)
 Estimated $t_{1/2} \sim 25$ to > 201 d under a variety of agronomic conditions in agriculture soils depending on depth of incorporation, soil moisture, soil temperature, soil air, and soil organic matter content (summary of literature data, Grover et al. 1997)
 Biota: $t_{1/2} = 22\text{--}31$ d in river saugers, $t_{1/2} = 17\text{--}57$ d in river shorthead redhorse, $t_{1/2} = 23$ d in river golden redhorse, $t_{1/2} = 3$ d in lab. fathead minnow (Spacie & Hamelink 1979);
 biochemical $t_{1/2} = 132$ d (Jury et al. 1987a,b; Jury & Ghodrati 1989).

TABLE 17.1.1.79.1

Reported vapor pressures of trifluralin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
Spencer & Cliath 1974		Rordorf 1989	
gas saturation method		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
20	0.0065	25	0.010
30	0.0323	50	0.32
40	0.155	75	6.30
		100	82.0
		125	780
			for solid
		eq. 1	P_s/Pa
		A	17.46
		B	5800.6
			for liquid
		eq. 1	P_L/Pa
		A	13.65
		B	4573.1

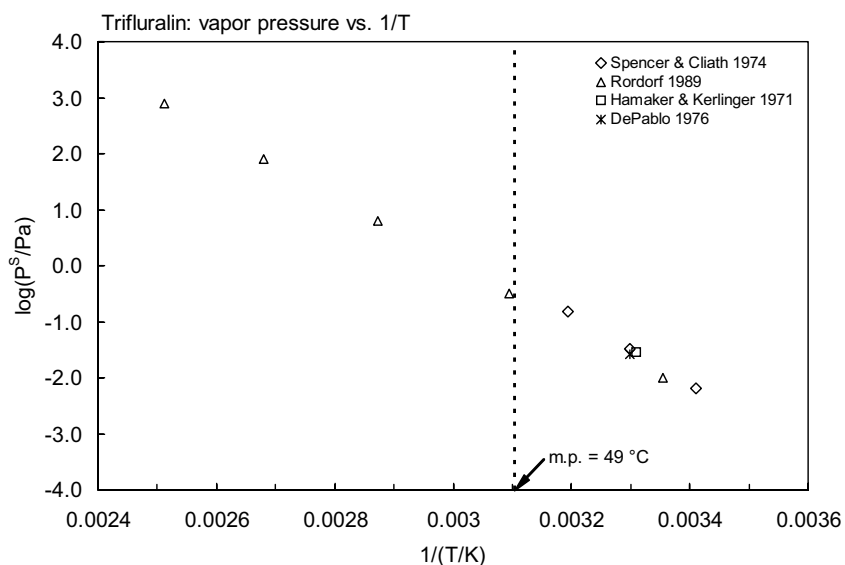
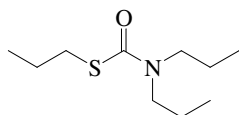


FIGURE 17.1.1.79.1 Logarithm of vapor pressure versus reciprocal temperature for trifluralin.

17.1.1.80 Vernolate



Common Name: Vernolate

Synonym: PPTC, R1607, Vanalate, Vernam, Vernnolaolate

Chemical Name: *S*-propyldipropylthiocarbamate; *S*-propyldipropylcarbamothioate

Uses: herbicide incorporated with soil for pre-planting or pre-emergence control of broadleaf and grass weeds in groundnuts, soybeans, maize, tobacco, and sweet potatoes.

CAS Registry No: 1929-77-7

Molecular Formula: $C_{10}H_{21}NOS$

Molecular Weight: 203.345

Melting Point (C): liquid

Boiling Point (°C):

150 (at 30 mmHg, Herbicide Handbook 1989; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

149–150 (at 30 mmHg, Budavari 1989)

Density (g/cm³ at 20°C):

0.954 (Ashton & Crafts 1981; Herbicide Handbook 1989; Worthing & Hance 1991)

0.952 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm³/mol):

269.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

107 (Martin & Worthing 1977)

90 (20°C, Khan 1980; Spencer 1982; Ashton & Crafts 1981; Herbicide Handbook 1989)

107 (21°C, Verschueren 1983)

90 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991)

107 (Budavari 1989; Milne 1995)

95 (Wauchope 1989)

108 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.84 (20°C, Hartley & Graham-Bryce 1980)

1.386 (Khan 1980; Spencer 1982; Herbicide Handbook 1989)

1.333 (Ashton & Crafts 1981)

0.244 (20°C, GC-RT correlation, Kim 1985)

1.39 (Hartley & Kidd 1987)

0.9 (20°C, selected, Suntio et al. 1988)

1.386 (Budavari 1989)

1.39 (Worthing & Hance 1991; Tomlin 1994)

1.293 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

2.05 (20°C, calculated-P/C, Suntio et al. 1988)

2.034 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

3.84 (20°C, Worthing & Hance 1991; Tomlin 1994)

- 3.84 (20°C, Milne 1995)
- 3.84 (recommended, Hansch et al. 1995)
- 3.86 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

- 1.64 (calculated-S, Kenaga 1980)
- 1.70 (calculated, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

- 2.52 (calculated-S, Kenaga 1980)
- 2.41 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.03, 1.93 (quoted exptl.; calculated-MCI and fragment contribution method, Meylan & Howard 1992)
- 2.41 (estimated-chemical structure, Lohninger 1994)
- 2.33 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 2.33; 2.40, 2.11 (soil, quoted exptl.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: microbial degradation $t_{1/2} = 8\text{--}16$ d at 27°C, $t_{1/2} > 64$ d at 4°C in soil (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} \sim 1.5$ wk in moist loam soil at 21–27°C (Herbicide Handbook 1989);
selected field $t_{1/2} = 12$ d (Wauchope et al. 1992; Hornsby et al. 1996);
soil $t_{1/2} = 11$ d (Pait et al. 1992);
microbial degradation $t_{1/2} = 8\text{--}16$ d at 27°C, $t_{1/2} > 64$ d at 4°C (Tomlin 1994).

Biota:

17.2 SUMMARY TABLES

TABLE 17.2.1

Common names, chemicals names and physical properties of herbicides

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK _a	pK _b
Alachlor [15972-60-8]	Lasso, Metachlor	α -chloro-2,6-diethyl- <i>N</i> -methoxy-methylacetanilide	C ₁₄ H ₂₀ ClNO ₂	269.768	40	0.713	0.62	
Ametryn [834-12-8]	Evik, Gesapax	2-methylthio-4-(ethylamino)-6-(isopropylamino)- <i>s</i> -triazine	C ₉ H ₁₇ N ₅ S	227.330	88	0.241	4.00 4.10	10.07
Amitrole [61-82-5]	Amerol, Aminotriazole	3-amino-1 <i>H</i> -1,2,4-triazole	C ₂ H ₄ N ₄	84.080	159	0.0484		9.83
Atrazine	Gesaprim	2-chloro-4-(ethylamino)-6-(isopropylamino)- <i>s</i> -triazine	C ₈ H ₁₄ ClN ₅	215.684	173	0.0353	1.68 1.70	12.32
Barban [101-27-9]	Carbyne	4-chlorobut-2-ynyl-3-chlorocarbamate	C ₁₁ H ₉ Cl ₂ NO ₂	258.101	75	0.323		
Benefin [1861-40-1]	Balan, Bonalan Benfluralin	<i>N</i> -butyl- <i>N</i> -ethyl- α,α,α -trifluoro-2,6-di-nitro- <i>p</i> -toluidine	C ₁₃ H ₁₆ N ₃ O ₄ F ₃	335.279	66	0.396		
Bifenox [42576-02-3]	Modown	methyl-5-(2,4-dichlorophenoxy)-2-nitrobenzoate	C ₁₄ H ₉ Cl ₂ NO ₅	342.131	85	0.258		
Bromacil [314-40-9]	Borea, Hyvar X	5-bromo-3- <i>sec</i> -butyl-6-methyl-uracil	C ₉ H ₁₃ BrN ₂ O ₂	261.115	158	0.0496	9.10 < 7.0	
Bromacil lithium salt			C ₉ H ₁₂ N ₂ O ₃ Li	267.0			9.27	
Bromoxynil [1689-84-5]	Brominal, Buctril	3,5-dibromo-4-hydroxybenzonitrile	C ₇ H ₃ Br ₂ NO	276.913	190	0.0241	4.06 4.20	
Bromoxynil butyrate ester [3861-41-4]			C ₁₃ H ₉ BrNO ₃	307.119			4.10	
Bromoxynil octanoate [1689-99-2]		2,6-dibromo-4-cyanophenyl octanoate	C ₁₅ H ₁₇ Br ₂ NO ₂	403.109	45–46	0.629	4.08	
<i>sec</i> -Bumeton [26259-45-0]	Etazine, Sumitol	<i>N</i> -ethyl-6-methoxy- <i>N'</i> -(1-methyl-propyl)-1,3,5-triazine-2,4-diamine	C ₁₀ H ₁₉ N ₅ O	225.291	87	0.246	4.40	
Butachlor [23184-66-9]	Machete	<i>N</i> -butoxymethyl-2-chloro-2',6'-diethylacetanilide	C ₁₇ H ₂₆ ClNO ₂	311.847	< –5	1		
Butralin [33629-47-9]	Amex, Tamex	<i>N</i> - <i>sec</i> -butyl-4- <i>tert</i> -butyl-2',6'- dinitroaniline	C ₁₄ H ₂₁ N ₃ O ₄	295.335	60	0.454		
Butylate [2008-41-5]	Sutan	<i>S</i> -ethyl bis(2-methylpropyl) carbamothioate	C ₁₁ H ₂₃ NOS	217.372	liquid	1		
Chloramben [133-90-4]	Amiben, Amoben	3-amino-2,5-dichlorobenzoic acid	C ₇ H ₅ Cl ₂ NO ₂	206.027	200	0.0192	3.40	

(Continued)

TABLE 17.2.1 (Continued)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK _a	pK _b
Chloramben salts [133-90-4]	Amiben	ammonium or sodium salt of chloramben	C ₇ H ₅ Cl ₂ NO ₂	206.027				
Chlorazine [580-48-3]		6-chloro- <i>N,N,N'</i> -tetraethyl-1,3,5-triazine-2,4-diamine	C ₁₁ H ₂₀ ClN ₅	257.764	27	0.956		
Chlorbromuron [13360-45-7]	Maloran	3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea	C ₉ H ₁₀ BrClN ₂ O ₂	293.544	96	0.201		
Chlorfenac [85-34-7]	Fenac	(2,3,6-trichlorophenyl)acetic acid	C ₈ H ₅ Cl ₃ O ₂	239.484	161	0.046		
Chlorpropham [101-21-3]	Furloe	isopropyl 3-chlorocarbanilate	C ₁₀ H ₁₂ ClNO ₂	213.661	41	0.697		
Chlorsulfuron [64902-72-3]	Glean, Telar	1-(2-chlorophenylsulfonyl)-3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)urea	C ₁₂ H ₁₂ ClN ₅ O ₄ S	357.773	176	0.0330	3.60	
Chlortoluron [15545-48-9]	Dicuran	3-(3-chloro- <i>p</i> -tolyl)-1,1-dimethylurea	C ₁₀ H ₁₃ ClN ₂ O	212.675	147	0.0635		
Cyanazine [21725-46-2]	Bladex, Fortrol	2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methylpropionitrile	C ₉ H ₁₃ ClN ₆	240.692	168	0.0395	1 0.63	12.9
2,4-D [94-75-7]	Agratect, Farmco, Weed Tox	2-(2,4-dichlorophenoxy)acetic acid	C ₈ H ₆ Cl ₂ O ₃	221.038	140.5	0.0736	2.64 3.31	
2,4-D dimethylamine salt [2008-39-1]			C ₁₀ H ₁₃ Cl ₂ NO ₃	266.121	85-87	0.252		
2,4-D esters			C ₈ H ₆ Cl ₂ O ₃ (a)	221.038			2.80	
Dalapon [75-99-0]	Dowpon, Radapon	2,2-dichloropropionic acid	C ₃ H ₄ Cl ₂ O ₂	142.969	liquid	1	1.74 1.84	
Dalapon sodium salt [120-20-8]		sodium 2,2-dichloropropionate	C ₃ H ₃ Cl ₂ Na	164.95	166.5 dec			
2,4-DB [94-82-6]	Embutox	4-(2,4-dichlorophenoxy)butyric	C ₁₀ H ₁₀ Cl ₂ O ₃	249.090	118	0.122	4.80	
2,4-DB butoxyethyl ester			C ₁₆ H ₂₂ O ₄ Cl ₂	349.249			4.80	
Diallate [2303-16-4]	Avadex	<i>S</i> -(2,3-dichloroallyl)diisopropylthiocarbamate	C ₁₀ H ₁₇ Cl ₂ NOS	270.219				
Dicamba [1918-00-9]	Banvel, Dianat, Mediben	3,6-Dichloro- <i>o</i> -anisic acid	C ₈ H ₆ Cl ₂ O ₃	221.038	115	0.131	1.91 1.95	
Dichlobenil [1194-65-6]	Casoron	2,6-dichlorobenzonitrile	C ₇ H ₃ Cl ₂ N	172.012	144.5	0.0672		
Dichlorophen (F.A.B) [97-23-4]	Super Mosstox	4,4'-dichloro-2,2'-methylenediphenol	C ₁₃ H ₁₀ Cl ₂ O ₂	269.123	177.5	0.0320		
Dichloroprop [120-36-5]	2,4-DP	(<i>RS</i>)-2-(2,4-dichlorophenoxy)-propionic acid	C ₉ H ₈ Cl ₂ O ₃	235.064	117.5	0.124	3.0	

Dichlorprop-P [15165-67-0]	Cornox RK	(<i>R</i>)-2-(2,4-dichlorophenoxy)propionic acid	C ₉ H ₈ Cl ₂ O ₃	235.064	122	0.112	3.0 2.86
Dichlorprop ester Diclofop [40843-25-2]	Weedone	butoxyethyl ester of (<i>R</i>)-2-(2,4-dichloro-2-(4-aryloxyphenoxy) propionic acid	C ₉ H ₈ Cl ₂ O ₃ C ₁₅ H ₁₂ Cl ₂ O ₄	335.3 327.159			2.85
Diclofop-methyl [51338-27-3]	Hoelon	2-(4-(2,4-dichlorophenoxy)phenoxy)- propanoic acid methyl ester	C ₁₆ H ₁₄ Cl ₂ O ₄	341.186	40	0.713	3.10
Dinitramine [29091-05-2]	Cobexo	<i>N,N</i> -diethyl-2,6-dinitro-4-trifluoro- methyl- <i>m</i> -phenylenediamine	C ₁₁ H ₁₃ N ₄ O ₄ F ₃	322.241	98	0.192	
Dinoseb [88-85-7]	Antox, Aretit, BNP 30, DNBP	2- <i>sec</i> -butyl-4,6-dinitrophenol	C ₁₀ H ₁₂ N ₂ O ₅	240.212	40	0.713	4.62
Dinoseb salts [88-85-7]	Premerge, Dinitro	2- <i>sec</i> -butyl-4,6-dinitrophenyl ammonium, amine, acetate salts					4.50
Diphenamid [957-51-7]	Dymid, Enide	<i>N,N</i> -dimethyldiphenylacetamide	C ₁₆ H ₁₇ NO	239.312	135	0.0833	
Diquat [2764-72-9]	Reglone, Pathclear Cleasweep, Weedol	1,1'-ethylene-2,2'-dipyridine	C ₁₂ H ₁₄ N ₂	186.236			
Diquat dibromide salt [85-00-7]			C ₁₂ H ₁₂ Br ₂ N ₂	344.1			10
Diuron [330-54-1]	DMU, Karmex DCMU	3-(3,4-dichlorophenyl)- 1,1-dimethylurea	C ₉ H ₁₀ Cl ₂ N ₂ O	233.093	158	0.0496	
EPTC [759-94-4]	Eptam, Eradicane	<i>S</i> -ethyl dipropylthiocarbamate	C ₉ H ₁₉ NOS	189.318	liquid	1	
Ethalfuralin [55283-68-6]	Benzenamine, Somilan, Sonalan, Sonalen	<i>N</i> -ethyl- <i>N</i> -(2-methyl-2-propenyl)- 2,6-dinitro-(trifluoromethyl)- benzenamine	C ₁₃ H ₁₄ F ₃ N ₃ O ₄	333.263	57	0.485	
Fenoprop (G.R.) [93-72-1]	Silvex, 2,4,5-TP	(±)-2-(2,4,5-trichlorophenoxy)- propionic acid	C ₉ H ₇ Cl ₃ O ₃	269.509	181.6	0.0291	
Fenuron [101-42-8]	Dybar, Urab	1,1-dimethyl-3-phenylurea	C ₉ H ₁₂ N ₂ O	164.203	132	0.0892	
Fenuron-TCA [4482-55-7]		1,1-dimethyl-3-phenyluronium trichloroacetate	C ₁₁ H ₁₃ Cl ₃ N ₂ O ₃	327.592	65-68	0.392	
Fluchloralin [33245-39-5]	Basalin Basalin, BAS-392H	<i>N</i> -(2-chloroethyl) α,α,α-trifluoro- 2,6-dinitro- <i>N</i> -propyl- <i>p</i> -toluidine	C ₁₂ H ₁₃ ClF ₃ N ₃ O ₄	355.697	42	0.681	
Fluometuron [2164-17-2]	Cotoran, Cottonex, Meturon	<i>N,N</i> -dimethyl- <i>N'</i> -[3-(trifluoromethyl)- phenyl]urea	C ₁₀ H ₁₁ F ₃ N ₂ O	232.201	164	0.0433	
Fluorodifen [15457-05-3]	Soyex	4-nitrophenyl α,α,α-trifluoro-2-nitro- <i>p</i> -tolyl ether	C ₁₃ H ₇ F ₃ N ₂ O ₅	328.200	94	0.210	
Fluridone [59756-60-4]	Fluridon, Pride, Sonar	1-methyl-3-phenyl-5-[3-(trifluoromethyl) phenyl]-4-(1 <i>H</i>)-pyridinone	C ₁₉ H ₁₄ F ₃ NO	329.315	155	0.0530	12.3

(Continued)

TABLE 17.2.1 (Continued)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK _a	pK _b
Glyphosate [1071-83-6]	Roundup, Polado	<i>N</i> -(phosphoromethyl)glycine	C ₃ H ₈ NO ₅ P	169.074	230 dec	0.0097	5.70	
Glyphosate-mono(<i>iso</i> -propylammonium) [38641-94-0]			C ₆ H ₁₇ N ₂ O ₅ P	228.2	200	0.0190		
Ioxynil [1689-83-4]	Actril, Totril	4-hydroxy-3,5-di-iodobenzonitrile	C ₇ H ₃ I ₂ NO	370.914	201 dec	0.0190	3.96	
Ioxynil-octanoate [3681-47-0]		4-cyano-2,6-iodophenyl octanoate	C ₁₅ H ₁₇ I ₂ NO ₂	497.1	59–60	0.459		
Ioxynil-sodium salt [2961-62-8]			C ₇ H ₂ I ₂ NNaO	392.9	360	0.00052		
Isopropalin [33820-53-0]	Paralan	4-isopropyl-2,6-dinitro- <i>N</i> -dipropylaniline	C ₁₅ H ₂₃ N ₃ O ₄	309.362	liquid	1		
Isoproturon [34123-59-6]	Alon, Arelon, Graminon	3- <i>p</i> -cumenyl-1,1-dimethylurea	C ₁₂ H ₁₈ N ₂ O	206.284	155–156	0.0520		
Linuron [330-55-2]	Afalon, Lorox	3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea	C ₉ H ₁₀ Cl ₂ N ₂ O ₂	249.093	93	0.215		
MCPA (G.R., H) [94-74-6]	Metaxon, Agroxone, Agritox	4-chloro- <i>o</i> -tolylxyacetic acid	C ₉ H ₉ ClO ₃	200.618	120	0.117	3.05 3.13	
MCPA dimethylamine salt [94-74-6]			C ₁₁ H ₁₆ ClNO ₃	243.7			3.12	
MCPA ester	Weedone, Weedar		C ₉ H ₉ ClO ₃	200.6				
MCPA sodium salt			C ₉ H ₈ ClNaO ₃	222.6				
MCPA-thioethyl [25319-90-8]		<i>S</i> -ethyl 4-chloro- <i>o</i> -tolylxythioacetate	C ₁₁ H ₁₃ ClO ₂ S	244.7	41–42	0.689		
MCPB [94-81-5]	Tropotox	4-(4-chloro-2-methylphenoxy)butyric acid	C ₁₁ H ₁₃ ClO ₃	228.672	100	0.184	4.84 4.80	
MCPB sodium salt [6062-26-6]			C ₁₁ H ₁₂ ClNaO ₂	250.7				
Mecoprop [7085-19-0]	Iso-Cornox, MCPP	(±)-2-(4-chloro- <i>o</i> -tolylxy)-propionic acid	C ₁₀ H ₁₁ ClO ₃	214.645	94-95	0.208	3.78 3.75	
Mecoprop-P [16484-77-8]		(<i>R</i>)-2-(4-chloro- <i>o</i> -tolylxy)propionic acid	C ₁₀ H ₁₁ ClO ₃	214.645	95	0.206	3.78	
Metobromuron [3060-89-7]	Patoran	3-(4-bromophenyl)-1-methoxy-1-methyl urea	C ₉ H ₁₁ BrN ₂ O ₂	259.099	95	0.206		

Metolachlor [51218-45-2]	Codal, Dual, Primagram	2-chloro-6'-ethyl- <i>N</i> -(2-methoxy- 1-methylethyl)acet- <i>o</i> -toluidide	C ₁₅ H ₂₂ ClNO ₂	283.795	liquid	1	
Metoxuron [19937-59-8]	Dosanex	3-(3-chloro-4-methoxyphenyl)- 1,1-dimethylurea	C ₁₀ H ₁₃ ClN ₂ O ₂	228.675	126-127	0.101	
Metribuzin [21087-64-9]	Metribuzine, Lexone, Preview, Sencor	4-amino-6-(<i>t</i> -butyl)-3-(methylthio)- 1,2,4-triazin-5-(4 <i>H</i>)-one	C ₈ H ₁₄ N ₄ OS	214.288	126	0.102	
Molinate [2212-67-1]	Ordram	<i>S</i> -ethyl azepane-1-carbothioate	C ₉ H ₁₇ NOS	187.302	liquid	1	
Monolinuron [1746-81-2]	Aresin	3-(4-chlorophenyl)-1-methoxy- 1-methylurea	C ₉ H ₁₁ ClN ₂ O ₂	214.648	77	0.309	
Monuron [150-68-5]	Telvar, Urox	1,1-dimethyl-3-(<i>p</i> -chloro-phenyl)-urea	C ₉ H ₁₁ ClN ₂ O	198.648	170.5	0.0374	
Napropamide [15299-99-7]	Devrinol	2-(α -naphthloxy)- <i>N,N</i> - diethylpropionamide	C ₁₇ H ₂₁ NO ₂	271.355	75	0.323	2.93
Neburon [555-37-3]	Kloben	1-butyl-3-(3,4-dichlorophenyl)-1-methyl urea	C ₁₂ H ₁₆ Cl ₂ N ₂ O	275.174	102-103	0.174	
Nitralin [4726-14-1]	Planavin	4-(methylsulfonyl)-2,6-dinitro- <i>N,N</i> -dipropylaniline	C ₁₃ H ₁₉ N ₃ O ₆ S	345.371	150	0.0594	
Nitrofen [1836-75-5]	nitrophen, Tok, Tokkron	2,4-dichloro-1-(4-nitrophenoxy)benzene	C ₁₂ H ₇ Cl ₂ NO ₃	284.095	70	0.362	
Norfluorazon [27314-13-2]			C ₁₂ H ₉ ClF ₃ N ₃ O	303.666	184	0.0275	
Oryzalin [19044-88-3]	Rycelan, Ryceon, Surflan	4-(dipropylamino)-3,5-dinitro- benzenesulfonamide	C ₁₂ H ₁₈ N ₄ O ₆ S	346.359	141	0.0728	9.40 8.60
Paraquat [4685-14-7]	Cyclone, Gramoxone	1,1'-dimethyl-4,4'-pyridinium	C ₁₂ H ₁₄ N ₂	186.252	dec.		
Paraquat dichloride salt [1910-42-5]			C ₁₂ H ₁₄ Cl ₂ N ₂	257.2			< 4
Pebulate [1114-71-2]	Tillam	<i>s</i> -propyl butylethylcarbamothioate	C ₁₀ H ₂₁ NOS	203.345	liquid	1	
Pendimethalin [40487-42-1]	penoxalin	<i>N</i> -(1-ethylpropyl-3,4-dimethyl- 2,6-dinitrobenzenamine	C ₁₃ H ₁₉ N ₃ O ₄	281.308	56	0.496	
Pentachlorophenol [87-86-5]	PCP	pentachlorophenol	C ₆ Cl ₅ OH	266.336	174	0.0350	4.74
Pentachlorophenol sodium salt (Pentacon)							
Pentanochlor [2307-68-8]	Solan	3'-chloro-2-methylvaler- <i>p</i> -toluidide	C ₁₃ H ₁₈ ClNO	239.741	85-86	0.255	
Picloram [1918-02-1]	Tordon	4-amino-3,5,6-trichloro-picolinic acid	C ₆ H ₃ Cl ₃ N ₂ O ₂	241.459	218.5	0.0126	1.90 3.60

(Continued)

TABLE 17.2.1 (Continued)

Compound	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK _a	pK _b
Picloram-potassium salt [2425-60-0]			C ₆ H ₂ Cl ₃ KN ₂ O ₂	279.6				
Profluralin [26399-36-0]	Pregard	<i>N</i> -(cyclopropylmethyl)-2,6-dinitro- <i>N</i> -propyl-4-(trifluoromethyl)-benzenamine	C ₁₄ H ₁₆ F ₃ N ₃ O ₄	347.290	34	0.816		
Prometon [1610-18-0]	Primatol, Gesagram	2,4-bis(isopropylamino)-6-methoxy- <i>s</i> -triazine	C ₁₀ H ₁₉ N ₅ O	225.291	91.5	0.223	4.28 4.30	9.73
Prometryn [7287-19-6]	Caparol, Gesagard	<i>N,N</i> -1,3,5-triazine-2,4-diamine-bis(isopropylamino)-6-(methylthio)	C ₁₀ H ₁₉ N ₅ S	241.357	119	0.120	4.05 4.10	9.95
Pronamide [23950-58-5]	Kerb, Promamide	3,5-dichloro- <i>N</i> -(1,1-dimethyl-propynyl)-benzamide	C ₁₂ H ₁₁ Cl ₂ NO	256.127	155	0.0530		
Propachlor [1918-16-7]	Ramrod	2-chloro- <i>N</i> -(1-methylethyl)- <i>N</i> -phenylacetamide	C ₁₁ H ₁₄ ClNO	211.688	77	0.309		
Propanil [709-98-8]	Propanex, Riselect, Stampede 3E	<i>N</i> -(3,4-dichlorophenyl)-propionamide	C ₉ H ₉ Cl ₂ NO	218.079	92	0.220		
Propazine [139-40-2]	Gesamil, Milogard	2-chloro-4,6-bis(isopropylamino)- <i>s</i> -triazine	C ₉ H ₁₆ ClN ₅	229.710	213	0.0143	1.85 1.80	12.15
Propham [122-42-9]	IPC	isopropyl carbanilate	C ₁₀ H ₁₃ NO ₂	179.216	90	0.230		
Pyrazon [1698-60-8]	Chloridazon	5-amino-4-chloro-2-phenyl-3(2 <i>H</i>)-pyridazinone	C ₁₀ H ₈ ClON ₃	221.643	205	0.0171		
Simazine [122-34-9]	Gesatop, Weedex, Aquazine	2-chloro-4,6-di(ethylamino)- <i>s</i> -triazine	C ₇ H ₁₂ ClN ₅	201.657	226	0.0107	1.65 1.60	12.35
Simetryne [1014-70-6]	Gy-bon	<i>N,N'</i> -diethyl-6-methylthio-1,3,5-triazine-2,4-diyl-diamine	C ₈ H ₁₅ N ₂ S	171.283	82-83	0.273		11
2,4,5-T [93-76-5]	Gesatop	2,4,5-trichlorophenoxyacetic acid	C ₈ H ₅ Cl ₃ O ₃	255.483	153	0.0555	2.80 2.88	
2,3,6-TBA [50-31-7]	Trysben, Cambilene	2,3,6-trichlorobenzoic acid	C ₇ H ₃ Cl ₃ O ₂	225.457	124.5	0.106		
Terbacil [5902-51-2]	Sinbar	3- <i>tert</i> -butyl-5-chloro-6-methyluracil	C ₉ H ₁₃ ClN ₂ O ₂	216.664	176	0.0330	9.0	
Terbumeton [33693-04-8]	Caragard	<i>N-tert</i> -butyl- <i>N'</i> -ethyl-6-methoxy-1,3,5-triazine	C ₁₀ H ₁₉ N ₅ O	225.290	123-124	0.108		9.41
Terbuthylazine [5915-41-3]	Gardoprim	<i>N-tert</i> -butyl-6-chloro- <i>N'</i> -ethyl-1,3,5-triazine-2,4-diamine	C ₉ H ₁₆ ClN ₅	229.710	178	0.0320		12
Terbutryn [886-50-0]	Igran, Clarosan, Prebane	<i>N-tert</i> -butyl- <i>N'</i> -ethyl-6-methyl-thio-1,3,5-triazine-2,4-diamine	C ₁₀ H ₁₉ N ₅ S	241.357	104	0.168	4.30 4.07	9.7

Thiobencarb [28249-77-6]	Benthiocarb, Bolero, Saturno	<i>S</i> -4-chlorobenzyl-diethyl-thiocarbamate	C ₁₂ H ₁₆ ClNOS	257.779	1.7	1	
Triallate [2303-17-5]	Avadex BW, Far-Go	<i>S</i> -(2,3,3-trichloro-2-propenyl)- bis(1-methylethyl)carbamothioate	C ₁₀ H ₁₆ Cl ₃ NOS	304.664	29	0.914	
Triclopyr [55335-06-3]	Garlon, Truflon, Crossbow	3,5,6-trichloro-2-pyridinyloxyacetic acid	C ₇ H ₄ Cl ₃ NO ₃	256.471	148–150	0.0607	2.68
Trifluralin [1582-09-8]	Treflan, Triflurex, Elancolan	2,6-dinitro- <i>N,N</i> -dipropyl- 4-trifluoromethylaniline	C ₁₃ H ₁₆ F ₃ N ₃ O ₄	335.279	49	0.581	
Vernolate [1929-77-7]	Surpass, Vernam	<i>S</i> -propyldipropylthiocarbamate	C ₁₀ H ₂₁ NOS	203.345	liquid	1	

Note: F.A.B. – fungicide algicide bactericide; G.R. – growth regulator

pK_a – acid dissociation constant; pK_b – basicity constant

(a) ester is quickly converted to parent acid.

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 17.2.2
Summary of selected physical-chemical properties of herbicides at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m ³ /mol) calcd P/C	log K _{OC} reported
	Vapor pressure		Solubility			log K _{OW}		
	P ^s /Pa	P _L /Pa	S/(g/m ³)	C ^s /(mol/m ³)	C _L /(mol/m ³)			
Alachlor	0.0020	2.88 × 10 ⁻³	240	0.890	1.281	2.8	0.0022	2.23
Ametryn	0.0001	3.92 × 10 ⁻⁴	185	0.814	3.191	2.58	1.23 × 10 ⁻⁴	2.59
Amitrole	5.50 × 10 ^{-7*}	1.14 × 10 ⁻⁵	280000	3330	68850	0.52	1.65 × 10 ⁻¹⁰	2.04
Atrazine	4.00 × 10 ⁻⁵	1.19 × 10 ⁻³	30	0.139	4.140	2.75	2.88 × 10 ⁻⁴	2.00
Barban	5.00 × 10 ^{-5*}	1.60 × 10 ⁻⁴	11	0.043	0.1362	2.68	1.17 × 10 ⁻³	2.66
Benefin	0.0088	0.0226	0.1	0.003	0.0077	5.29	29.4	3.95
Bifenox	3.20 × 10 ⁻⁴	1.25 × 10 ⁻³	0.35	0.0010	0.0040	4.48	0.313	
Bromacil	4.00 × 10 ⁻⁵	8.46 × 10 ⁻⁴	815	3.121	66.018	2.11	1.28 × 10 ⁻⁵	1.86
Bromacil lithium salt	4.13 × 10 ⁻⁵							1.51
Bromoxynil	6.40 × 10 ⁻⁴	0.0307	130	0.469	22.54	< 2.0	1.36 × 10 ⁻³	
Bromoxynil octanoate	6.40 × 10 ⁻⁴	1.03 × 10 ⁻³				5.4		4.25
sec-Bumeton	0.00097	3.98 × 10 ⁻³	620	2.756	11.31		3.52 × 10 ⁻⁴	2.30
Butachlor	6.0 × 10 ⁻⁴	6.00 × 10 ⁻⁴	23	0.074	0.074	4.50	8.14 × 10 ⁻³	2.8
Butralin	0.0017	3.86 × 10 ⁻³	1	0.0034	7.69 × 10 ⁻³	4.54	0.502	3.75
Butylate	1.73	1.73	45	0.182	0.182	4.15	8.36	2.60
Chloramben	0.93	51.19	700	3.398	187.05	1.11	0.274	1.32
Chloramben salts	0		900000					1.18
Chlorbromuron	5.33 × 10 ⁻⁵	2.69 × 10 ⁻⁴	50	0.170	0.858		3.13 × 10 ⁻⁴	2.7
Chlorfenac	1	19.75	200	0.835	16.50		1.20	
Chlorpropham	0.001	0.001	89*	0.417	0.600	3.51	2.40 × 10 ⁻³	2.85, 2.8
Chlorsufuron	6.13 × 10 ^{-4*}	0.019	7000	19.56	609.4	-1.0	3.13 × 10 ⁻⁵	1.6
Chlortoluron	1.70 × 10 ⁻⁵	2.80 × 10 ⁻⁴	70	0.329	5.418	2.38	5.17 × 10 ⁻⁵	2.81
Cyanazine	2.13 × 10 ⁻⁷	5.41 × 10 ⁻⁶	171	0.710	18.03	2.22	3.00 × 10 ⁻⁷	2.3
2,4-D	8.0 × 10 ^{-5*}	1.11 × 10 ⁻³	400	1.810	25.12	2.81	4.42 × 10 ⁻⁵	1.68-2.73
2,4-D (a)	0.001	0.0139	890	4.026	55.92	2.81	2.48 × 10 ⁻⁴	
2,4-D DMA salt	0		796000	2991	12000			1.3
2,4-D esters			100					2.00
Dalapon	1.0 × 10 ^{-5*}	1.0 × 10 ⁻⁵	502000	3510	3510	0.78	2.85 × 10 ⁻⁹	0.48, 2.13
Dalapon sodium salt			900000	5455			0	
2,4-DB	0		46	0.185	1.539	3.53		2.64
2,4-DB butoxyethyl ester	0.00001		8					2.7
2,4-DB DMA salt	0		709000					1.30

Diallate	0.02	0.0224	50*	0.185	0.207	5.23	0.108	2.70
Dicamba	0.0045*	0.0349	4500	20.36	158.1	2.21	2.21×10^{-4}	0.342, -0.4
Dicamba salt			400000	1646				0.301
Dichlobenil	0.07*	1.076	18	0.105	1.609	2.74	0.669	2.91
Dichlorophen (F.A.B)	1.30×10^{-8}	4.24×10^{-7}	30	0.111	3.635		1.17×10^{-7}	
Dichloroprop	0.0004	3.25×10^{-3}	350	1.489	12.099	3.43	2.69×10^{-4}	3.0
Dichloroprop-P	6.20×10^{-5}	5.65×10^{-4}	590	2.510	22.855	1.95	2.47×10^{-5}	2.23
Dichloroprop(2,4-DP)ester	1.0×10^{-5}		50	0.149				3.00
Diclofop-methyl	$4.67 \times 10^{-4*}$	6.57×10^{-4}	0.8	2.34×10^{-3}	3.30×10^{-3}	4.58	0.199	4.2
Dinitramine	0.00048	2.59×10^{-3}	1	0.0031	0.017	4.30	0.155	3.6
Dinoseb	0.01*	0.0141	50	0.208	0.293	3.56	0.048	2.85
Diphenamid	$4.0 \times 10^{-6*}$	4.95×10^{-5}	260	1.087	13.46	1.92	3.68×10^{-6}	2.31
Diquat	1.30×10^{-5}	0.0170	700000	3800	4.96×10^6	-3.05*	3.42×10^{-9}	
Diquat dibromide	0		718000	2087				
Diuron	$9.2 \times 10^{-5*}$	1.9×10^{-3}	40	0.172	3.630	2.78	6.83×10^{-4}	2.6
EPTC	2*	2.0	370	1.954	1.954	3.2	1.023	2.3
Fenopro (H., G.R.)	$1.33 \times 10^{-5*}$	4.54×10^{-4}	140	0.519	17.73		2.56×10^{-5}	2.48
Fenuron	0.0267	0.305	3800	23.14	264.7	0.98	1.15×10^{-3}	1.43
Fenuron-TCA			4800	14.65	38.13			
Fluchloralin	0.004	6.03×10^{-3}	1	0.00281	0.0042	4.60*	1.343	3.50
Fluometuron	6.70×10^{-5}	1.61×10^{-3}	90	0.388	9.292	2.42	1.73×10^{-4}	2.24
Fluridone	1.3×10^{-5}	2.5×10^{-4}	12	0.036	0.7039	2.98	0.357	2.544-3.04
Fluorodifen	9.5×10^{-6}	4.47×10^{-6}	2	0.0061	0.0293	3.65		3.13
Glyphosate	$4.0 \times 10^{-5*}$	2.15×10^{-3}	12000	70.96	3818.4	-1.6	5.64×10^{-7}	3.43-3.69
Ioxynil	0.001	0.066	50	0.135	8.904		7.42×10^{-3}	
Ioxynil-octanoate	0.0037	8.21×10^{-3}						
Isopropalin	0.0019	0.0019	0.11	3.56×10^{-4}	3.56×10^{-4}	4.71	5.34	4.0
Isoproturon	3.30×10^{-6}	6.52×10^{-5}	55	0.267	5.266	2.25	1.24×10^{-5}	1.86
Linuron	0.023*	6.74×10^{-2}	75	0.301	1.449	3.0	7.54×10^{-2}	2.91
MCPA (H., G.R.)	0.0002	1.70×10^{-3}	1605	8.001	68.05	2.69*	2.50×10^{-5}	2.03-2.07
MCPA dimethylamine salt							1.30	
MCPA ester	0.0002		5.0					3.00
MCPA-thioethyl	0.021	0.0309	2.3	0.0094	0.0138		2.234	
MCPB	$5.77 \times 10^{-5*}$	3.18×10^{-4}	41	0.179	0.989	3.43	3.22×10^{-4}	
MCPB sodium salt	0		200000	798				1.30
Mecoprop	3.1×10^{-4}	1.53×10^{-3}	620	2.89	14.23	3.94	7.43×10^{-5}	
Mecoprop-P	4.0×10^{-4}	1.97×10^{-3}	860	4.007	19.73		9.98×10^{-5}	
Metobromuron	4.0×10^{-4}	2.02×10^{-3}	330	1.274	6.416	2.41	3.14×10^{-4}	

(Continued)

TABLE 17.2.2 (Continued)

Compound	Selected properties					log K _{OW}	Henry's law constant H/(Pa·m ³ /mol) calcd P/C	log K _{OC} reported
	Vapor pressure		Solubility					
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)			
Metolachlor	0.0042*	4.20 × 10 ⁻³	430	1.80	1.80	3.13	2.33 × 10 ⁻³	2.26
Metoxuron	0.0043	0.0439	678	2.965	30.26	1.6	1.45 × 10 ⁻³	
Molinate	0.75	0.750	970	5.179	5.179	3.21	0.145	1.92
Monolinuron	0.02	0.0732	735	3.425	12.54	2.30	5.84 × 10 ⁻³	2.3
Monuron	6.66 × 10 ⁻⁵	2.12 × 10 ⁻³	230	1.007	32.08	1.94	6.62 × 10 ⁻⁵	2.00
Neburon			4.8	0.017	0.1031	3.8		3.36
Nitralin	0.2	3.526	0.5	0.0014	0.0255		138.2	
Oryzalin	1.30 × 10 ⁻⁶	1.87 × 10 ⁻⁵	2.4	0.0069	0.0995	3.73	1.88 × 10 ⁻⁴	2.78
Paraquat	< 0.0001		~700000					
Paraquat dichloride salt	0		620000					6.0
Pebulate	1.2*	1.20	92*	0.452	0.452	3.84	2.653	2.63
Pentanochlor			8	0.033	0.134			
Picloram	6.0 × 10 ⁻⁵ *	4.98 × 10 ⁻³	430	1.781	147.7	0.3	3.37 × 10 ⁻⁵	1.23
Picloram-potassium salt			1430.6				1.20	
Profluralin	0.009	0.0116	0.10	2.88 × 10 ⁻⁴	3.7 × 10 ⁻⁴	6.34	31.35	4.0
Prometon	0.0003	1.38 × 10 ⁻³	750	3.329	15.31	2.99	9.01 × 10 ⁻⁵	2.54
Prometryn	0.0001	8.70 × 10 ⁻⁴	48	0.199	1.730	3.51	5.03 × 10 ⁻⁴	2.60
Pronamide	0.011	0.208	15	0.059	1.105	3.26	0.188	2.90
Propachlor	0.03	0.0958	600	2.834	9.055	2.18	0.011	1.90
Propanil	0.005*	0.0230	200	0.917	4.218	3.07	5.45 × 10 ⁻³	2.17
Propazine	3.90 × 10 ⁻⁶	2.89 × 10 ⁻⁴	8.6	0.037	2.766	2.90	1.04 × 10 ⁻³	2.19
Propham	sublime		250	1.395	5.804	2.60		1.71
Propyzamide	5.80 × 10 ⁻⁵	1.15 × 10 ⁻³	15	0.059	1.157	3.28	9.90 × 10 ⁻⁴	2.90
Pyrazon (chloridazon)	7*	441.8	360	1.625	102.5	1.14	4.309	2.08
Simazine	8.50 × 10 ⁻⁶	8.27 × 10 ⁻⁴	5	0.025	2.412	2.18	3.43 × 10 ⁻⁴	2.11
Simetryne	9.47 × 10 ⁻⁵	3.55 × 10 ⁻⁴	450	2.110	7.904		4.49 × 10 ⁻⁵	2.30
2,4,5-T	0.005*	0.0922	220	0.861	15.89	3.13	5.81 × 10 ⁻³	1.72
2,3,6-TBA			7700	34.15	340.6	4.34		
Terbacil	5.0 × 10 ⁻⁵	1.56 × 10 ⁻³	710	3.277	102.1	1.89	1.53 × 10 ⁻⁵	1.74
Terbumeton	2.70 × 10 ⁻⁴	2.57 × 10 ⁻³	130	0.577	5.500	3.04	4.68 × 10 ⁻⁴	
Terbuthylazine	1.50 × 10 ⁻⁴	4.89 × 10 ⁻³	8.5	0.037	1.206	3.04	4.05 × 10 ⁻³	2.21-2.44
Terbutryn	0.00013*	8.04 × 10 ⁻⁴	22	0.091	0.564	3.74	1.43 × 10 ⁻³	2.85
Thiobencarb	2.2	2.20	19.1	0.074	0.0741	3.42	29.69	

Triallate	0.015	0.0164	4	0.013	0.0144	4.29	1.14	3.38
Trifluralin	0.026*	0.0259	0.5*	1.49×10^{B3}	2.57×10^{B3}	5.34	10.08	4.14
Vernolate	0.90	0.90	90	0.443	0.443	3.84	2.034	2.414

Note: F.A.B. – fungicide algicide bactericide; G.R. – growth regulator, H - herbicide

2,4-D(a) physical-chemical properties modified from values used in Vol. IV.

* The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to large error.

TABLE 17.2.3**Suggested half-life classes of herbicides in various environmental compartments 25°C**

Compound	Air class	Water class	Soil class	Sediment class
Atrazine	1	8	6	6
2,4-D	2	3	5	6
Dalapon	5	6	6	6
2,4-DB	3	4	4	5
Diallate	2	6	6	7
Dicamba	3	5	5	6
Diuron	2	5	6	7
EPTC	2	4	4	6
Glyphosate	4	6	6	7
Isopropalin	2	5	6	7
Linuron	2	5	6	7
Mecoprop	2	4	4	6
Metolachlor	4	6	6	7
Simazine	3	5	6	7
2,4,5-T	3	5	5	6
Triallate	4	6	4	5
Trifluralin	4	6	6	7

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

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18 Insecticides

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18.1. List of Chemicals and Data Compilations (by Functional Group):

Organophosphorus compounds:

a) Phosphates:

Chlorfenvinphos	3758
Crotoxyphos	3767
Dichlorvos	3811
Dicrotophos	3816
Mevinphos	3925
Monocrotophos	3930
Naled	3932

b) Phosphorothioates:

Acephate	3715
Bromophos	3734
Bromophos-ethyl	3736
Chlorpyrifos	3760
Chlorpyrifos-methyl	3765
Demeton	3800
Diazinon	3804
Fenitrothion	3851
Fensulfothion	3857
Fenthion	3859
Leptophos	3896
Parathion	3936
Parathion-methyl	3942
Ronnel	3969
Trichlorfon	3980

c) Phosphorodithioates (Phosphorothiolothionates):

Azinphos-methyl	3729
Carbophenothion	3746
Dialifor	3802
Dimethoate	3829
Disulfoton	3832
Ethion	3847
Ethoprop	3849
Fonofos	3867
Malathion	3912
Phenthoate	3957
Phorate	3959
Phosmet	3962
Terbufos	3971

Carbamates:

Aldicarb	3717
Aminocarb	3728
Bendiocarb	3732
Carbaryl	3738
Carbofuran	3742
Carbosulfan	3748
Ethiofencarb	3845
Fenoxycarb	3854
Methiocarb	3916
Methomyl	3918
Oxamyl	3934
Pirimicarb	3964
Propoxur	3966
Thiodicarb	3973

Organochlorines:

Aldrin	3721
Chlordane	3750
DDD	3774
DDE	3779
DDT	3785
Dieldrin	3819
Endrin	3840
α -HCH	3869
β -HCH	3876
δ -HCH	3881
Heptachlor	3885
Heptachlor epoxide	3890
Kepone	3893
Lindane (γ -HCH)	3898
Methoxychlor	3920
Mirex	3927
Toxaphene	3975

Phenols:

Pentachlorophenol (PCP)	3947
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Synthetic pyrethroids:

Cypermethrin	3772
Cyhalothrin	3769
Lambda-cyhalothrin	3770
Deltamethrin	3798
Fenpropathrin	3855
Fenvalerate	3862
Permethrin	3953

Miscellaneous:

Diflubenzuron	3827
Endosulfan	3835
Flucythrinate	3865

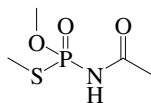
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18.1 LIST OF CHEMICALS AND DATA COMPILATIONS

18.1.1 INSECTICIDES

18.1.1.1 Acephate



Common Name: Acephate

Synonym: Chevron RE 12420, ENT 27822, Orthene, Ortho 12420, Ortran, Ortril, RE 12420, 75 SP, Tornado

Chemical Name: acetylphosphoramidothioic acid *O,S*-dimethyl ester; *O,S*-dimethyl acetylphosphoramidothioate; *N*-[methoxy(methylthio)phosphinoyl]acetamide

Uses: systemic insecticide with contact and stomach action to control a wide range of chewing and sucking insects in fruit, cotton, hops, vines, soybeans, olives, groundnuts, beet, brassicas, celery, potatoes, rice ornamentals, forestry and other crops; also used as cholinesterase inhibitor.

CAS Registry No: 30560-19-1

Molecular Formula: $C_4H_{10}NO_3PS$

Molecular Weight: 183.166

Melting Point ($^{\circ}C$):

88 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.35 (Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

135.7 (calculated from density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F : 0.241 (mp at $88^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

650000 (Spencer 1973, 1982; Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)
 > 5000 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a)
 790000 ($20^{\circ}C$, Hartley & Kidd 1987)
 818000 (Wauchope 1989)
 818000 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 790000 ($20^{\circ}C$, Montgomery 1993; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

2.26×10^{-4} ($20^{\circ}C$, Hartley & Kidd 1987)
 2.26×10^{-4} ($24^{\circ}C$, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)
 2.27×10^{-4} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.27×10^{-4} ($20^{\circ}C$, Montgomery 1993)
 0.513; 0.759, 0.457 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

5.27×10^{-8} (20 – $25^{\circ}C$, calculated-P/C, Montgomery 1993)
 6.37×10^{-8} (20 – $25^{\circ}C$, calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)
 5.06×10^{-8} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

-0.85 (shake flask, Log P Database, Hansch & Leo 1987)
 -1.87 (calculated, Montgomery 1993)

-0.85	(recommended, Sangster 1993)
-0.886	(Tomlin 1994)
1.12	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

-0.523	(calculated-S, Kenaga 1980)
0.053	(wet wt. basis, rainbow trout, Geen et al. 1984)

Sorption Partition Coefficient, log K_{OC} :

0.477	(calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
0.30	(soil, 20–25°C, selected, Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996)
0.48	(Montgomery 1993)
0.30	(estimated-chemical structure, Lohninger 1994)
3.50, 3.00	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: calculated rate constant $k \sim 51 \times 10^{-12} \text{ cm}^3/\text{molecules}$ for the vapor phase reaction with hydroxyl radical in air (Winer & Atkinson 1990).

Hydrolysis: persistent to hydrolysis between pH 4.0 and 6.0 under laboratory condition at 20 and 30°C regardless of temperature while strongly affected by temperature at pH 8.2; and more persistent in pond than creek water (Szeto et al. 1979)

$t_{1/2} = 60 \text{ h}$ at pH 9 and $t_{1/2} = 710 \text{ h}$ at pH 3 both at 40°C (Montgomery 1993).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: resistant to hydrolysis in distilled, buffered water at pH 4.0 to 6.9, but not at pH 8.2; and more persistent in pond than creek water, 45% found after 50 d when incubated at 9°C in creek water (Szeto et al. 1979)

Ground water:

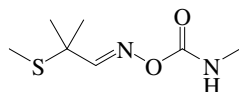
Sediment: degradation increased greatly when treated samples were incubated in the presence of sediments, ~ 20% recovered after 42 d and ~ 28% recovered after 58 d after incubating acephate-treated pond and creek water with their respective sediments (Szeto et al. 1979)

Soil: selected field $t_{1/2} = 3.0 \text{ d}$ (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{1/2} = 7\text{--}10 \text{ d}$ in soil (Tomlin 1994).

Biota:

18.1.1.2 Aldicarb



Common Name: Aldicarb

Synonym: Ambush, Carbanolate, ENT 27093, NCI-C08640, matadan, OMS 771, Pounce, Temik, Union Carbide 21149

Chemical Name: 2-methyl-2-(methylthio)propionaldehyde *O*-(methylcarbamoyl) oxime; 2-methyl-2-(methylthio)propional *O*-(methylamino)carbonyl) oxime

Uses: systemic insecticide, acaricide, and nematocide with contact and stomach action; also used as cholinesterase inhibitor.

CAS Registry No: 116-06-3

Molecular Formula: C₇H₁₄N₂O₂S

Molecular Weight: 190.263

Melting Point (°C):

99 (Lide 2003)

Boiling Point (°C):

100 (decomposes above this temp., Howard 1991)

Density (g/cm³ at 20°C):

1.195 (25°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm³/mol):

224.3 (calculated-Compiled method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.94 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K, F: 0.188 (mp at 99°C)

Water Solubility (g/m³ or mg/L at 25°C):

4000 (24°C, shake flask-GC, Felsot & Dahm 1979)

7800 (Kenaga 1980a; Kenaga & Goring 1980)

6000 (Khan 1980; Verschueren 1983)

6016, 6000 (exptl., corrected-mp, Briggs 1981)

6000 (20°C, shake flask-GC, Bowman & Sans 1983b)

6000 (Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Budavari 1989; Montgomery 1993; Milne 1995)

5730 (Seiber 1987)

6000 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

4930 (20°C at pH 7, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations.):

6.67 (20°C, Khan 1980)

0.00707 (20°C, selected exptl. value, Kim 1985)

0.102, 0.016 (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)

0.013 (20°C, Hartley & Kidd 1987; Tomlin 1994)

0.013 (selected, Suntio et al. 1988)

0.013 (Worthing & Hance 1991)

0.004 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0046 (Montgomery 1993)

Henry's Law Constant (Pa·m³/mol at 25°C):

2.48 × 10⁻⁴ (Jury et al. 1987a, Jury & Ghodrati 1989)

3.20 × 10⁻⁴ (calculated-P/C, Suntio et al. 1988)

1.47×10^{-4} (20–25°C, calculated-P/C, Montgomery 1993)

1.27×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.85	(shake flask, Felsot & Dahm 1979)
1.10	(Hansch & Leo 1979)
1.57	(shake flask-UV, Lord et al. 1980)
0.70	(Rao & Davidson 1980)
1.57	(20°C, shake flask-UV, Briggs 1981)
1.13	(20°C, shake flask-GC, Bowman & Sans 1983b)
1.13	(Hansch & Leo 1985)
0.70, 1.13	(Montgomery 1993)
1.13	(recommended, Sangster 1993)
1.13	(recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.62	(fish in static water, Metcalf & Sanborn 1975; Kenaga & Goring 1980)
0.85	(vegetation, correlated- K_{OW} , Iwata et al. 1977; Maitlen & Powell 1982)
0.602	(calculated-S, Kenaga 1980; quoted, Howard 1991)
1.64	(earthworm, Lord et al. 1980; quoted, Connell & Markwell 1990)
1.00, 1.18	($\log BCF_{lipid}$, $\log BCF_{protein}$, Briggs 1981)

Sorption Partition Coefficient, $\log K_{OC}$:

1.36–1.57	(Felsot & Dahm 1979)
0.91, 1.20	(Bromilow & Leistra 1980)
1.51	(calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
1.39	(reported as $\log K_{OM}$, Briggs 1981)
1.51	(estimated, Kenaga 1980; quoted, Howard 1991)
1.30–1.40	(Bilkert & Rao 1985; quoted, Howard 1991)
1.56	(soil, screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
1.48	(soil, 20–25°C, selected, Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996)
0.85–1.67	(Montgomery 1993)
1.48	(estimated-chemical structure, Lohninger 1994)
1.50	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.40, 1.97	(estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
1.30	(soil: organic carbon OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 1\text{--}9.5$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$t_{1/2} = 1.7\text{--}12$ d in soil for pH 1–10 with little change in rate between pH 4.4–10 (Lemley et al. 1988; quoted, Howard 1991)

$k(aq.) = 5.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) = (4.4 \pm 0.1) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.1; $k = (4.3 \pm 0.2) \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.0 and $24 \pm 1^\circ\text{C}$, with $t_{1/2} = 0.08$ s at pH 7 (Yao & Haag 1991).

$k(aq.) = (8.1 \pm 1.1) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to acetophenone) with hydroxyl radical in aqueous solutions at pH 3.5 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992)

Hydrolysis: $t_{1/2} = 23$ d at pH 7.2 (Smelt et al. 1978; quoted, Howard 1991)

$t_{1/2} = 9.9$ d at pH 6.3–7.0 at 15°C (Bromilow & Leistra 1980; quoted, Howard 1991)

$t_{1/2} = 4580$ d, based on a first-order $k = 1.51 \times 10^{-4} \text{ d}^{-1}$ at pH 5.5 and 5°C (Hansen & Spiegel 1983; quoted, Howard et al. 1991)

$t_{1/2} = 4.0$ min at pH 12.9, $t_{1/2} = 1.3$ min at pH 13.39 and 15°C (Lemley & Zhong 1983)

$t_{1/2} = 0.4$ – 3.2 d in soil at pH 4.5–4.9 and 25°C (Rao et al. 1984; quoted, Howard 1991)

Pseudo-first order $k = 5.3 \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 131$ d at pH 3.95, $k = 1.3 \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 559$ d at pH 6.02, $k = 2.1 \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 324$ d at pH 7.96, $k = 1.3 \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 55$ d at pH 8.85 in period of 89 d; and $k = 1.2 \times 10^{-1} \text{ d}^{-1}$ with $t_{1/2} = 6$ d at pH 9.85 for period of 15 days at 20°C in pH-buffered distilled water (Given & Dierberg 1985; Mink et al. 1989)

For pH buffered distilled water at 20°C: $t_{1/2} = 131$ d at pH 3.95, $t_{1/2} = 559$ d at pH 6.02, $t_{1/2} = 324$ d at pH 7.96, $t_{1/2} = 55$ d at pH 8.85, and $t_{1/2} = 6$ d at pH 9.85 (Montgomery 1993)

$t_{1/2} = 16$ d in aqueous montmorillonite suspensions (10 g/L) at pH 3.7 (Wei et al. 2001).

Biodegradation:

$k = 0.000222 \text{ h}^{-1}$ for discharge rate of 30 cm/year and $k = 0.000233 \text{ h}^{-1}$ for discharge rate of 61 cm/year with $t_{1/2} = 30$ d (Jones & Back 1984)

Aerobic mineralization $k = (1.93\text{--}34.2) \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 20\text{--}361$ d in surface soils and $k = 2.97\text{--}5.28) \times 10^{-3} \text{ d}^{-1}$ with $t_{1/2} = 131\text{--}233$ d in subsurface soils; anaerobic mineralization $k = (8.09\text{--}31.1) \times 10^{-4} \text{ d}^{-1}$ with $t_{1/2} = 223\text{--}1130$ d in surface soils after 63 d incubation (Ou et al. 1985)

$t_{1/2} = 70$ d in 0–10 cm depth of soil (Jury et al. 1987a, b; Jury & Ghodrati 1989).

$t_{1/2}(\text{aq. aerobic}) = 480\text{--}8664$ h, based on unacclimated aerobic soil grab sample data; $t_{1/2}(\text{aq. anaerobic}) = 1488\text{--}15240$ h, based on anaerobic ground water grab sample data (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 1\text{--}9.5$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991; Howard et al. 1991).

Surface water: $t_{1/2} = 5$ d in pond water, $t_{1/2} = 6$ d in lake water (Moorefield 1974; Mink et al. 1989)

Hydrolysis $t_{1/2} = 6$ to 131 d in pH-buffered distilled water at 20°C (Given & Dierberg 1985)

$t_{1/2} = 480\text{--}8664$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 0.08$ s for direct reaction with ozone in water at pH 7 and $24 \pm 1^\circ\text{C}$ (Yao & Haag 1991)

Ground water: $t_{1/2} = 960\text{--}15240$ h, based on estimated aqueous aerobic biodegradation half-life and water grab sample data (Miles & Delfino 1985; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 9, 7,$ and 12 d in clay, silty clay loam and fine sandy loam at an application rate of 20 ppm (Coppedge et al. 1967; quoted, Montgomery 1993);

hydrolysis $t_{1/2} = 23$ d at pH 7.2 (Smelt et al. 1978; quoted, Howard 1991),

$t_{1/2} = 9.9$ d at pH 6.3–7.0 at 15°C (Bromilow et al. 1980; Bromilow & Leistra 1980; quoted, Howard 1991; Montgomery 1993);

$t_{1/2} = 0.4\text{--}3.2$ d at pH 4.5–4.9 and 25°C (Rao et al. 1984; quoted, Howard 1991);

degradation rate constants $k = 0.000222 \text{ h}^{-1}$ for discharge rate of 30 cm/year and $k = 0.000233 \text{ h}^{-1}$ for discharge rate of 61 cm/yr with $t_{1/2} = 30$ d (Jones & Back 1984);

Mineralization $t_{1/2} = 20\text{--}361$ d in surface soils and $t_{1/2} = 131\text{--}233$ d in surface soils under aerobic condition, anaerobic $t_{1/2} = 223\text{--}1130$ d in surface soils after 63 d incubation (Ou et al. 1985)

reported $t_{1/2} = 70$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);

oxidation $t_{1/2} = 1.7\text{--}12$ d for pH 1–10 with little change in rate between pH 4.4–10 (Lemley et al. 1988; quoted, Howard 1991);

Rapidly oxidized to sulfoxide with $t_{1/2} \sim 7$ d in some soils, much more slowly to sulfone, pH dependent with $t_{1/2}$ varying from a few minutes at a pH of > 12 to ~ 560 d at a pH of 6.0. $t_{1/2}$ from 2 to > 8 wk in laboratory experiment, and $t_{1/2} < 1$ wk in field studies (Mink et al. 1989)

$t_{1/2} \leq 2$ wk, field study over 218-d period in the unsaturated zone beneath a citrus grove (Hornsby et al. 1990)

$t_{1/2}$ = 480–8664 h, based on unacclimated aerobic soil grab sample data (Howard 1991);

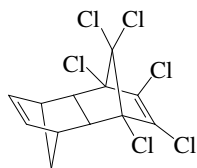
selected field $t_{1/2}$ = 30 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{1/2}$ between 0.3 and 3.5 months in surface soils (Jones & Norris 1998);

$t_{1/2}$ = 12.0 d in sterile soil, $t_{1/2}$ = 2.7 d in non-sterile soil; $t_{1/2}$ = 1.6, 1.4 and 1.7 d in soil grown with corn, mung bean and cowpea, respectively (Sun et al. 2004)

Biota: biochemical $t_{1/2}$ = 70 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

18.1.1.3 Aldrin



Common Name: Aldrin

Synonym: Aldrec, Aldrex, Aldrite, Aldrosol, Alttox, Compound 118, Drinox, ENT 15949, HHDN, NA 2761, NA 2762, Octalene, Seedrin

Chemical Name: 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4-endoexo-5,8-dimethano-naphthalene

Uses: Insecticide/Fumigant

CAS Registry No: 309-00-2

Molecular Formula: $C_{12}H_8Cl_6$

Molecular Weight: 364.910

Melting Point ($^{\circ}C$):

104 (Lide 2003)

Boiling Point ($^{\circ}C$):

145 (at 2 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.70 (Montgomery 1993)

Molar Volume (cm^3/mol):

316.8 (calculated-Le Bas method at normal boiling point)

214.7 (calculated-density)

Dissociation Constant, pK_a :

80.20 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

16.19 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.168 (mp at $104^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.20* (shake flask-GC/UV, measured range $25-45^{\circ}C$, Richardson & Miller 1960)

0.20 (Stephen & Stephen 1963)

0.027 ($25-29^{\circ}C$, shake flask-GC/ECD, Park & Bruce 1968)

0.013*, 0.14*, 0.18* (particle size: 0.01, 0.05 and 5.0μ , shake flask-GC/ECD, Biggar & Riggs 1974)

0.017 (generator column-GC/ECD, Weil et al. 1974)

0.027 (Martin & Worthing 1977)

0.01–0.2 ($20-25^{\circ}C$, Wauchope 1978; Willis & McDowell 1982)

0.013 (Kenaga 1980a, b; Kenaga & Goring 1980; Garten & Trabalka 1983)

0.027 ($27^{\circ}C$, Spencer 1982; Worthing & Walker 1987)

<0.05 (rm. temp., Hartley & Kidd 1987, Milne 1995)

0.017–0.18 (Montgomery 1993)

0.027 ($20-25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

1.06, 0.985 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

$\log [C_L/(mol m^{-3})] = -1480/(T/K) + 2.42$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00308 (Porter 1964a)

$\log (P/mmHg) 2,351 - 2035.35/(T/K)$; temp range $20-50^{\circ}C$ (Porter 1964a)

0.0008 (Günther & Günther 1971)
 0.0031 (20°C, Martin 1972)
 0.075 (20°C, Khan 1980)
 0.001 (20°C, estimated-relative volatilization rate, Dobbs & Cull 1982)
 0.0086* (20°C, extrapolated, gas saturation-GC, measured range 35.5–70°C, Grayson & Fosbraey 1982)
 $\ln(P/\text{Pa}) = 32.9 - 11044/(T/\text{K})$; temp range 35.5–70°C (Antoine eq., gas saturation-GC, Grayson & Fosbraey 1982)
 0.023, 0.033 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
 0.105 (supercooled liquid P_{L} , converted from literature P_{S} with ΔS_{fus} Bidleman 1984)
 0.0092, 0.0071 (20°C, gas saturation-GC, gas saturation-mixed bed-GC, Kim 1985)
 $\log(P/\text{mmHg}) = 10.4514 - 4281.065/(T/\text{K})$; temp range 25–45°C (gas saturation, Kim 1985)
 0.0086 (20°C, Hartley & Kidd 1987)
 0.0010 (20°C, Budavari 1989)
 0.0081* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
 $\log(P_{\text{S}}/\text{Pa}) = 15.561 - 5262.3/(T/\text{K})$; measured range 45–65.2°C (solid, gas saturation-GC, Rordorf 1989)
 $\log(P_{\text{L}}/\text{Pa}) = 12.489 - 4189.8/(T/\text{K})$; measured range 105–181°C (liquid, gas saturation-GC, Rordorf 1989)
 0.105, 0.0757 (supercooled P_{L} , converted from literature P_{S} with different ΔS_{fus} values, Hinckley et al. 1990)
 0.0231, 0.0202 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log(P_{\text{L}}/\text{Pa}) = 12.04 - 3924/(T/\text{K})$ (GC-RT correlation, Hinckley et al. 1990)
 0.0031 (20°C, Montgomery 1993)
 0.0009 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 0.061, 0.064 (supercooled liquid P_{L} : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
 $\log(P_{\text{L}}/\text{Pa}) = -4106/(T/\text{K}) + 12.56$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

1.418 (calculated-P/C, Thomas 1982)
 50.25 (20°C, gas stripping-GC, Warner et al. 1987)
 91.23 (20°C, calculated-P/C, Suntio et al. 1988)
 39.2 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
 50.25 (calculated-P/C, Montgomery 1993)
 50.8 (quoted from Howard 1989–1991, Capel & Larson 1995)
 91.23 (calculated-P/C, this work)
 4.46 (wetted wall column-GC, Altschuh et al. 1999)
 15, 23 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.01 (Lu & Metcalf 1975)
 5.67 (Callahan et al. 1979)
 5.66 (calculated, Kenaga 1980a, b)
 7.50 (RP-TLC-RT correlation, Lord et al. 1980)
 7.40 (extrapolated from RP-TLC, Briggs 1981)
 5.66 (shake flask, Geyer et al. 1984)
 6.496 ± 0.035 (shake flask/slow-stirring-GC, De Bruijn et al. 1989)
 5.17–7.40 (Montgomery 1993)
 5.74 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
 6.50 (selected, Hansch et al. 1995)
 5.74, 5.49, 5.39 (RP-HPLC-RT correlation, CLOGP, calculated-S, Finizio et al. 1997)
 6.50, 6.24 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:

8.08* (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
 $\log K_{\text{OA}} = -4.37 + 3709/(T/\text{K})$, temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
 8.08, 8.26 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

- 0.398 (bioaccumulation factor log BF, adipose tissue in female Albino rats, Quaife et al. 1967)
- 3.56–4.88 (earthworms, Wheatley & Hardman 1968)
- 2.80 (lake bacteria, Leshniowsky et al. 1970)
- 4.36; 4.50; 5.15 (*Diptera*; *Epimeoptera*; *Cladocera*; non-steady-state, Johnson et al. 1971)
- 4.55 (*Daphnia magna*, wet wt. basis, Johnson et al. 1971)
- 3.56–4.60 (*Oedogonium sp.*, Metcalf et al. 1973)
- 3.50 (Metcalf 1974)
- 3.11 (*Anabaena cylindrica*, Schaubberger & Wildman 1977)
- 2.30 (*Acacystis nidulans*, Schaubberger & Wildman 1977; quoted, Baughman & Paris 1981)
- 2.99 (*Acacystis nidulans*, Schaubberger & Wildman 1977; quoted, Baughman & Paris 1981)
- 4.03, 3.50 (fish: flow water, static water; Kenaga 1980b)
- 3.85, 1.34 (calculated-S, K_{OC} , Kenaga 1980a)
- 0.431 (average beef fat diet, Kenaga 1980b)
- 4.10 (*Chlorella fusca*, Geyer et al. 1981)
- 3.59 (golden orfe, Freitag et al. 1982)
- 4.10 (algae, Freitag et al. 1982)
- 4.26 (activated sludge, Freitag et al. 1982, 1984)
- 4.03 (Garten & Trabalka 1983; quoted, Howard 1991)
- 4.13 (clam fat, 60-d expt., Hartley & Johnson 1983)
- 4.09 (*Chlorella fusca*, Geyer et al. 1984)
- 4.09, 3.44, 4.26 (algae, golden ide, activated sludge, Freitag et al. 1985)
- 3.66 (molluscs, Hawker & Connell 1986; quoted, Howard 1991)
- 1.07 (beef biotransfer factor log B_b , correlated- K_{OW} from Radeleff et al. 1952 & Kenaga 1980; Travis & Arms, 1988)
- 1.62 (milk biotransfer factor log B_m , correlated- K_{OW} from Saha 1969; Travis Arms 1988)
- 1.67 (vegetation, correlated- K_{OW} from Lichtenstein 1960 & Weisgerber et al. 1974; Travis & Arms, 1988)
- 4.09, 4.79 (algae *Chlorella*: wet wt basis, dry wt basis, Geyer et al. 2000)
- 4.55, 6.55 (*Daphnia*: wet wt basis, lipid wt basis, Geyer et al. 2000)
- 3.66, 5.66 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{OC} :

- 2.61 (soil, Hamaker & Thompson 1972; quoted, Kenaga 1980a, b; Kenaga & Goring 1980)
- 4.68 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 4.69 (soil, sorption isotherm, converted from K_{OM} multiplied by 1.724, Briggs 1981)
- 4.36 (calculated- K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
- 4.69 (derived from exptl., Meylan et al. 1992)
- 5.02 (calculated-MCI χ , Meylan et al. 1992)
- 6.18 (estimated by QSAR & SPARC, Kollig 1993)
- 2.61, 4.69 (Montgomery 1993)
- 3.70 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 4.69; 4.68 (soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)
- 6.50; 4.70 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: half-life of a few hours to a few days (Callahan et al. 1979);
calculated $t_{1/2}$ = 68 h from water (Thomas 1982).

Photolysis:

Oxidation: photooxidation $t_{1/2}$ = 0.9–9.1 h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: not readily hydrolyzable with $t_{1/2}$ > 4 yr (Callahan et al. 1979);

first-order $t_{1/2}$ = 760 d, based on a first-order rate constant $k = 3.8 \times 10^{-5} \text{ h}^{-1}$ at pH 7.0 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991);

no disappearance in sealed glass ampoules after two weeks at pH 11 and 85°C (Kollig 1993)

$t_{1/2}$ = 760 d at pH 7 and 25°C (Montgomery 1993)

$t_{1/2} = 760$ d at pH 7 in natural waters (Capel & Larson 1995).

Biodegradation: aqueous aerobic $t_{1/2} = 504\text{--}14200$ h, based on unacclimated aerobic river die-away test data and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991);

rate constant $k = 0.013\text{ d}^{-1}$ by soil incubation studies from die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic $t_{1/2} = 24\text{--}168$ h, based on soil and freshwater mud grab sample data (Maule et al. 1987; quoted, Howard et al. 1991);

$t_{1/2} = 43\text{--}63$ d in a sandy loam soil incubated in the dark (McLean et al. 1988; quoted, Howard 1991)

$t_{1/2}(\text{aerobic}) = 21$ d, $t_{1/2}(\text{anaerobic}) = 1$ d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} \sim 35.5$ min for the vapor phase reaction with hydroxyl radical in air (GEMS 1986; quoted, Howard 1991);

$t_{1/2} = 0.9\text{--}9.1$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 504\text{--}14200$ h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991).

Biodegradation $t_{1/2}(\text{aerobic}) = 21$ d, $t_{1/2}(\text{anaerobic}) = 1$ d, hydrolysis $t_{1/2} = 760$ d at pH 7 in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 24\text{--}28400$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 5\text{--}10$ yr persistence in soil (Nash & Woolson 1967);

$t_{1/2} = 504\text{--}14200$ h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and soil field test data (Lichtenstein et al. 1971; quoted, Howard et al. 1991);

persistence of 2 yr (Edwards 1973; quoted, Morrill et al. 1982);

more than 24 months of persistence in soil (Wauchope 1978);

estimated first-order $k = 0.013\text{ d}^{-1}$ with $t_{1/2} = 53.3$ d from biodegradation by soil incubation studies from die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent with a $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982; quoted, Howard 1991);

$t_{1/2} = 43\text{--}63$ d in a sandy loam soil incubated in the dark (McLean et al. 1988; quoted, Howard 1991);

selected field $t_{1/2} = 365$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

$t_{1/2} = 5\text{--}9$ d (Geyer et al. 2000)

Biota:

TABLE 18.1.1.3.1

Reported aqueous solubilities and octanol-air partition coefficients of aldrin at various temperatures

Aqueous solubility						log K _{OA}	
Richardson & Miller 1960		Biggar & Riggs 1974				Shoeib & Harner 2002	
shake flask-UV spec.		shake flask-GC				generator column-GC/MS	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	S/g·m ⁻³	S/g·m ⁻³	t/°C	log K _{OA}
		particle size	0.01μ	0.05μ	5.0μ		
25	0.20	15	0.0055	0.052	0.105	5	9.0091
35	0.39	25	0.0135	0.140	0.180	10	8.6780
45	0.79	35	0.030	0.235	0.350	15	8.5419
		45	0.065	0.455	0.600	20	8.2987
						25	8.0801
						25	8.080
log K _{OA} = A + B/(T/K)							
A -4.366							
B 3709							
enthalpy of phase change							
ΔH _{OA} /(kJ mol ⁻¹) = 71.0							

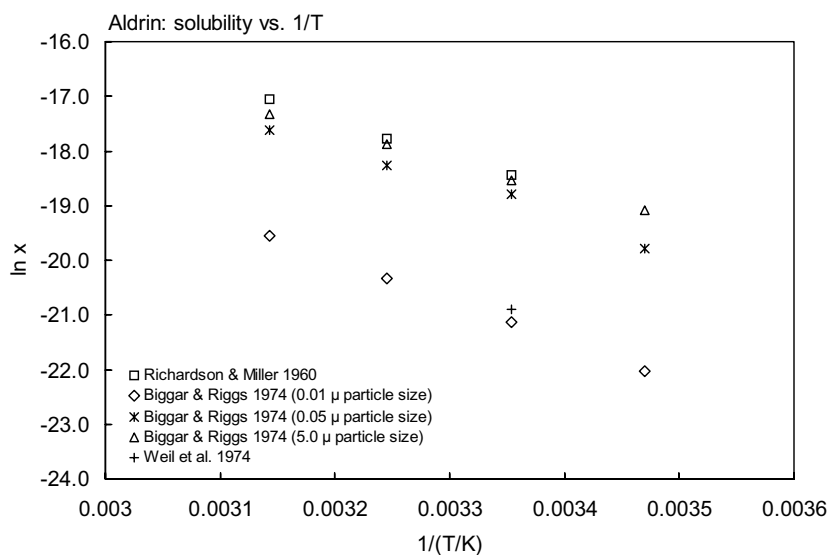


FIGURE 18.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for aldrin.

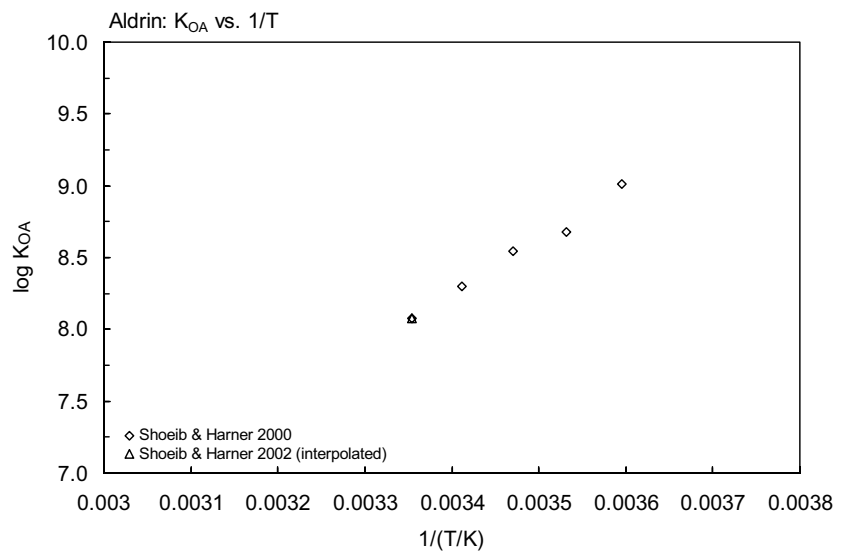


FIGURE 18.1.1.3.2 Logarithm of K_{OA} versus reciprocal temperature for aldrin.

TABLE 18.1.1.3.2
Reported vapor pressures of aldrin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$		(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)		

Grayson & Fosbracey 1982		Rordorf 1989	
gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
35.5	0.063	25	0.0081
41.0	0.101	50	0.19
41.6	0.112	75	2.80
45.6	0.163	100	29.0
50.8	0.329	125	220
63.3	1.033		
70.0	2.213	eq. 1	P_s/Pa
20	0.0086	A	15.561
		B	5262.3
eq. 1a	P/Pa		
A	11044		for liquid
B	32.9	eq 1	P_L/Pa
		A	12.489
		B	4189.8

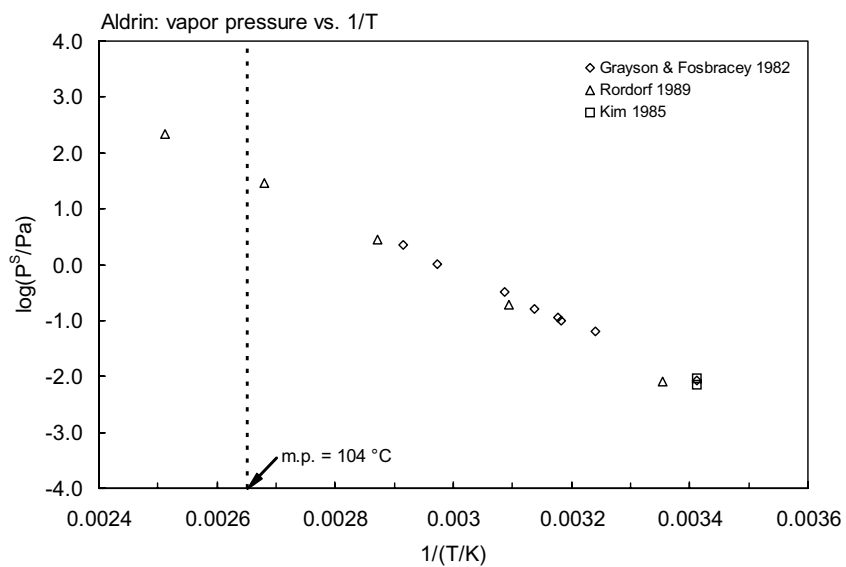
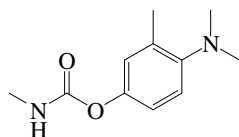


FIGURE 18.1.1.3.3 Logarithm of vapor pressure versus reciprocal temperature for aldrin.

18.1.1.4 Aminocarb



Common Name: Aminocarb

Synonym: A 363, Bay 44646, Bayer 5080, ENT 25784, Matacil, Mitacil

Chemical Name: 4-dimethylamino-*m*-tolyl methylcarbamate, 4-dimethylamino-3-methylphenol methylcarbamate

Uses: nonsystemic, broad-spectrum insecticide used to control the spruce budworm in forests and also as molluscicide.

CAS Registry No: 2032-59-9

Molecular Formula: $C_{11}H_{16}N_2O_2$

Molecular Weight: 208.257

Melting Point ($^{\circ}C$):

94 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

250.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.210 (mp at $94^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

915 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

915, 1360 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

915 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00227 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

5.17×10^{-4} (20 – $25^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.74 (Zitko & McLeese 1980)

1.73 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983b)

1.90 ($22^{\circ}C$, shake flask-GC, pH 9, Bowman & Sans 1983b)

0.91, 1.90 (pH 5, pH 9, shake flask-GC, Weinberger & Greenhalgh 1983)

1.70 (Richardson & Qadri 1986)

1.73 (Montgomery 1993)

1.90 (recommended, Sangster 1993)

1.90 (pH 9, selected, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

0.690 (mussel, McLeese et al. 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

1.92 (calculated, Montgomery 1993)

2.00 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

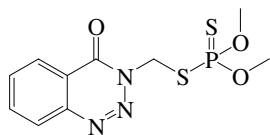
2.52, 1.94 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: selected field $t_{1/2} = 6$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

18.1.1.5 Azinphos-methyl



Common Name: Azinphos-methyl

Synonym: Bay or Bayer 9027, Bay 17147, Carfene, Cotnion, Cotnion methyl, Crysthion 21, DBD, ENT 23233, Gothnion, Guthion, Gusathion, Metiltriazotion, R 1582

Chemical Name: *O,O*-dimethyl-*S*-[4-*oxo*-1,2,3-benzotriazin-3(4*H*)-yl)methyl] phosphorodithioate; *O,O*-dimethyl-*S*-[3,4-dihydro-4-keto-1,2,3-benzotriazinyl-3-methyl] dithiophosphate

Uses: nonsystemic insecticide and acaricide for control of insects and pests in blueberry, grape, maize, vegetable, cotton, and citrus crops.

CAS Registry No: 86-50-0

Molecular Formula: $C_{10}H_{12}N_3O_3PS_2$

Molecular Weight: 317.324

Melting Point ($^{\circ}C$):

73 (Lide 2003)

Boiling Point ($^{\circ}C$):

> 200 (dec., Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

1.518 (Tomlin 1994)

1.44 (Milne 1995; Montgomery 1993)

Molar Volume (cm^3/mol):

270.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

96.65 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.96 (DSC method, Plato & Glasgow 1969)

20.5 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

59 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F : 0.338 (mp at $73^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

33 (rm. temp., Spencer 1973; Worthing 1979; Khan 1980; Budavari 1989)

30 ($20^{\circ}C$, Melnikov 1971; Spencer 1982)

33 (20 – $25^{\circ}C$, Willis & McDowell 1982)

20.9 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

29 (Hartley & Kidd 1987; Lohninger 1994)

28 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

29 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

30 (Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.93×10^{-5} ($20^{\circ}C$, Melnikov 1971)

0.0510 ($20^{\circ}C$, Khan 1980)

1.00×10^{-6} ($20^{\circ}C$, Worthing & Walker 1983)

1.11×10^{-5} ($20^{\circ}C$, GC-RT correlation without mp correction, Kim et al. 1984; Kim 1985)

3.10×10^{-6} ($20^{\circ}C$, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)

<0.0010 ($20^{\circ}C$, Hartley & Kidd 1987)

3.00×10^{-5} ($20^{\circ}C$, selected, Suintio et al. 1988)

7.80×10^{-7} , 3.0×10^{-5} , 6.90×10^{-4} , 0.010, 0.11 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log (P_s/P_a) = 14.416 - 6119.2/(T/K)$; measured range 80.3–145°C (solid, gas saturation-GC, Rordorf 1989)
 $\log (P_L/P_a) = 11.327 - 5048.6/(T/K)$; measured range 80.3–145°C (liquid, gas saturation-GC, Rordorf 1989)
 $<1.8 \times 10^{-4}$ (20°C, Worthing & Hance 1991)
 1.80×10^{-4} (20°C, Tomlin 1994)
 2.67×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.13×10^{-4} (20°C, Montgomery 1993)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.0032 (20°C, calculated-P/C, Suntio et al. 1988)
 1.52×10^{-5} (calculated-P/C, Howard 1991)
 3.17×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.99 (Callahan et al. 1979)
 2.69 (20°C, shake flask-GC, Bowman & Sans 1983b)
 2.75 (Hansch & Leo 1985)
 2.43 (HPLC-RT correlation, Moody et al. 1987)
 2.69, 2.75 (Montgomery 1993)
 2.75 (recommended, Sangster 1993)
 2.96 (Tomlin 1994)
 2.75 (recommended, Hansch et al. 1995)
 2.62 (Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, $\log \text{BCF}$:

1.96 (calculated-S as per Kenaga 1980, this work)
 1.86 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

2.61 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
 2.28 (Fröbe et al. 1989)
 1.30 (selected, USDA 1989; Neary et al. 1993)
 2.28 (derived from exptl., Meylan et al. 1992)
 1.84 (calculated-MCI χ , Meylan et al. 1992)
 3.00 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.47–3.53 (Montgomery 1993)
 2.95 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
 2.28 (soil, calculated- QSAR MCI χ , Sabljic et al. 1995)
 2.95; 1.84 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 3.67, 3.69, 2.73, 2.74, 2.91 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
 3.30, 2.89, 2.75, 2.799, 3.231 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
 2.69 (sandy loam soil, column equilibrium method, 20°C, Xu et al. 1999)
 3.299, 2.894, 2.755, 2.799, 3.231 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, HPLC-k' correlation, Gawlik et al. 2000)
 2.28; 1.80, 2.04 (soil, quoted exptl.; estimated-class specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 1.3$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order $t_{1/2} = 36.4, 27.9, 7.2$ d in water at pH 8.6 and 6°C, 25°C and 40°C (Heuer et al. 1974; quoted, Howard 1991);

$t_{1/2} = 27.9$ d at pH 8.6 and 25°C (Montgomery 1993);

$t_{1/2} = 87$ d at pH 4, $t_{1/2} = 50$ d at pH 7, and $t_{1/2} = 4$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: studies with aquatic water/sediment microorganisms at 5 mg/L and pH 6.7 indicate $t_{1/2} = 3.3$ d in microcosms compared to $t_{1/2} = 2.7$ d in field studies (Portier 1985; quoted, Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 1.3$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 415$ d at 6°C, $t_{1/2} = 115$ d at 22°C in darkness for Milli-Q water; $t_{1/2} = 278$ d at 6°C, $t_{1/2} = 42$ d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 506$ d at 6°C, $t_{1/2} = 35$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 26$ d at 22°C in darkness, $t_{1/2} = 11$ d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment:

Soil: for dry soil with 2–3% moisture, $t_{1/2} = 484, 88,$ and 32 d at 6, 25, and 40°C, respectively; while for moist soil with 50% moisture content, half-lives were much shorter: 64, 13, and 5 d at 6, 25, and 40°C, respectively (Yaron et al. 1974; quoted, Montgomery 1993);

selected field $t_{1/2} = 10$ d (Wauchope et al. 1992; Hornsby et al. 1996);

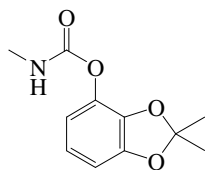
average $t_{1/2} = 40$ d (Dowd et al. 1993);

half-life in soil ranges from a few days to many weeks, depending on soil type (Tomlin 1994);

$t_{1/2} = 10$ d (selected, Halfon et al. 1996).

Biota: average $t_{1/2} = 30$ d in forest (selected, USDA 1989; quoted, Neary et al. 1993).

18.1.1.6 Bendiocarb



Common Name: Bendiocarb

Synonym: Bencarbate, Dycarb, Ficam, Garvox, Multamat, Multimet, NC 6897, Niomil, Rotate, Seedox, Tatto, Turcam

Chemical Name: 2,3-isopropylidenedioxyphenyl methylcarbamate; 2,2-dimethyl-1,3-benzodioxol-4-yl methyl-carbamate

Uses: contact insecticide used to control beetles, wireworms, flies, wasps, and mosquitoes in beets and maize.

CAS Registry No: 22781-23-3

Molecular Formula: $C_{11}H_{13}NO_4$

Molecular Weight: 223.226

Melting Point ($^{\circ}C$):

130 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.25 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

231.7 (calculated-Le Bas method at normal boiling point)

178.6 (calculated-density)

Dissociation Constant, pK_a :

8.80 (Worthing & Hance 1991; Wauchope et al. 1992; Montgomery 1993; Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0933 (mp at $130^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

40 (Spencer 1973, 1982)

40 (Martin & Worthing 1977; Worthing & Walker 1987; Kenaga 1980;)

40 ($20^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

40 ($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

40 (Lohninger 1994)

280 ($20^{\circ}C$ at pH 7, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

6.6×10^{-4} (Hartley & Kidd 1987)

0.00467 ($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

6.6×10^{-4} ($20^{\circ}C$, Montgomery 1993)

0.0046 (quoted, gas saturation-GC, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.365 ($20^{\circ}C$, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.29 (selected, Dao et al. 1983)

1.70 (Worthing & Hance 1991; Montgomery 1993; Milne 1995)

1.72 (at pH 6.55, Tomlin 1994)

1.70 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.89 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

- 2.76 (calculated-S, Kenaga 1980)
- 2.76 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.76 (Montgomery 1993)
- 2.76 (estimated-chemical structure, Lohninger 1994)
- 1.45–1.60 (Tomlin 1994)
- 1.30, 1.83 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} = 4$ d at pH 7 and 25°C (Spencer 1982; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: hydrolysis half-life of 4 d at 25°C and pH 7 under EPA guidelines (Spencer 1982)

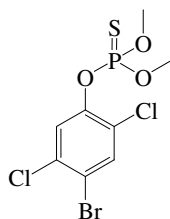
Ground water:

Sediment:

Soil: half-life of several days to a few weeks (Hartley & Kidd 1987; quoted, Montgomery 1993);
selected field $t_{1/2} = 5.0$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

18.1.1.7 Bromophos



Common Name: Bromophos

Synonym: Nexion, S-1942, Omexan, Brofene

Chemical Name: *o*-4-bromo-2,5-dichlorophenyl *O,O*-dimethyl phosphorothioate

CAS Registry No: 2104-96-3

Uses: insecticide

Molecular Formula: $C_8H_8BrCl_2PS$

Molecular Weight: 317.999

Melting Point ($^{\circ}C$):

54 (Lide 2003)

Boiling Point ($^{\circ}C$):

140–142 at 0.01 mmHg (Hartley & Kidd 1987; Worthing & Walker 1987)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.519 (mp at $54^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

40 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987)

0.30 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1979)

0.652 ($20^{\circ}C$, correlated, Bowman & Sans 1983b)

0.70 ($20^{\circ}C$, Worthing & Walker 1987)

Vapor Pressure (Pa at $25^{\circ}C$):

0.017 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.88 (shake flask-concn ratio-GC, Bowman & Sans 1983b)

5.208 ± 0.009 (slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1991)

4.88 (recommended, Sangster 1993)

5.21 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.89 (calculated, Kenaga 1980b)

4.65 ± 0.06 (guppy, calculated on an extractable liquid wt basis, De Bruijn & Hermens 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

2.76 (calculated-solubility, Kenaga 1980b)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: hydrolyzed in alkaline media (Worthing 1987).

Biodegradation:

Biotransformation:

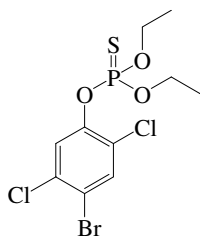
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 0.01307 \text{ mL g}^{-1} \text{ d}^{-1}$; $k_2 = 0.33 \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = 12 \text{ d}^{-1}$ (guppy, calculated- K_{OW} , De Bruijn & Hermens 1991)

Half-Lives in the Environment:

18.1.1.8 Bromophos-ethyl



Common Name: Bromophos-ethyl

Synonym: Nexagan, Filariol

Chemical Name: *O*-(4-bromo-2,5-dichlorophenyl) *O,O*-diethyl phosphorothioate

CAS Registry No: 4824-78-6

Uses: insecticide, acaricide

Molecular Formula: $C_{10}H_{12}Cl_2O_3PS$

Molecular Weight: 394.049

Melting Point ($^{\circ}C$):

colorless liquid (Spencer 1982)

Boiling Point ($^{\circ}C$):

122–123 (at 0.001 mmHg, Hartley & Kidd 1987; Worthing & Walker 1987)

Density (g/cm^3 at $20^{\circ}C$):

1.52–1.55 (Hartley & Kidd 1987; Worthing & Walker 1987)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.0 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987)

0.44 ($20^{\circ}C$, Bowman & Sans 1983b)

0.14 ($20^{\circ}C$, Worthing & Walker 1987)

Vapor Pressure (Pa at $25^{\circ}C$):

6.1×10^{-3} ($30^{\circ}C$, Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)

Henry's Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.68 (shake flask-concn-ration, Bowman & Sans 1983b)

6.149 ± 0.019 (slow-stirring-GC; De Bruijn et al. 1989)

5.68 (recommended, Sangster 1993)

6.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.62 (fish, calculated, Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{OC}$:

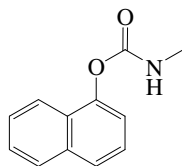
3.48 (soil, calculated-solubility, Kenaga 1980b)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: at room temp., stable in aqueous suspension at $\text{pH} < 9$, hydrolysed at $\text{pH} > 9$, particularly at higher temperature (Worthing & Walker 1987).

Half-Lives in the Environment:

18.1.1.9 Carbaryl



Common Name: Carbaryl

Synonym: Arylam, Atoxan, Caproline, Carbamine, Carbatox, Carpolin, Carylderm, Cekubaryl, Crag sevin, Denapon, Devicarb, Dicarbam, ENT 23969, Gamonil, Germain's, Hexavin, Karbaspray, Karbatox, Karbosep, OMS 29, naphthyl carbamate, Panam, Ravyon, Rylam, Seffein, Septene, Sevimol, Sevin, Sok, Tercyl, Toxan, Union Carbide 7744

Chemical Name: carbamic acid, methyl-, 1-naphthyl ester; 1-naphthalenol, methyl carbamate; 1-naphthyl-*N*-methyl carbamate; 1-naphthyl methylcarbamate; 1-naphthalenyl methylcarbamate

Uses: contact insecticide used to control most insects on fruits, vegetables, and ornamentals; also used as growth regulator for fruit thinning of apples.

CAS Registry No: 63-25-2

Molecular Formula: $C_{12}H_{11}NO_2$

Molecular Weight: 201.221

Melting Point ($^{\circ}C$):

145 (Lide 2003)

Boiling Point ($^{\circ}C$): dec. on distillation

Density (g/cm^3 at $20^{\circ}C$):

1.232 (Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

0.52–0.61 (Worthing & Hance 1991)

Molar Volume (cm^3/mol):

218.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.27 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0665 (mp at $145^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

40 (shake flask, David et al. 1960)

40 ($30^{\circ}C$, Spencer 1973; Worthing & Hance 1991)

40 (Martin & Worthing 1977)

34 (20 – $25^{\circ}C$, shake flask-GC, Kanazawa 1981)

50 ($20^{\circ}C$, Spencer 1982)

104 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

82.6 (generator column-GC, Swann et al. 1983)

590 (RP-HPLC-RT correlation, Swann et al. 1983)

120 ($30^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)

120 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

104, 130 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

40, 1000 (Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

<0.665 ($26^{\circ}C$, Melnikov 1971)

2.80×10^{-3} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

<0.133 (20 – $25^{\circ}C$, Weber et al. 1980)

1.81×10^{-4} (Ferreira & Seiber 1981)

7.75×10^{-3} , 5.39×10^{-4} ($20^{\circ}C$, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)

< 0.665	(26°C, Hartley & Kidd 1987)
< 0.0053	(Worthing & Hance 1991)
1.60×10^{-4}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
8.77×10^{-4}	(Montgomery 1993)
2.00×10^{-4}	(23.5°C, Tomlin 1994)

Henry's Law Constant (Pa m³/mol):

0.0013	(calculated-P/C, Suntio et al. 1988;)
4.41×10^{-4}	(calculated-P/C as known LWAPC, Meylan & Howard 1991)
3.18×10^{-4}	(calculated-bond contribution method LWAPC, Meylan & Howard 1991)
1.287	(20°C, calculated-P/C, Montgomery 1993)
< 0.010	(estimated, Mabury & Crosby 1996)
4.48×10^{-5}	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow}:

2.36	(shake flask-UV, Fujita et al. 1974)
2.36	(Freed et al. 1976)
2.81	(Hansch & Leo 1979; Rao & Davidson 1980)
2.32	(shake flask-UV, Lord et al. 1980)
2.32	(20°C, shake flask-UV, Briggs 1981)
2.29	(20°C, shake flask-GC, Kanazawa 1981)
2.36	(Lyman et al. 1982; Magee 1991; Trapp & Pussemier 1991)
2.31	(22°C, shake flask-GC, Bowman & Sans 1983b)
2.36	(Hansch & Leo 1985)
2.14	(RP-HPLC-RT correlation, Trapp & Pussemier 1991)
2.63	(HPLC-RT correlation, average, Hu & Leng 1992)
2.31–2.81	(Montgomery 1993)
1.99	(RP-HPLC-RT correlation, Saito et al. 1993)
1.59	(Tomlin 1994)
2.36	(recommended, Hansch et al. 1995)
2.24	(RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

< 0.0	(fish in static water, Metcalf & Sanborn 1975; Freed et al. 1976)
1.89	(calculated-S, Kenaga 1980)
1.08	(calculated-K _{OC} , Kenaga 1980)
1.64	(earthworm, Lord et al. 1980)
0.95	(<i>Pseudorasbora parva</i> , Kanazawa 1981)
1.86	(algae, Freitag et al. 1982)
1.53	(golden orfe, Freitag et al. 1982)
1.95	(activated sludge, Freitag et al. 1982, 1984)
0.954	(topmouth gudgeon, Kanazawa 1983)
1.45	(golden ide, Freitag et al. 1984)
1.85, 1.48, 1.95	(algae, golden ide, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC}:

2.36	(soil, Leenheer & Atrichs 1971; LaFleur 1976)
2.36	(Kenaga 1980; Kenaga & Goring 1978)
2.76	(calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
2.49	(average of 3 soils, McCall et al. 1980)
2.49	(average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
2.02	(soil slurry/shake flask-UV method, converted form reported as log K _{OM} of 1.78, Briggs. 1981)
3.04, 2.50, 2.42	(estimated-S, calculated-S and mp, estimated-K _{OW} , Karickhoff 1981)

- 2.76, 2.66 (estimated-S, K_{OW} , Lyman 1982)
 2.59 (soil slurry method, Swann et al. 1983)
 2.57 (reverse phase HPLC-RT correlation, Swann et al. 1983)
 2.14 (calculated- MCI χ , Gerstl & Helling 1987)
 2.36 (soil, screening model calculations, Jury et al. 1987b)
 2.23 (calculated-MCI χ , Bahnick & Doucette 1988)
 2.30 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)
 2.04 (estimated as $\log K_{OM}$, Magee 1991)
 2.48 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.30 (soil, Dowd et al. 1993)
 2.02–2.59 (Montgomery 1993)
 2.71 (estimated-chemical structure, Lohninger 1994)
 2.40 (soil, calculated-MCI χ , Sabljic et al. 1995)
 2.21, 2.39 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
 2.49–2.62 (sediments of San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 3000$ d estimated from Henry's law constant for a body of water 1 m deep, flowing at 1 m/s and with a wind speed of 3 m/s (Howard 1991).

Photolysis: $t_{1/2} = 6.6$ d for a mid-summer day at latitude 40°, photolysis is about 4 times faster than in the winter months (Wolfe et al. 1978)

$t_{1/2}(\text{air}) = 52\text{--}200$ h in the atmosphere, based on aqueous photolysis data; $t_{1/2}(\text{aq.}) = 52\text{--}200$ h, based on reported photolysis half-life for summer and winter sunlight at 40°N (Howard et al. 1991)

$k(\text{aq.}) = 6.4 \times 10^{-4} \text{ h}^{-1}$ (Armbrust 2000)

$k(\text{aq.}) = (5.6 \pm 0.3) \times 10^{-5} \text{ s}^{-1}$ in the presence of UV light, a 30 ppm carbaryl solution at 298 K; in the presence of silver-doped zeolite Y catalyst with 2.42% Ag by weight, the photodecomposition rate becomes 80 times faster. The addition of Suwannee River natural organic matter had a minimal effect on this system, increases or decreases the catalytic photodecomposition rate by a factor of 3 at most (Kanan et al. 2003).

Oxidation: photooxidation $t_{1/2} = 4.5\text{--}7.4$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)

$k_{OH}(\text{aq.}) = 3.40 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies and the field dissipation $t_{1/2} = 8.8$ h (Mabury & Crosby 1996).

Hydrolysis: $k(\text{alkaline}) = (5.02 \pm 0.03) \text{ M}^{-1} \text{ h}^{-1}$ with $t_{1/2} = 1500$ d at pH 5, $t_{1/2} = 15$ d at pH 7 and $t_{1/2} = 0.15$ d at pH 9 and 28°C (Wolfe et al. 1978)

$t_{1/2} = 312$ h, based on base rate constant at pH 7 and 25°C (Howard et al. 1991)

$t_{1/2} = 1500$ d at pH 5, $t_{1/2} = 15$ d at pH 7, and $t_{1/2} = 0.15$ d at pH 9 at 27°C (Montgomery 1993)

$t_{1/2} = 12$ d at pH 7 and $t_{1/2} = 3.2$ h at pH 9 (Tomlin 1994)

$t_{1/2} = 1500$ d at pH 2, $t_{1/2} = 13$ d at pH 7 and $t_{1/2} = 0.00013$ d at pH 12 in natural waters (Capel & Larson 1995)

$k = 0.066 \text{ d}^{-1}$ at pH 7, $k = 5.2 \text{ d}^{-1}$ at pH 9; dissipation by hydrolysis from a simulated aquatic system after 30 d: 53.9%, 59.1% of depth of 10 cm, 1 m, respectively, at pH 6; 64.2%, 70.7% of depth of 10 cm, 1 m, respectively, at pH 7; and 85.7%, 81.0% of depth of 10 cm, 1 m, respectively, at pH 7 (Armbrust 2000) Biodegradation:

$t_{1/2}(\text{aerobic}) = 40\text{--}720$ h, based on unacclimated aerobic river die-away test data and freshwater grab sample data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991)

$t_{1/2} > 3 \times 10^4$ d, assuming a bacterial population of 0.1 mg/L (Wolfe et al. 1978b)

$k(\text{aq.}) = 2.4 \times 10^{-10} \text{ mL cell}^{-1} \text{ d}^{-1}$ in aquatic system (Scow 1982)

$t_{1/2}(\text{anaerobic}) = 160\text{--}2880$ h, based on unacclimated aerobic biodegradation (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1.7$ d, $t_{1/2}(\text{anaerobic}) = 6.7$ d in natural waters (Capel & Larson 1995)

$k(\text{aerobic}) = 1.70 \times 10^{-3} \text{ h}^{-1}$ (Armbrust 2000) .

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives or Fate Rate Constants in the Environment:

Air: $t_{1/2}$ = 12.6 h, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Howard 1991);

$t_{1/2}$ = 4.5–7.4 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994).

Surface water: hydrolysis $t_{1/2}$ = 1500 d at pH 5, $t_{1/2}$ = 15 d at pH 7 and $t_{1/2}$ = 0.15 d at pH 9; direct photolysis $t_{1/2}$ = 6.6 d; and biolysis $t_{1/2}$ > 3×10^4 d assuming a bacterial population of 0.1 mg/L (Wolfe et al. 1978b); 18–20% recovered from pond water after 42 d, 37–42% recovered after 50 d from creek water (Szeto et al. 1979)

$t_{1/2}$ = 3.2–200 h, based on aqueous hydrolysis half-life at pH 9 and 28°C and photolysis half-life for winter sunlight at 40°N (Howard et al. 1991)

Biodegradation $t_{1/2}$ (aerobic) = 1.7 d, $t_{1/2}$ (anaerobic) = 6.7 d, hydrolysis $t_{1/2}$ = 1500 d at pH 2, $t_{1/2}$ = 13 d at pH 7 and $t_{1/2}$ = 0.00013 d at pH 12 in natural waters (Capel & Larson 1995)

$t_{1/2}$ = 37 d at 22°C for Milli-Q water at pH 6.1; $t_{1/2}$ = 31 d at 6°C, $t_{1/2}$ = 11 d at 22°C in darkness, $t_{1/2}$ = 9 d under sunlight conditions for river water at pH 7.3; $t_{1/2}$ = 45 d at 6°C, $t_{1/2}$ < 2 d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2}$ = 22 d at 6°C, $t_{1/2}$ < 2 d at 22°C in darkness and $t_{1/2}$ = 13 d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995);

dissipation by hydrolysis from a simulated aquatic system after 30 d, 53.9%, 59.1% of depth of 10 cm, 1 m, respectively, at pH 6, 64.2%, 70.7% of depth of 10 cm, 1 m, respectively, at pH 7 and 85.7%, 81.0% of depth of 10 cm, 1 m, respectively, at pH 7 (Armbrust 2000).

Ground water: $t_{1/2}$ = 3.2–1440 h, based on aqueous hydrolysis half-life at pH 9 and 28°C, and unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment: ~ 55% recovered after 50 d in autoclaved water and sediment samples (Szeto et al. 1979)

first-order degradation k = 0.392 d⁻¹ with $t_{1/2}$ = 1.8 d under aerobic conditions, k = 0.005 d⁻¹ with $t_{1/2}$ = 125 d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation k = 0.141 d⁻¹ with $t_{1/2}$ = 4.9 d under aerobic conditions, k = 0.0009 d⁻¹ with $t_{1/2}$ = 746 d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: $t_{1/2}$ = 97–251 h in dry soil and 4458–688 h in wet or saturated soil (Hautala 1978; quoted, Howard 1991); persistence of less than one month (Wauchope 1978);

$t_{1/2}$ = 3.2–720 h, based on aqueous hydrolysis half-life at pH 9 and 28°C and unacclimated aerobic biodegradation half-life (Howard et al. 1991);

biodegradation rate constant k = 0.037 d⁻¹ in soil by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);

$t_{1/2}$ = 22 d from screening model calculations (Jury et al. 1987b);

selected field $t_{1/2}$ = 10 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{1/2}$ = 8 d (Pait et al. 1992);

degradation $t_{1/2}$ = 7–14 d in a sandy loam and $t_{1/2}$ = 14–28 d in a clay loam under aerobic conditions for concn. at 1 ppm (Tomlin 1994);

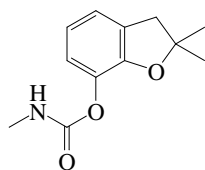
$t_{1/2}$ = 10 d (selected, Halfon et al. 1996)

Field dissipation $t_{1/2}$ = 8.8 h (Mabury & Crosby 1996)

$t_{1/2}$ = 14 d in an aerobic soil, $t_{1/2}$ = 72 d in an anaerobic aquatic soil (quoted, Bondarenko & Gan 2004)

Biota: biochemical $t_{1/2}$ = 22 d from screening model calculations (Jury et al. 1987b).

18.1.1.10 Carbofuran



Common Name: Carbofuran

Synonym: Bay 70143, Curaterr, ENT 27164, Furadan, NIA 10242, Niagara 10242, Yaltox

Chemical Name: 2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate; 2,3-dihydro-2,2-dimethyl-7-benzo-furanyl methylcarbamate

Uses: broad-spectrum systemic insecticide, nematocide and acaricide applied in soil to control insects and nematodes; also to control insects and mites on foliage.

CAS Registry No: 1563-66-2

Molecular Formula: $C_{12}H_{15}NO_3$

Molecular Weight: 221.252

Melting Point ($^{\circ}C$):

151 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.18 (Hartley & Kidd 1987; Trotter et al. 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

240.8 (calculated-Le Bas method at normal boiling point)

187.5 (calculated-density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0580 (mp at $151^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

700	(Spencer 1973, 1982; Khan 1980; Weber et al. 1980)
250	(Caro et al. 1976)
415	(Martin & Worthing 1977; Herbicide Handbook 1978, 1983)
320	($19^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983b)
700	(Verschuereen 1983; Windholz 1983, Budavari 1989)
480	(generator column-HPLC/RI, Swann et al. 1983)
670	(RP-HPLC-RT correlation, Swann et al. 1983)
700	(Hartley & Kidd 1987; Worthing & Walker 1987; Milne 1995)
351	($20-25^{\circ}C$, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)
320	($20^{\circ}C$, Montgomery 1993; Tomlin 1994; Milne 1995)
375	($30^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.12×10^{-3}	(Knudsen effusion method, Cook 1973)
1.11×10^{-3}	(Caro et al. 1976; Fuhrmann & Lichtenstein 1980)
8.67×10^{-4}	($20^{\circ}C$, Hartley & Graham-Bryce 1980)
2.70×10^{-3}	($33^{\circ}C$, Khan 1980)
2.67×10^{-3}	($20-25^{\circ}C$, Weber et al. 1980)
2.70×10^{-4}	(Thomas 1982)
2.20×10^{-3} , 1.08×10^{-4}	($20^{\circ}C$, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)
2.70×10^{-3}	($33^{\circ}C$, Hartley & Kidd 1987)
8.00×10^{-5}	($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.10×10^{-5} , 7.20×10^{-5}	(20 , $25^{\circ}C$, Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

- 3.95 × 10⁻⁴ (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
- 7.69 × 10⁻⁴ (Jury et al. 1984)
- 9.42 × 10⁻⁶ (Jury et al. 1987a, b; Jury & Ghodrati 1989)
- 5.10 × 10⁻⁴ (calculated-P/C, Suntio et al. 1988)
- 7.69 × 10⁻⁴ (calculated-P/C, Taylor & Glotfelty 1988)
- < 0.010 (estimated, Mabury & Crosby 1996)
- 5.04 × 10⁻⁵ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow}:

- 2.32 (Hansch & Leo 1979, 1985)
- 1.60 (from Dow Chemical data, Kenaga & Goring 1980)
- 2.88 (Belluck & Felsot 1981)
- 2.07 (quoted, Karickhoff 1981)
- 1.60 (calculated, Lyman 1982)
- 1.82 (RP-HPLC-RT correlation, Trapp & Pussemier 1991)
- 1.60–2.32 (Montgomery 1993)
- 1.60 (RP-HPLC-RT correlation, Saito et al. 1993)
- 2.32 (recommended, Sangster 1993)
- 1.52 (20°C, Tomlin 1994)
- 1.23–1.42 (Milne 1995)
- 2.32 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 1.00 (estimated-log K_{ow}, Neely et al. 1974)
- 1.32 (calculated-S, Kenaga 1980)
- 0.60 (*Triaenodes tardus*, Belluck & Felsot 1981)
- 1.00 (selected, Schnoor & McAvoy 1981; Schnoor 1992)
- 1.53 (calculated-log K_{ow}, Lyman et al. 1982; quoted, Howard 1991)
- 1.18 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
- 2.07 (*Tilapia nilotica*, Tejada & Magallona 1985)
- 1.00 (*Pila luzonica*, Tejada & Magallona 1985)
- 2.07 (paddy field fish, Tejada 1995)

Sorption Partition Coefficient, log K_{oc}:

- 2.20 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 1.67 (calculated values for 6 samples while high organic carbon >15% were omitted from calculation by Felsot & Wilson 1980)
- 1.78–2.20 (3 soils of org. content 0.68–2.01, McCall et al. 1980)
- 2.02 (average of 3 soils, McCall et al. 1980)
- 1.46 (soil/sediments, Rao & Davidson 1980)
- 2.46; 1.51; 1.68 (estimated-S; estimated-S and mp; estimated-K_{ow}, Karickhoff 1981)
- 2.70 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
- 2.25 (calculated-S, Lyman 1982)
- 1.47 (average of 5 different soils, Rao & Davidson 1982)
- 2.11 (retention times of RP-HPLC-RT correlation, Swann et al. 1983)
- 2.00 (soil slurry/shake flask method, Swann et al. 1983; quoted, Howard 1991)
- 1.45 (soil, screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
- 1.73 (calculated-Freund isotherm linearized for 12 samples, Sukop & Cogger 1992)
- 0.903 (selected, USDA 1989)
- 1.34 (soil, 20–25°C, selected, Wauchope et al. 1992; Tomlin 1994; Hornsby et al. 1996)
- 1.98–2.32 (Montgomery 1993)
- 1.80, 2.01 (soil, estimated-class specific model, estimated-general model, Gramatica et al. 2000)

- 1.63, 1.64 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)
 1.55 (sediment: organic carbon OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: initial rate constant $k = 1.2 \times 10^{-3} \text{ h}^{-1}$ and a predicted rate constant $k = 2.9 \times 10^{-4} \text{ h}^{-1}$ from soil with $t_{1/2} = 2390 \text{ h}$ (Thomas 1982).

Photolysis: near surface direct sunlight photolysis rate constant $k = 0.003 \text{ d}^{-1}$ with $t_{1/2} \sim 200 \text{ d}$ (Schnoor & McAvoy 1981; Schnoor 1992);

$t_{1/2} \sim 2, 6, 12 \text{ h}$ for degradation in river, lake and seawater, respectively, from Greece which were irradiated with sunlight (Samanidou et al. 1988; quoted, Howard 1991)

Photodegradation ($\lambda > 290 \text{ nm}$) half-lives in aqueous carbofuran solutions: $t_{1/2} \sim 50 \text{ min}$ with TiO_2 (160 mg/L) + O_2 , $t_{1/2} \sim 40 \text{ min}$ with H_2O_2 ($6 \times 10^{-3} \text{ mg/L}$); $t_{1/2} \sim 30 \text{ min}$ with O_3 (10^{-3} mg/L) and $t_{1/2} \sim 65 \text{ h}$ in water/oil suspension. (Mansour et al. 1997)

Oxidation: photooxidation $t_{1/2} = 4.6 \text{ h}$, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k(\text{aq.}) = (620 \pm 60) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 3.7 and 21°C , with $t_{1/2} = 54 \text{ s}$ at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = 7 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in aqueous solutions at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992);

$k_{\text{OH}}(\text{aq.}) = 2.20 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in irradiated field water both in the laboratory and sunlit rice paddies with field dissipation $t_{1/2} = 16.3 \text{ h}$ (Mabury & Crosby 1996).

Hydrolysis: aqueous hydrolysis $t_{1/2} = 5.1 \text{ wk}$ at pH 7.0 and at 27°C and $t_{1/2} = 1.2 \text{ h}$ at pH 10 (Seiber et al. 1978; quoted, Howard 1991);

alkaline chemical hydrolysis rate constant $k = 6 \times 10^{-5} \text{ M}^{-1} \cdot \text{s}^{-1}$ with $t_{1/2} > 10,000 \text{ d}$ (Schnoor & McAvoy 1981; Schnoor 1992);

$t_{1/2} = 690, 8.2, \text{ and } 1.0 \text{ wk}$ in water at 25°C and pH 6.0, 7.0 and 8.0, respectively (Chapman & Cole 1982; quoted, Howard 1991);

hydrolysis rate constants: $k = (30.6 \pm 0.6) \text{ L min}^{-1} \text{ mol}^{-1}$ at 15°C , $k = (67.0 \pm 0.4) \text{ L/min} \cdot \text{mol}$ at 25°C and $k = (163 \pm 1.0) \text{ L min}^{-1} \text{ mol}^{-1}$ at 35°C (Trotter et al. 1991);

$t_{1/2} = 170 \text{ wk}$ at pH 4.5, $t_{1/2} = 690 \text{ wk}$ at pH 5–6, $t_{1/2} = 8.2 \text{ wk}$ at pH 7 and $t_{1/2} = 1 \text{ wk}$ at pH 8.0 at 25°C (Montgomery 1993);

$t_{1/2} > 1 \text{ yr}$ at pH 4, $t_{1/2} = 121 \text{ d}$ at pH 7, and $t_{1/2} = 31 \text{ d}$ at pH 9 at 22°C (Tomlin 1994);

rate constant $k = 5.0 \times 10^{-3} \text{ M}^{-1} \text{ h}^{-1}$ at 24°C ; $t_{1/2} = 737 \text{ h}$ at pH 7.0, $t_{1/2} = 93.7 \text{ h}$ at pH 8.0 and $t_{1/2} = 1.17 \text{ h}$ at pH 10.0 in aqueous solutions; $t_{1/2} = 630 \text{ d}$ at pH 7, $t_{1/2} = 133 \text{ d}$ at pH 8, and $t_{1/2} = 0.87 \text{ d}$ at pH 10 in aqueous solutions with montmorillonite suspensions (23.9 g/L); $t_{1/2} = 937 \text{ d}$ at pH 7, $t_{1/2} = 76.2 \text{ d}$ at pH 8, $t_{1/2} = 0.98 \text{ d}$ at pH 10 in aqueous solutions with beidellite suspensions (4.9 g/L); $t_{1/2} = 889 \text{ d}$ at pH 7, $t_{1/2} = 113 \text{ d}$ at pH 8, $t_{1/2} = 0.78 \text{ d}$ at pH 10 in aqueous solutions with illite suspensions (9.2 g/L); and $t_{1/2} = 753 \text{ d}$ at pH 7, $t_{1/2} = 80.6 \text{ d}$ at pH 8, $t_{1/2} = 0.91 \text{ d}$ at pH 10 in aqueous solutions with vermiculite suspensions (8.5 g/L) with an initial carbofuran concentration of $1.0 \times 10^{-4} \text{ M}$ (Wei et al. 2001).

Biodegradation: rate constants $k = 0.047 \text{ d}^{-1}$ from soil incubation studies and $k = 0.026 \text{ d}^{-1}$ in anaerobic system from flooded soil incubation studies both by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2} = 40 \text{ d}$ in 0 to 10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 4.6 \text{ h}$, based on estimated rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Atkinson 1987; quoted, Howard 1991).

Surface water: average $t_{1/2} = 57 \text{ h}$ in rice paddy water, but pH dependent, e.g., $t_{1/2} = 1.2 \text{ h}$ at pH 10 and $t_{1/2} = 864 \text{ h}$ at pH 7; $t_{1/2} = 48$ and 55 h for two farm ponds (Seiber et al. 1978);

$t_{1/2} = 2, 6, 12 \text{ h}$ for degradation in river, lake and seawater, respectively, from Greece which were irradiated with sunlight (Samanidou et al. 1988; quoted, Howard 1991);

measured rate constant $k = (620 \pm 60) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 3.7 and 21°C , with $t_{1/2} = 54 \text{ s}$ at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil: persistence of less than one month (Wauchope 1978);

$t_{1/2} = 11\text{--}13$ d at pH 6.5, and $t_{1/2} = 60\text{--}75$ d for a granular formulation (Ahmad et al. 1979; quoted, Montgomery 1993);

estimated first-order $t_{1/2} = 15$ d in soil from biodegradation rate constant $k = 0.047\text{ d}^{-1}$ by die-away test from soil incubation studies and $t_{1/2} = 26$ d from biodegradation rate constant $k = 0.026\text{ d}^{-1}$ in anaerobic system from flooded soil incubation studies by die-away test (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982);

$t_{1/2} = 1\text{--}2$ months (Hartley & Kidd 1987; quoted, Montgomery 1993);

$t_{1/2} = 40$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);

selected field $t_{1/2} = 50$ d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

soil $t_{1/2} = 81$ d (Pait et al. 1992);

$t_{1/2} = 30$ d for soil depth <5 cm, $t_{1/2} = 60$ d for soil depth $5\text{--}20$ cm and $t_{1/2} = 120$ d for soil depth >20 cm (Dowd et al. 1993);

$t_{1/2} = 60$ d in forest soil (Neary et al. 1993);

$t_{1/2} = 42.4$ d in loam and $t_{1/2} = 95.5$ d in sand (Behrendt & Brüggemann 1993);

$t_{1/2} = 30\text{--}60$ d in soil (Tomlin 1994)

Disappearance rate constants $k = (1.33\text{--}5.16) \times 10^{-2}\text{ h}^{-1}$ and $k = (0.36\text{--}1.13) \times 10^{-2}\text{ h}^{-1}$ in non-sterile soil suspensions; $k = (1.20\text{--}5.07) \times 10^{-2}\text{ h}^{-1}$ in sterile soil suspension at 30°C for 5 Spanish soils. Kinetic profiles in 3 consecutive steps assumed as sorption and fast and slow degradation. Disappearance $t_{1/2} = 24$ h at 30 and $t_{1/2} = 5$ h at 40°C for all 5 soil suspensions; $t_{1/2} = 48$ h at 30°C and $t_{1/2} = 12$ h at 40°C in Soil 3 (Mora et al. 1996)

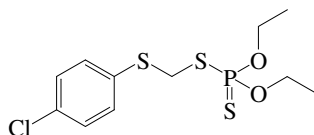
First order rate constants for photolytic decline in sandy soil: $k = 1.88 \times 10^{-3}\text{ h}^{-1}$ with $t_{1/2} = 370$ h irradiated in moisture-maintained soil, $k = 0.86 \times 10^{-3}\text{ h}^{-1}$ with $t_{1/2} = 800$ h, irradiated in air-dried soil, $k = 1.15 \times 10^{-3}\text{ h}^{-1}$ with $t_{1/2} = 600$ h in dark control moist sandy soil, but not degraded in the dark control air-dry system. The photolytic $k = 7.31 \times 10^{-4}\text{ h}^{-1}$ with $t_{1/2} = 950$ h in moist soil and the contribution of moisture to irradiated metabolism $k = 1.02 \times 10^{-3}\text{ h}^{-1}$ with $t_{1/2} = 680$ h (Graebing & Chib 2004)

Biota: biochemical $t_{1/2} = 40$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);

$t_{1/2} = 4$ d in wheat/barley (Behrendt & Brüggemann 1993);

average $t_{1/2} = 60$ d in the forest (USDA 1989; quoted, Neary et al. 1993)

18.1.1.11 Carbophenothion



Common Name: Carbophenothion

Synonym: Carbofenotion, Acarithion, Akarithion, Trithion, Garrathion, Nephocarb, Dagadip

Chemical Name: *S*-chlorophenylthio methyl *O,O*-diethyl phosphorothioate

Uses: insecticide/acaricide

CAS Registry No: 786-19-6

Molecular Formula: $C_{11}H_{16}ClO_2PS_3$

Molecular Weight: 342.866

Melting Point ($^{\circ}C$):

colorless liquid (Spencer 1982, Hartley & Kidd 1987, Tomlin 1994)

< 25 (Montgomery 1993)

Boiling Point ($^{\circ}C$):

82 (at 0.01 mmHg, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

Density (g/cm^3):

1.274 (Spencer 1982)

1.271 ($20^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993, Milne 1995)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

< 2.0 (Martin 1961; Spencer 1982)

0.34 (Gunther et al. 1968; Kenaga 1980b; Kenaga & Goring 1980)

< 40 (Verschuere 1983)

0.63 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

< 1.0 (room temp., Hartley & Kidd 1987, Worthing & Walker 1987)

0.61, 0.63, 0.73 (10, 20, $30^{\circ}C$, Montgomery 1993)

0.34 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

40, < 1 (Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.40 (Menn et al. 1964)

4.13×10^{-5} ($20^{\circ}C$, Eichler 1965)

4.07×10^{-5} ($20^{\circ}C$, Melnikov 1971)

4.0×10^{-5} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

1.07 (Spencer 1982)

7.73×10^{-5} ($20^{\circ}C$, GC-RT correlation, Kim et al. 1984, Kim 1985)

1.07×10^{-3} (Hartley & Kidd 1987; Montgomery 1993)

1.107×10^{-3} (selected, Augustijn-Beckers et al. 1994, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.046 ($20^{\circ}C$, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.53 (Callahan et al. 1979)

5.12 (shake flask-concn ratio-GC, Bowman & Sans 1983b)

- 5.66 (shake flask-GC, De Bruijn et al. 1989)
 5.50 (recommended, 1993)
 5.33 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 3.07, 3.63 (calculated-solubility, K_{OW} , Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.66 (Kenaga & Goring 1980)
 3.90 (calculated, Kenaga 1980b)
 4.98, 4.72, 3.92, 4.48 (Elkhorn sandy loam at pH 6.0, Hugo gravelly sandy loam at pH 5.5, Sweeney sandy clay loam at pH 6.3 and Tierra clay loam at pH 6.2, Rao & Davidson 1982)
 3.56 (calculated-MCI χ , Gerstl & Helling 1987)
 3.92–4.98 (Montgomery 1993)
 5.10, 4.66, 5.07, 4.76, 5.09, 4.69, 4.90 (mg/L, quoted, Augustijn-Beckers et al. 1994)
 4.70 (recommended, soil, Augustijn & Beckers 1994; Hornsby et al. 1996)
 4.66 (calculated-MCI χ , Sabljic et al. 1995)
 4.47, 4.08 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation: $t_{1/2} \geq 100$ d in soil (Verschuere 1983; quoted, Montgomery 1993).

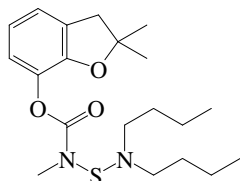
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Soil: $t_{1/2} \geq 100$ d (Verschuere 1983; quoted, Montgomery 1993);

field $t_{1/2} = 30$ d (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

18.1.1.12 Carbosulfan



Common Name: Carbosulfan

Synonym: Marshal, Adventage, Posse, FMC 35001

Chemical Name: 2,3-dihydro-2,2-dimethylbenzofuran-7-yl(dibutylaminothio) methylcarbamate

Uses: insecticide/acaricide/nematicide

CAS Registry No: 55285-14-8

Molecular Formula: $C_{20}H_{32}N_2O_3S$

Molecular Weight: 380.544

Melting Point ($^{\circ}C$):

viscous brown liquid (Hartley & Kidd 1987)

Boiling Point ($^{\circ}C$):

124–128 (Tomlin 1994; Milne 1995)

Density (g/cm^3):

1.056 ($20^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.30 (Hartley & Kidd 1987; Tomlin 1994)

0.03 (Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

0.041×10^{-3} (Hartley & Kidd 1987, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.30 (Tomlin 1994)

2.20 (Milne 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives. $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: hydrolyzed in aqueous media with $t_{1/2} < 1$ h in pure water at pH 4; $t_{1/2} = 22$ h at pH 6, $t_{1/2} = 7.6$ d at pH 7, $t_{1/2} = 14.2$ d at pH 8 and $t_{1/2} > 58.3$ d at pH 9 (Hartley & Kidd 1987; Tomlin 1994)

Biodegradation: in soil, rapidly degraded under both aerobic and anaerobic conditions with $t_{1/2} = 2-3$ d (Hartley & Kidd 1987).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air:

Surface water: hydrolyzed in aqueous media with half-lives at 25°C are, $t_{1/2} < 1$ h in pure water at pH 4; $t_{1/2} = 22$ h at pH 6, $t_{1/2} = 7.6$ d at pH 7, $t_{1/2} = 14.2$ d at pH 8 and $t_{1/2} > 58.3$ d at pH 9 (Hartley & Kidd 1987; Tomlin 1994)

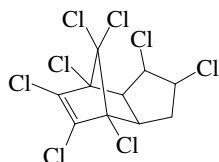
Ground water:

Sediment:

Soil: rapidly degraded under both aerobic and anaerobic conditions with $t_{1/2} = 2-3$ d (Hartley & Kidd 1987).

Biota:

18.1.1.13 Chlordane



Common Name: Chlordane

Synonym: A 1068, Aspon-chlordane, Belt, beta-chlordane, CD-68, Chlorindan, Chlor-Kill, Chlortox, Corodane, Cortilan-neu, Dichlorochlordene, Dowchlor, ENT 9932, ENT 25552, HCS 3260, Kypchlor, M 140, Octachlor, Octaterr, Orthoklor, Shell SD 5532, Synklor, Tat chlor 4, Topichlor, Toxichlor, Velsicol

Chemical Name: 1,2,4,5,6,7,8,8-octachloro-3a,4,7,7a-tetrahydro-4,7-methano-1*H*-indane; 1,2,4,5,6,7,8,8-octa-chloro-3a,4,7,7a-tetrahydro-4,7-methanoindane

Uses: nonsystemic insecticide with contact, stomach, and respiratory action and also used as fumigant.

CAS Registry No: 57-74-9 (nonstereospecific chlordane); 5103-71-9 (*cis*- or α -isomer); 5103-74-2 (*trans*- or β -isomer); 5564-34-7 (γ -isomer); 12789-03-6 (technical grade chlordane)

Molecular Formula: C₁₀H₆Cl₈

Molecular Weight: 409.779

Melting Point (°C):

107–108.8 (*cis*-isomer, Callahan et al. 1979; Howard 1991)

103–105 (*trans*-isomer, Callahan et al. 1979; Howard 1991)

106–107, 104–105 (*cis*-isomer, *trans*-isomer, Hartley & Kidd 1987; Tomlin 1994)

Boiling Point (°C):

175 (at 2 mmHg, Roark 1951; Callahan et al. 1979; Howard 1991; Montgomery 1993)

262, 363, 365 (estimated from structure, Tucker et al. 1983)

175 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Density (g/cm³ at 20°C):

1.59–1.63 (25°C, Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

1.59–1.63 (Montgomery 1993)

Molar Volume (cm³/mol):

340.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, p*K*_a:

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.22, 80.26, 82.92 (mixture, α -chlordane, β -chlordane, Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.033 (*cis*-isomer, DSC method, Plato 1972)

16.45 (*trans*-isomer, DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.4 (Passivirta et al. 1999)

Fugacity Ratio at 25°C, F:

0.162 (assuming $\Delta S_{fus} = 56$ J/mol K, Mackay et al. 1986)

0.140 (20°C, assuming $\Delta S_{fus} = 56$ J/mol K, Suntio et al. 1988)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):

1.850 (generator column-GC/ECD, Weil et al. 1974)

0.056 (shake flask-LSC, Sanborn et al. 1976)

0.056 (Martin & Worthing 1977)

0.10 (Hartley & Kidd 1987; Worthing & Walker 1987, 1991)

0.56 (Agency for Toxic Substances and Disease Registry 1988; quoted, Burmaster et al. 1991)

0.05 (20°C, selected, Suntio et al. 1988)

0.032; 0.009–0.056 (shake flask-LSC; lit. range, Johnson-Logan et al. 1992)

1.83 (selected, Yalkowsky & Banerjee 1992)

0.056 (Montgomery 1993)

0.06 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

- 0.127 (calculated-group contribution fragmentation method, Kühne et al. 1995)
 0.10 (Tomlin 1994; Milne 1995)
 0.061, 0.002 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
 $\log [S_L/(\text{mol/L})] = -0.880 - 1124/(T/K)$ (liquid, *cis*-isomer, Passivirta et al. 1999)
 $\log [S_L/(\text{mol/L})] = -0.880 - 1118/(T/K)$ (liquid, *trans*-isomer, Passivirta et al. 1999)
 0.451, 0.402 (*cis*-chlordane, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
 0.451, 0.615 (*trans*-chlordane, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

- 0.0013 (Martin 1972, Spencer 1973, 1982)
 0.0013 (SRI International 1980; Tucker et al. 1983)
 0.00227, 1.6×10^{-5} , 1.3×10^{-5} (estimated-bp, Tucker et al. 1983)
 2.9×10^{-3} , 3.86×10^{-3} (*cis*-, *trans*-chlordane, 20°C, supercooled liquid P_L , Bidleman et al. 1986)
 0.0013 (Hartley & Kidd 1987)
 0.0011 (20°C, selected, Suntio et al. 1988)
 0.0613, 0.00133 (technical, refined, Worthing & Walker 1987)
 0.00293, 0.00040 (*cis*-isomer, GC-RT correlation, supercooled liquid P_L , solid crystal P_S , Foreman & Bidleman 1987)
 0.00387, 0.00052 (*trans*-isomer, GC-RT correlation, supercooled liquid P_L , solid crystal P_S , Foreman & Bidleman 1987)
 0.0013 (Agency for Toxic Substances and Disease Registry 1988)
 0.027, 0.31, 2.40, 14.0, 69.0 (25, 50, 70, 100, 125°C, chlordane mixture, gas saturation-GC, Rordorf 1989)
 $\log (P_L/\text{Pa}) = 11.968 - 4033.7/(T/K)$; measured range 70.4–115°C (chlordane mixture, liquid, gas saturation-GC, Rordorf 1989)
 0.0080, 0.011, 0.98, 6.70, 36 (α -chlordane, 25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
 $\log (P_L/\text{Pa}) = 12.435 - 4332.5/(T/K)$; measured range 50.1–135°C (α -chlordane, liquid, gas saturation-GC, Rordorf 1989)
 0.013, 0.16, 1.40, 9.30, 48 (β -chlordane, 25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
 $\log (P_S/\text{Pa}) = 12.318 - 4235.5/(T/K)$; measured range 50/1–135°C (β -chlordane, liquid, gas saturation-GC, Rordorf 1989)
 $\log (P_L/\text{Pa}) = 13.396 - 4803.6/(T/K)$; measured range 49.5–140°C (gas saturation-GC, Rordorf 1989)
 4.5×10^{-3} , 5.1×10^{-3} , 4.8×10^{-3} (*cis*-chlordane, GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990)
 6.3×10^{-3} , 6.9×10^{-3} , 6.7×10^{-3} (*trans*-chlordane, GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990)
 $\log (P_L/\text{Pa}) = 12.04 - 4284/(T/K)$ (*cis*-chlordane, supercooled liquid P_L , GC-RT correlation, Hinckley et al. 1990; quoted, Passivirta et al. 1999)
 $\log (P_L/\text{Pa}) = 11.95 - 4216/(T/K)$ (*trans*-chlordane, supercooled liquid P_L , GC-RT correlation, Hinckley et al. 1990)
 0.0013 (refined grade, Worthing & Hance 1991; Tomlin 1994)
 0.0610 (technical grade, Worthing & Hance 1991)
 0.00269, 0.00813 (*cis*-chlordane, supercooled liquid P_L at 20°C, 30°C, calculated from Hinckley et al. 1990; Cotham & Bidleman 1992)
 0.000133 (20°C, Montgomery 1993)
 0.00133 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 4.59×10^{-4} (quoted as mean of *cis* and *trans* forms from Howard 1991, Mortimer & Connell 1995)
 4.68×10^{-3} , 4.15×10^{-3} , 6.57×10^{-4} (*cis*-chlordane, supercooled liquid P_L : calculated, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 6.58×10^{-3} , 5.84×10^{-3} , 9.66×10^{-4} (*trans*-chlordane, supercooled liquid P_L : calculated, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 14.99 - 5407/(T/K)$ (*cis*-chlordane, solid, Passivirta et al. 1999)
 $\log (P_S/\text{Pa}) = 14.91 - 5333/(T/K)$ (*trans*-chlordane, solid, Passivirta et al. 1999)
 0.080, 0.0073 (*cis*-chlordane, supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

0.013, 0.010 (*trans*-chlordane, supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

$\log(P_L/\text{Pa}) = -4238/(T/K) + 12.32$ (*cis*-chlordane, supercooled liquid P_L : linear regression, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

2.92–9.5 (Callahan et al. 1979)
 4.92 (gas stripping-GC, Warner et al. 1980)
 112 (batch stripping, average of *cis*- and *trans*- isomers, Atlas et al. 1982)
 87.7, 134 (exptl.: α -chlordane, γ -chlordane, Atlas et al. 1982;)
 9.12 (Mabey et al. 1982)
 3.44 (estimated-group method of Hine & Mookerjee 1975, Tucker et al. 1983)
 9.64 (calculated-P/C, Mackay et al. 1986)
 0.248 (calculated-P/C, Jury et al. 1990)
 4.86 (gas stripping-GC, Warner et al. 1987)
 9.02 (20°C , calculated-P/C, Suntio et al. 1988; quoted, Cotham & Bidleman 1991; Majewski & Capel 1995)
 9.66 (Ryan et al. 1988)
 0.97 (Agency for Toxic Substances and Disease Registry 1988; quoted, Burmaster et al. 1991)
 4.91 (technical chlordane, Howard 1991)
 8.37 (23°C , γ -chlordane, wetted-wall column-GC/ECD, Fendinger et al. 1989)
 5.66, 5.91 (22 – 24°C , γ -chlordane, fog chamber-GC/ECD, Fendinger et al. 1989)
 0.87 (0°C , selected, Cotham & Bidleman 1991)
 7.12 (calculated-bond contribution method, Meylan & Howard 1991)
 9.02 (20°C), 140, 570 (23°C), 9.64 (25°C) (*trans*-chlordane, quoted, Iwata et al. 1993)
 9.02 (20°C), 89, 420 (23°C), 9.64, 11.2 (25°C) (*cis*-chlordane, quoted, Iwata et al. 1993)
 8.42 (γ -chlorane, wetted-wall column-concn ratio-GC/ECD, Fendinger et al. 1989)
 5.45 (γ -chlorane, fog chamber-concn ratio-GC/ECD, Fendinger et al. 1989)
 8.11 (calculated-bond contribution, Meylan et al. 1991)
 $\log[H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 12.92 - 3160/(T/K)$ (*cis*-chlordane, Passivirta et al. 1999)
 $\log[H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 12.84 - 3098/(T/K)$ (*trans*-chlordane, Passivirta et al. 1999)
 6.0, 5.7 (*cis*-chlordane, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
 6.0, 6.8 (*trans*-chlordane, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.78 (shake flask-LSC, Sanborn et al. 1976)
 6.00 (Veith et al. 1979, 1980; Veith & Kosian 1983)
 5.16 (calculated, Kenaga 1980a, b)
 3.32 (Rao & Davidson 1980)
 5.89 (selected, Dao et al. 1983)
 5.54 (CLOGP 1986; Thor 1989; Howard 1991)
 2.78, 5.48 (Schnoor et al. 1987)
 5.9, 6.1 (*cis*-, *trans*-chlordane, Kawano et al. 1988)
 6.21 (estimated by QSAR & SPARC, Kollig 1993)
 5.16; 2.78, 3.32; 5.08, 6.00 (quoted lit. exptl. values; Sangster 1993)
 6.00 (Montgomery 1993; Devillers et al. 1996)
 5.08 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
 5.80 (LOGSTAR or CLOGP, Sabljic et al. 1995)
 5.66, 5.62, 5.44, 6.10, 6.22 (α -, β -, γ -, *cis*-, *trans*-chlordane, shake flask/slow stirring-GC, Simpson et al. 1995)
 5.08, 5.80, 4.75 (RP-HPLC-RT correlation, ClogP, calculated-S, Finizio et al. 1997)
 6.10, 6.20 (*cis*-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
 6.23, 6.27 (*trans*-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:

8.70 (*cis*-chlordane, calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
 8.50 (*trans*-chlordane, calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)

9.027*, 8.916 (*cis*-chlordane, gas saturation-GC/MS interpolated, measured range 5–25°C, Shoeib & Harner 2002)
 $\log K_{OA} = -8.29 + 5217/(T/K)$, temp range 5–25°C (*cis*-chlordane, gas saturation-GC, Shoeib & Harner 2002)
 8.967*, 8.872 (*trans*-chlordane, gas saturation-GC/MS, interpolated, measured range 5–25°C, Shoeib & Harner 2002)
 $\log K_{OA} = -8.03 + 5036/(T/K)$, temp range 5–25°C (*trans*-chlordane, gas saturation-GC, Shoeib & Harner 2002)
 8.3887*, 8.387 (oxychlordane, gas saturation-GC/MS, interpolated, measured range 5–25°C, Shoeib & Harner 2002)
 $\log K_{OA} = -5.636 + 4179/(T/K)$, temp range: 5–25°C (oxychlordane, gas saturation-GC, Shoeib & Harner 2002)
 8.91, 8.85 (*cis*-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
 8.86, 8.85 (*trans*-chlordane, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF at 25°C or as indicated:

3.51–3.92; 3.60–3.78; 3.28–3.36; 4.10–4.27 (wet wt. basis 96-h test, eastern oysters; pink shrimp; grass shrimp; pin fish, Parrish et al. 1976)
 4.69 (*Oedogonium cardiacum*, Sanborn et al. 1976)
 3.66 (spot fish, 24-h flow system, *trans*-chlordane, Schimmel et al. 1976)
 3.57–4.23 (96 h exposures of *trans*-chlordane to whole marine fish, Schimmel et al. 1976)
 4.11–4.34 (186-d chronic exposures, *trans*-chlordane to sheephead minnow, Parrish et al. 1978)
 3.85–4.46 (exposures *trans*-chlordane to 28-d old second generation sheephead minnow, Parrish et al. 1978)
 4.58 (fathead minnows, 32-d exposure, Veith et al. 1979, 1980; Veith & Kosian 1983)
 4.01 (green algae, Glooschenko et al. 1979)
 4.06, 3.92 (fish: flowing water, static ecosystem, Kenaga 1980a, b; Kenaga & Goring 1980)
 3.50 (calculated-S, Kenaga 1980a)
 –0.523 (average beef fat diet, Kenaga 1980b)
 2.08, 4.32 (estimated-S, K_{OW} , Bysshe 1982)
 3.68, 3.64 (α -, γ -chlordane, clam fat, 60-d expt., Hartley & Johnson 1983)
 4.06–4.58 (fish, Bysshe 1987)
 5.04–5.88 (earthworms, Gish & Hughes 1982;)
 3.57–4.20 mean 4.20; 3.36–4.34 mean 4.34 (α -chlordane, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
 33.30–4.18 mean 4.18; 3.26–4.30 mean 4.30 (γ -chlordane, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
 4.23, 4.26 (α -, γ -chlordane, rainbow trout, steady-state BCF-concentration ratio., Oliver & Niimi 1985)
 4.45, 4.20 (α -, γ -chlordane, rainbow trout, kinetic state BCF-ratio of rate const., Oliver & Niimi 1985)
 6.15, 4.88 (α -, γ -chlordane, rainbow trout, Lake Ontario field BCF., Oliver & Niimi 1985)
 4.58; 4.33, 4.40 (measured for fathead minnow; calculated- K_{OW} for sheepshead minnows, Zaroogian et al. 1985)
 4.58; 3.90, 3.92 (measured for fathead minnow; calculated- K_{OW} for pinfish, Zaroogian et al. 1985)
 4.58; 4.33, 4.40 (measured for fathead minnow; calculated- K_{OW} for oyster, Zaroogian et al. 1985)
 3.70 (oyster, Hawker & Connell 1986)
 6.73, 6.99 (total chlordanes, zooplankton, thick-billed murre, Kawano et al. 1986)
 3.78, 4.30 (juvenile and adult sheepshead minnow, 28–129 d exposure, Parrish et al. 1978)
 6.0–7.0 (zooplankton and Chum salmon, Kawano et al. 1988)
 5.57 (Markwell et al. 1989)
 3.52, 2.60 (large mouth bass, clams, 106–127 d exposure, NRC 1974)
 3.86 (eastern oyster, 10-d exposure, NRC 1974)
 3.74 (white sucker and redbreast, Roberts et al. 1977)
 2.03, 2.51, 3.0 (frogs, bluegills, goldfish, Verschuere 1983)
 6.73, 7.89, 6.99 (total chlordane: zooplankton, Dall's porpoise, thick-billed murre, Kawano et al. 1986)
 4.58 (estimated-S and K_{OW} , Isnard & Lambert 1988)
 –2.13 (beef biotransfer factor $\log B_b$, correlated- K_{OW} from Kenaga 1980, Travis & Arms 1988)
 –3.43 (milk biotransfer factor $\log B_m$, correlated- K_{OW} from Dorough & Hemken 1973, Travis & Arms 1988)
 –1.81 (vegetation, correlated- K_{OW} from Dorough & Pass 1973; Tafuri et al. 1977; Travis & Arms 1988)
 3.03 (*Hydrilla*, Hinman & Klaine 1992)
 4.01, 3.50; 2.80 (estimated: fish-based, duckweed-based, Hinman & Klaine 1992)

- 3.117, 3.098 (*cis*-, *trans*-chlordane, goldfish, Park & Erstfeld 1997)
 >4.58, >5.56 (fathead minnow, uptake 32-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.38, 5.20 (*Daphnia*: wet wt basis, lipid wt basis, α -chlordane, Geyer et al. 2000)
 4.45, 5.58 (fathead minnow: wet wt basis, lipid wt basis, α -chlordane, Geyer et al. 2000)
 5.26, 6.31 (Chum salmon, 91% lipid: wet wt basis, lipid wt basis, α -chlordane, Geyer et al. 2000)
 3.04, 3.74 (algae: wet wt basis, dry wt basis, γ -chlordane, Geyer et al. 2000)
 3.04, 3.74 (*Daphnia*: wet wt basis, lipid wt basis, γ -chlordane, Geyer et al. 2000)
 4.21, 5.35 (fathead minnow: wet wt basis, lipid wt basis, γ -chlordane, Geyer et al. 2000)
 5.04, 6.18 (chum salmon, 9.2% lipid: wet wt basis, lipid wt basis, γ -chlordane, Geyer et al. 2000)
 3.68; 3.67 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 4.33 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980a, b)
 1.58 (screening model calculations, Jury et al. 1987b)
 4.64, 4.09 (calculated- K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
 5.50, 5.60 (α -chlordane: field sediment trap material, calculated- K_{OW} , Oliver & Charlton 1984)
 5.40, 5.60 (γ -chlordane, field sediment trap material, calculated- K_{OW} , Oliver & Charlton 1984)
 4.58 (soil, screening model calculations, Jury et al. 1987b, 1990)
 4.39, 4.19 (calculated- K_{OW} and solubility, Howard 1991)
 4.77, 4.94 (α -chlordane: quoted, calculated-MCI χ , Meylan et al. 1992)
 5.45, 4.40–4.86 (Aldrich humic acid, soil, Johnson-Logan et al. 1992)
 5.90 (estimated by QSAR and SPARC, Kollig 1993)
 4.85–5.57 (Montgomery 1993)
 4.30 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 5.15 (soil, calculated-MCI χ , Sabljic et al. 1995)
 4.33, 4.42 (log K_P *cis*-, *trans*-chlordane, Park & Erstfeld 1997)
 5.15; 5.03 (soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: the volatilization $t_{1/2} \sim 7.3$ and 7.9 h for γ - and α -chlordane, respectively, from a model river 1 m deep flowing 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982, Howard 1991); and $t_{1/2} \sim 18$ –26, 3.6–5.2, 14.4–20.6 d from a model environmental pond (2 m deep), river (3 m deep) and lake (5 m deep), respectively, (Lyman et al. 1982; Howard 1991); $t_{1/2} \sim 43$ h from a model river 1-m deep flowing 1 m/s based, on the Henry's law constant of technical chlordane (Lyman et al. 1982, Howard 1991); measured rate constant $k = 0.3 \text{ d}^{-1}$ (Glottfelty et al. 1984; Glottfelty et al. 1989); calculated rate constant $k = 1.0 \text{ d}^{-1}$ (Glottfelty et al. 1989).

Photolysis:

Oxidation: $t_{1/2} = 5.2$ –51.7 h in air, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);

$k_{OH}(aq.) = 8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 3.3 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) < 0.04$ – $> 300 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 6.2–6.4 and $19 \pm 2^\circ\text{C}$, with 2 min $> t_{1/2} > 10$ d at pH 7 (Yao & Haag 1991).

$k(aq.) = (6$ – $170) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (photo-Fenton with reference to acetophenone) with hydroxyl radicals in aqueous solutions at pH 3.3 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992).

Hydrolysis: $t_{1/2} > 4$ yr (Callahan et al. 1979);

first-order $t_{1/2} > 197000$ yr, based on base rate constant $k = 4.3 \times 10^{-3} \text{ M}^{-1} \text{ h}^{-1}$ at pH 7.0 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991).

$t_{1/2} = 7.2 \times 10^7$ d at pH 7 and $t_{1/2} = 670$ d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 5712$ –33264 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991);

$k = 0.0024 \text{ d}^{-1}$ with a biodegradation $t_{1/2} = 1214$ d under field conditions (Rao & Davidson 1980);

aqueous anaerobic $t_{1/2}$ = 24–168 h, based on soil and freshwater mud grab sample data for aldrin, dieldrin, endrin and heptachlor epoxide (Maule et al. 1987; quoted, Howard et al. 1991);

$t_{1/2}$ = 100 d in soil (Jury et al. 1990)

$t_{1/2}$ (aerobic) = 240 d, $t_{1/2}$ (anaerobic) = 1 d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

k_1 = 340 d⁻¹ (α -, γ -chlordane, rainbow trout, Oliver & Niimi 1985)

k_2 = 1.92 d⁻¹ (α -chlordane, rainbow trout, Oliver & Niimi 1985)

k_2 = 0.021 d⁻¹ (γ -chlordane, rainbow trout, Oliver & Niimi 1985)

k_2 = 0.0974 d⁻¹ (γ -chlordane from rats, Dearth & Hites 1991)

k_2 = 0.1170 d⁻¹ (α -chlordane from rats, Dearth & Hites 1991)

Half-Lives in the Environment:

Air: $t_{1/2}$ = 5.2–51.7 h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991; Mortimer & Connell 1995);

atmospheric transformation lifetime was estimated to be >1 d (Kelly et al. 1994);

$t_{1/2}$ = in the Great Lake's atmosphere. 16 ± 5.7 yr at Eagle Harbor, 10 ± 2.3 yr at Sleeping Bear Dunes and 6.8 ± 0.8 yr at Sturgeon Point (Buehler et al. 2004).

Surface water: $t_{1/2}$ = 5712–33264 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991; Mortimer & Connell 1995) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991; Mortimer & Connell 1995)

measured rate constant $k < 0.04$ – > 300 M⁻¹ s⁻¹ for direct reaction with ozone in water at pH 6.2–6.4 and $19 \pm 2^\circ\text{C}$, with a half-life, 2 min $> t_{1/2} > 10$ d at pH 7 (Yao & Haag 1991)

Biodegradation $t_{1/2}$ (aerobic) = 240 d, $t_{1/2}$ (anaerobic) = 1 d; hydrolysis $t_{1/2}$ = 7.2×10^7 d at pH 7 and $t_{1/2}$ = 670 d at pH 12 in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2}$ = 11424–66528 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2}$ = 20000 h (quoted mean value from Howard et al. 1991, Mortimer & Connell 1995).

Soil: $t_{1/2}$ ~ 6 yr persistence in soil (Nash & Woolson 1967);

estimated persistence of 5 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

$t_{1/2}$ = 5712–33264 h, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenberg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991);

rate constant $k = 0.0024$ d⁻¹ with a biodegradation $t_{1/2}$ = 1214 d under field conditions (Rao & Davidson 1980); field $t_{1/2}$ = 9 d in fallow soil (Glotfelty 1981; quoted, Nash 1983);

persistent with $t_{1/2} > 100$ d (Willis & McDowell 1982);

microagroecosystem $t_{1/2}$ = 10–13 d in moist fallow soil (Nash 1983);

$t_{1/2}$ ~ 1 yr in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);

$t_{1/2}$ = 3500 d from screening model calculations (Jury et al. 1987b);

$t_{1/2} > 50$ d when subject to plant uptake via volatilization (Ryan et al. 1988);

degradation $t_{1/2}$ = 100 d in soil (Jury et al. 1990);

mean $t_{1/2}$ = 3.3 yr under field conditions (Howard 1991);

estimated field $t_{1/2}$ ~ 350 d (Augustijn-Beckers et al. 1994; Tomlin 1994; Hornsby et al. 1996);

$t_{1/2}$ = 1–20 yr in soil, $t_{1/2}$ = 5015 yr in the environment (Geyer et al. 2000)

$t_{1/2}$ = 240 and 7.2 yr for control and sludge-amended Luddington soils, respectively, for *cis*-chlordane and $t_{1/2}$ = 12.9 and 9.2 yr for control and sludge-amended Luddington soils, respectively, for *trans*-chlordane (Meijer et al. 2001).

Biota: $t_{1/2}$ = 1 d for daphnids and $t_{1/2}$ = 60 d for fish (Callahan et al. 1979; quoted, Wilcock et al. 1993);

elimination $t_{1/2}$ ~ 60 d for α -chlordane and $t_{1/2}$ = 33 d for γ -chlordane in rainbow trout (Oliver & Niimi 1985);

biochemical $t_{1/2}$ = 3500 d from screening model calculations (Jury et al. 1987b);

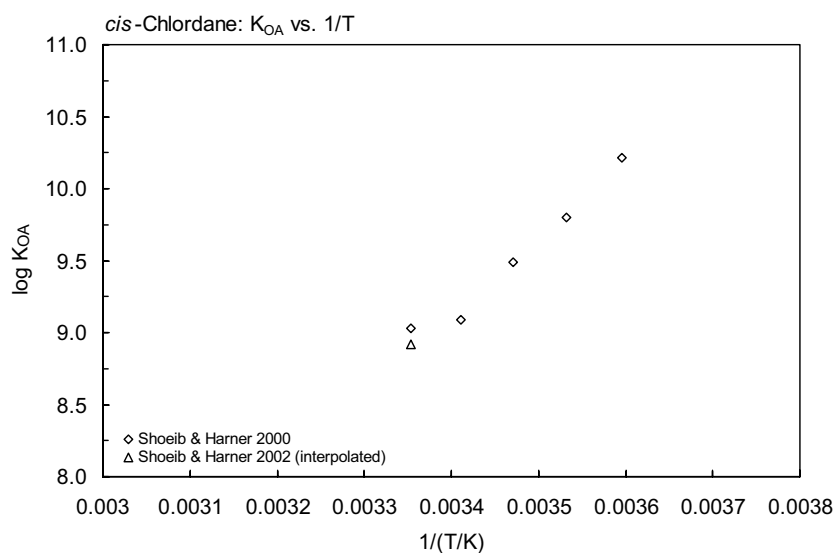
depuration $t_{1/2}$ = 7.1 d for γ -chlordane, and $t_{1/2}$ = 5.9 d for α -chlordane (rats, Dearth & Hites 1991);

$t_{1/2}$ = 12 d for elimination from *T. liliana* (Wilcock et al. 1993).

TABLE 18.1.1.13.1

Reported octanol-air partition coefficients of chlordane at various temperatures

<i>cis</i> -chlordane		<i>trans</i> -chlordane		oxychlordane	
Shoeib & Harner 2002		Shoeib & Harner 2002		Shoeib & Harner 2002	
generator column-GC/MS		generator column-GC/MS		generator column-GC/MS	
t/°C	log K _{OA}	t/°C	log K _{OA}	t/°C	log K _{OA}
5	10.2162	5	10.1292	5	9.4204
10	9.7963	10	9.7568	10	9.0757
15	9.4916	15	9.4375	15	8.9090
20	9.0896	20	9.0500	20	8.6184
25	9.0271	25	8.9671	25	8.3887
25	8.916	25	8.872	25	8.387
log K _{OA} = A + B/(T/K)		log K _{OA} = A + B/(T/K)		log K _{OA} = A + B/(T/K)	
A	-8.289	A	-8.027	A	-5.636
B	5127	B	5036	B	4179
enthalpy of phase change ΔH _{OA} /(kJ mol ⁻¹) = 97.5		enthalpy of phase change ΔH _{OA} /(kJ mol ⁻¹) = 96.4		enthalpy of phase change ΔH _{OA} /(kJ mol ⁻¹) = 80.0	

FIGURE 18.1.1.13.1A Logarithm of K_{OA} versus reciprocal temperature for *cis*-chlordane.

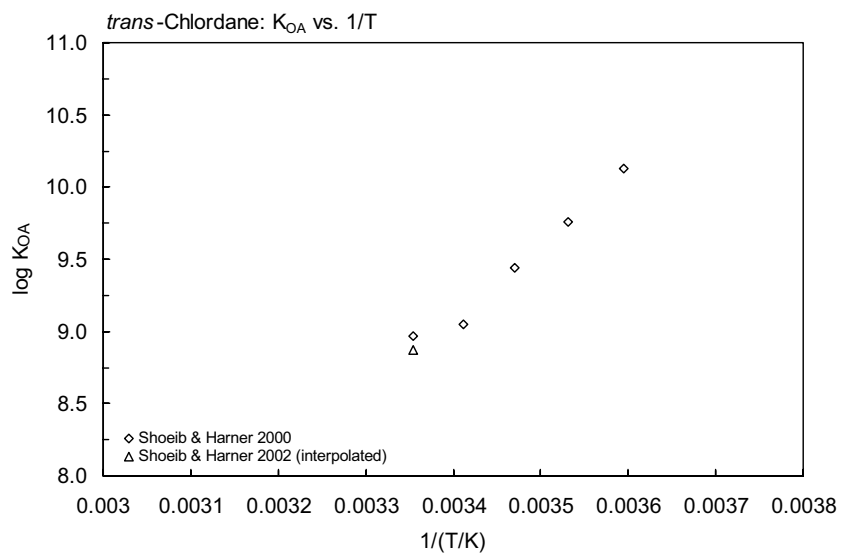


FIGURE 18.1.1.13.1B Logarithm of K_{OA} versus reciprocal temperature for *trans*-chlordane.

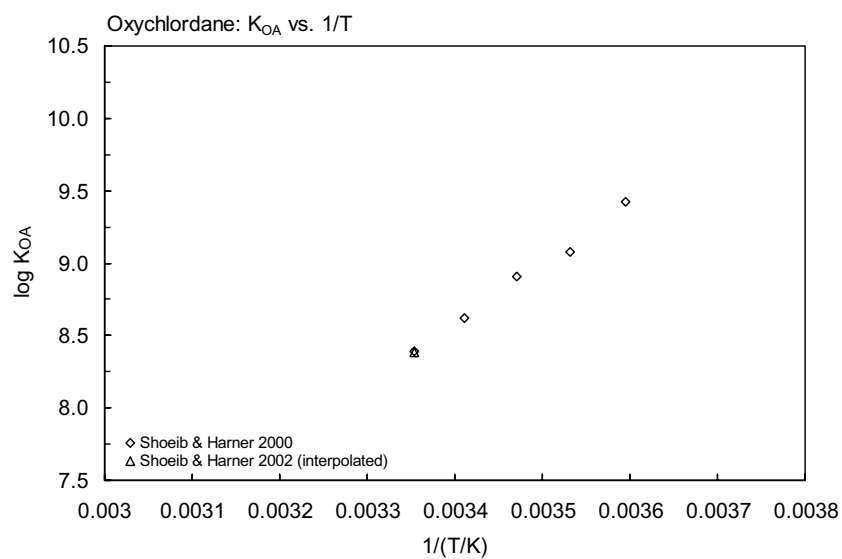
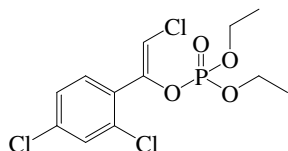


FIGURE 18.1.1.13.1C Logarithm of K_{OA} versus reciprocal temperature for oxychlordane.

18.1.1.14 Chlorfenvinphos



Common Name: Chlorfenvinphos

Synonym: Apachlor, Birlane, Clofenvenfos, GC 4092, Sapecron, SD 7859

Chemical Name: 2-chloro-1-(2,4-dichlorophenyl)vinyl diethyl phosphate; 2-chloro-1-(2,4-dichlorophenyl)ethenyl diethyl phosphate

Uses: soil application of insecticide to control root flies, root worms and other soil insects in vegetables; foliar application to control Colorado beetles on potatoes; scale insects and mite eggs on citrus fruit; stem borers and leafhoppers on rice, maize and sugar cane; and white flies on cotton; aside from control of mosquito larvae, it is also used as acaricide and animal ectoparasiticide.

CAS Registry No: 470-90-6 (*Z*)-isomer, 18708-87-7 (*E*)-isomer or *cis*-chlorfenvinphos, 18708-86-6 *trans*-chlorfenvinphos

Molecular Formula: $C_{12}H_{14}Cl_3O_4P$

Molecular Weight: 359.569

Melting Point ($^{\circ}C$):

-19 (Lide 2003)

Boiling Point ($^{\circ}C$):

167–170 (at 0.5 mmHg, Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.36 (Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm^3/mol):

321.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

96.34 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

145 ($20^{\circ}C$, Melnikov 1971)

145 (Martin & Worthing 1977; Milne 1995)

145 ($23^{\circ}C$, Khan 1980)

146 ($20^{\circ}C$, Briggs 1981)

124 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

145 ($23^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987, 1991; Tomlin 1994)

130 ($20^{\circ}C$, selected, Suntio et al. 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00053 ($20^{\circ}C$, Khan 1980)

2.7×10^{-5} (Verschuere 1983)

0.0010 (Hartley & Kidd 1987; Tomlin 1994)

0.00010 ($20^{\circ}C$, selected, Suntio et al. 1988)

8.20×10^{-4} , 1.70×10^{-2} , 0.22, 2.0, 14.0 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 13.794 - 5032.8/(T/K)$; measured range 36.9 – $129^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

0.00053 ($20^{\circ}C$, Worthing & Hance 1991)

8.91×10^{-4} ; 1.35×10^{-3} , 0.0038 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 0.00028 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.00029 (calculated-P/C, this work)
- 0.324 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
- $\log K_{\text{AW}} = 0.173 - 1187/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 3.23 (shake flask-UV, Lord et al. 1980)
- 3.10 (20°C, shake flask-GC, Briggs 1981)
- 3.81 (shake flask-GC, Bowman & Sans 1983)
- 3.84 (shake flask, Eadsforth & Moser 1983)
- 3.79 (HPLC-RT correlation method, Eadsforth & Moser 1983)
- 3.56 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 3.81 (recommended, Sangster 1993)
- 3.85, 4.22 (*Z* isomer, *E* isomer, Tomlin 1994)
- 3.10 (recommended, Hansch et al. 1995)
- 3.56 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.57 (calculated-S, Kenaga 1980)
- 2.30 (earthworms, Lord et al. 1980; quoted, Connell & Markwell 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.45 (calculated-S, Kenaga 1980)
- 2.47 (soil, sorption isotherm, converted from reported $\log K_{\text{OM}}$ of 2.23, Briggs 1981)
- 2.77 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 2.47 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 2.47; 2.42, 3.04 (soil, *cis*-chlorfenvinphos, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 2.47; 2.40, 3.11 (soil, *trans*-chlorfenvinphos, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

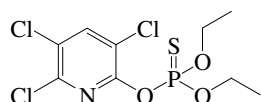
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: at 38°C : $t_{1/2} > 700$ h at pH 1.1 and $t_{1/2} > 400$ h at pH 9.1; $t_{1/2} = 1.28$ h at pH 13 and 20°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} < 1.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 1.0$ wk in nonsterile organic soil (Miles et al. 1979).

18.1.1.15 Chlorpyrifos



Common Name: Chlorpyrifos

Synonym: Brodan, Chlorpyrifos-ethyl, Detmol UA, Dowco 179, Dursban, ENT 27311, Eradex, Killmaster, Lorsban, NA 2783, OMS 971, Pyrinex

Chemical Name: *O,O*-diethyl *O*-3,5,6-trichloro-2-pyridyl phosphorothioate; *O,O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) phosphorothioate

Uses: insecticide used to control insects on a wide variety of crops including fruits, vegetables, ornamentals and trees.

CAS Registry No: 2921-88-2

Molecular Formula: $C_9H_{11}Cl_3NO_3PS$

Molecular Weight: 350.586

Melting Point ($^{\circ}C$):

42 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

298.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.94 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.681 (mp at $42^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.40, 0.47 (23, $25^{\circ}C$, Brust 1966)

2.0 (Spencer 1973; Windholz 1983; Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Milne 1995)

1.12 (shake flask-GC, Felsot & Dahm 1979)

0.70, 0.73 (19, $20^{\circ}C$, shake flask-GC, Bowman & Sans 1979)

0.30 ($23^{\circ}C$, Kenaga 1980a, b)

0.30 (Dow Chemical Data, Kenaga & Goring 1980)

2.00 ($35^{\circ}C$, Khan 1980)

2.00 (20 – $25^{\circ}C$, Willis & McDowell 1982)

0.40 (Verschueren 1983)

0.73 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

1.07, 0.42 (generator column, RP-HPLC-RT correlation, Swann et al. 1983)

0.30 (Kanazawa 1989)

0.40 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.93 (Racke 1993)

0.73, 1.30 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

1.40 (Tomlin 1994)

1.18 (quoted lit., Armbrust 2000)

1.61, 1.94 (supercooled liquid S_L : literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ at $25^{\circ}C$ or as indicated):

0.00145 ($20^{\circ}C$, Eichler 1965; Wolfdietrich 1965)

0.0025 (Brust 1966; Neely & Blau 1977)

0.0037 (Hamaker 1975)

0.00253 (Melnikov 1971)

0.0104 ($30^{\circ}C$, NIEHS 1975)

0.0012 ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

0.00088 (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
 0.00052 (20°C, GC-RT with mp correction, Kim et al. 1984; Kim 1985)
 0.0025 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)
 0.0015 (20°C, selected, Suntio et al. 1988)
 0.0067 (supercooled liquid P_L , GC-RT correlation method, Hinckley et al. 1990)
 0.0022; 0.0040 (liquid P_L , GC-RT correlation; quoted lit., Donovan 1996)
 0.0023 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.0022 (gradient GC method, Tsuzuki 2000)
 2.18×10^{-3} ; 1.86×10^{-3} , 0.00407 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)
 0.0038, 0.0031 (supercooled liquid P_L : literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

1.0 (Mackay 1985)
 1.75 (20°C, calculated-P/C, Suntio et al. 1988)
 0.418 (calculated-P/C, Fendinger & Glotfelty 1990; Fendinger et al. 1990)
 7.902 (calculated-P/C, Howard 1991)
 4.06×10^{-3} (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
 0.421 (23°C, quoted, Schomburg et al. 1991)
 0.421 (calculated-P/C, Montgomery 1993)
 0.317, 0.492 (20°C, distilled water, salt water 33.3l, wetted wall column-GC, Rice et al. 1997b)
 $\log K_{AW} = -1187.0/(T/K) + 0.173$; temp range 8.3–43.5°C, (distilled water, wetted-wall column-GC, Rice et al. 1997b)
 $\log K_{AW} = -916.0/(T/K) - 0.674$; temp range 8.3–43.5°C, (salt water solution, 33.3l NaCl, wetted-wall column-GC, Rice et al. 1997b)
 0.366, 0.366; 0.390 (20°C, microlayer, subsurface natural water of salinity 17l and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
 0.341, 0.390; 0.390 (20°C, microlayer, subsurface natural water of salinity 16l and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
 0.317, 0.341; 0.366 (20°C, microlayer, subsurface natural water of salinity 12l, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
 0.366, 0.414; 487 (20°C, microlayer, subsurface water of salinity 32l, TOC 2.2–46 ppm, ocean water from Bering/Chukchi Sea; estimated value adjusted to salinity, Rice et al. 1997b)
 0.340, 0.414, 0.869 (8.3, 20, 43.5°C, subsurface water from Bering Sea, TOC 2.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
 0.284, 0.356; 0.738 (8.3, 20, 43.5°C, surface microlayer water from Bering Sea, TOC 3.14 ppm, wetted-wall column-GC, Rice et al. 1997b)
 0.337, 0.424, 0.782 (8.3, 20, 43.5°C, subsurface water from Chukchi Sea, TOC 3.3 ppm, wetted-wall column-GC, Rice et al. 1997b)
 0.294, 0.369; 0.750 (8.3, 20, 43.5°C, surface microlayer water from Chukchi Sea, TOC 45.5 ppm, wetted-wall column-GC, Rice et al. 1997b)
 0.224, 0.268, 0.674 (8.3, 20, 43.5°C, melted surface ice from the Arctic Ocean, TOC 48.8 ppm, wetted-wall column-GC, Rice et al. 1997b)
 $\log K_{AW} = -872/(T/K) - 0.775$; temp range 8.3–43.5°C, (ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)
 $\log K_{AW} = -633/(T/K) - 1.665$; temp range 8.3–43.5°C, (surface microlayer of ocean water from the Chukchi Sea, wetted-wall column-GC, Rice et al. 1997b)
 0.74 (quoted lit., Armbrust 2000)
 1.090 (calculated-P/C, this work)
 0.472, 0.568 (literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.11 (20°C, shake flask-GC, Chiou et al. 1977; Freed et al. 1977, 1979)
 4.99 (Kenaga 1980b; Kenaga & Goring 1980)
 4.82 (Veith et al. 1979)

- 4.67, 4.77 (RP-HPLC correlation, McDuffie 1981)
- 4.96 (22°C, shake flask-GC, Bowman & Sans 1983b)
- 5.20 (shake flask-GC, Schimmel et al. 1983)
- 4.77 (HPLC-RT correlation, De Kock & Lord 1987)
- 5.14 (HPLC-RT correlation, Liu & Qian 1988)
- 5.267 (shake flask/slow-stirring method, De Bruijn et al. 1989)
- 4.70 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)
- 3.31–5.27 (Montgomery 1993)
- 4.73 (RP-HPLC, Saito et al. 1993)
- 3.99 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 4.96 (recommended, Sangster 1993)
- 5.25 (shake flask-HPLC, Ankley et al. 1994)
- 5.27 (recommended, Hansch et al. 1995)
- 4.96 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)
- 5.11 (literature-derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 8.75 (final adjusted value FAV, Muir et al. 2004)

Bioconcentration Factor, $\log BCF$:

- 2.67 (rainbow trout, Neely & Blau 1977; quoted, McLeese et al. 1976)
- 2.67 (mosquito fish for 35-d exposure, Veith et al. 1979; Veith & Kosian 1983)
- 2.65, 2.51 (fish: flowing water, static water; Kenaga 1980b; Kenaga & Goring 1980)
- 3.09; 3.04 (calculated-S; calculated- K_{OC} , Kenaga 1980a)
- 1.70 (average beef fat diet, Kenaga 1980b)
- 2.67 (mosquito fish for 30-d exposure, Veith et al. 1980)
- 2.65; 2.38 (quoted exptl., calculated- K_{OW} , Briggs 1981)
- 3.54 (estimated-regression from $\log K_{OW}$, Lyman et al. 1982)
- 3.08 (estimated-regression from S, Lyman et al. 1982; quoted, Howard 1991)
- 3.50 (calculated- K_{OW} , Mackay 1982)
- 2.67 (mosquito fish, Veith & Kosian 1983)
- 3.55 (beef biotransfer factor $\log B_b$, correlated- K_{OW} from Kenaga 1980, Travis & Arms 1988)
- 4.73 (milk biotransfer factor $\log B_m$, correlated- K_{OW} from McKellar et al. 1976, Travis & Arms 1988)
- 2.67; 2.51 (rainbow trout; mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)
- 4.32 (stickleback, lipid-based lab data, Deneer 1994)
- 2.68 (Pait et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.13 (soil, quoted from Dow Chemical Data, Kenaga 1980a, b; Kenaga & Goring 1980)
- 3.93 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 3.78 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
- 3.96, 4.87 (estimated-S, calculated-S and mp, Karickhoff 1981)
- 2.92, 4.43, 4.72 (estimated- K_{OW} , Karickhoff 1981)
- 4.11 (soil, Thomas 1982; quoted, Nash 1988)
- 3.79, 4.0 (soil slurry method, RP-HPLC, Swann et al. 1983)
- 1.61 (av. value calculated from Freundlich coeffs. without Baldwin Lake site data, Corwin & Farmer 1984)
- 3.35 (calculated-MCI χ , Gerstl & Helling 1987)
- 3.78 (soil, screening model calculations, Jury et al. 1987b)
- 3.27 (average of 2 soils, Kanazawa 1989)
- 3.78 (soil, 20–25°C, selected, Wauchope et al. 1992)
- 3.77–4.13 (Montgomery 1993)
- 3.93 (average, Racke 1993)
- 4.37 (selected, Lohninger 1994)
- 3.70 (soil, calculated-MCI χ , Sabljic et al. 1995)

- 3.46 (sediment, estimated, Paraiba et al. 1999)
 3.78 (soil, 20–25°C, recommended, Hornsby et al. 1996)
 4.00 (quoted lit., Armbrust 2000)
 3.70; 3.83, 3.76 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)
 3.62, 3.63 (soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)
 3.46–4.23 (sediments of San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Sorption Partition Coefficient, log K_{OM} :

- 3.42 (Felsot & Dahm 1979)
 3.78 (average of 3 soils, McCall et al. 1980)
 3.90 (exptl., Briggs 1981)
 3.10–4.31 (Mingelgrin & Gerstl 1983)
 4.24 (quoted, Karickhoff 1985; Neely & Blau 1985)
 4.50 (best estimate at low sediment concn., Karickhoff 1985)
 4.13, 3.74 (selected, estimated, Magee 1991)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: based on Henry's law constant, $t_{1/2} \sim 9.0$ d for a model river 1 m deep, flowing 1 m/s with a wind velocity of 3 m/s (Howard 1991);
 initial $k = 8.8 \times 10^{-2} \text{ h}^{-1}$ and predicted $k = 1.3 \times 10^{-3} \text{ h}^{-1}$ from soil with $t_{1/2} = 533$ h (Thomas 1982);
 $t_{1/2} = 0.3\text{--}3.2$ d for disappearance from an inert surface at 25°C (Meikle et al. 1983).

Photolysis: $t_{1/2}(\text{exptl}) = 22$ d determined under midday summer sunlight in California (Meikle et al. 1983; quoted, Howard 1991)

$k_p = (2.19 \pm 0.17) \times 10^{-2} \text{ h}^{-1}$, $(2.09 \pm 0.17) \times 10^{-2} \text{ h}^{-1}$ at different initial solute concentrations in aqueous solution at pH 7.0 and 25°C irradiated with a 450-W Hanovia mercury arc lamp. Under various environmental conditions, the estimated $t_{1/2} = 31$ d at a depth of 0.001 cm, $t_{1/2} = 43$ d at a depth of 1-m pure water, $t_{1/2} = 2.7$ yr at 1-m depth river water for midsummer conditions; $t_{1/2} = 345$ d at a depth of 1-m pure water under midwinter surface conditions, all at pH 2 at 40°N latitude, with average light attenuation (Dilling et al. 1984; quoted, Howard 1991; Montgomery 1993)

Oxidation: photooxidation $t_{1/2} = 6.34$ h for the vapor phase reaction with OH radical in air (Howard 1991).

Hydrolysis:

$t_{1/2} = 53$ d at pH 7.4 and 20°C (NIEHS 1975; quoted, Freed et al. 1977, 1979);
 $t_{1/2} = 120$ d at pH 6.1 and $t_{1/2} = 53$ d at pH 7.4 in water and soil at 20°C as per Ruzicka et al. 1967 using GC-RT correlation for hydrolysis rates determination (Freed et al. 1979; quoted, Montgomery 1993)
 $k(\text{alkaline}) = 0.1 \text{ M}^{-1} \text{ s}^{-1}$, $k(\text{neutral}) = 1 \times 10^{-7} \text{ s}^{-1}$, $10^{-7}\text{--}10^{-9} \text{ M}$ in aqueous buffer at 20°C (Harris 1982)
 $k = (1.08 - 2.0) \times 10^{-3} \text{ h}^{-1}$ corresponding to half-lives of 13–27 d at pH 7 buffer solution and 25°C (Dilling et al. 1984)
 $t_{1/2} = 78$ d relatively independent of pH 1 to 7 (Macalady & Wolfe 1983; quoted, Howard 1991)
 $t_{1/2} = 1.5$ d in water at pH 8 and 25°C (Worthing & Hance 1991; Tomlin 1994)

Hydrolytic $k(\text{acidic}) < 0.008 \text{ d}^{-1}$ in acidic soils with pH ≤ 7.0 , corresponding to $t_{1/2} = 92\text{--}341$ d and $k(\text{alkaline}) = (0.006 - 0.063) \text{ d}^{-1}$ in alkaline soils corresponding to $t_{1/2} = 11\text{--}200$ d in abiotic hydrolysis in 37 different soils with pH 3.8–8.5. (Racke et al. 1996)

$k = 0.0009 \text{ d}^{-1}$ at pH 5, $k = 0.023 \text{ d}^{-1}$ at pH 7, $k = 0.044 \text{ d}^{-1}$ at pH 9; measured hydroxy radical rate constant for chlorpyrifos $1.3 \times 10^{13} \text{ M}^{-1} \text{ h}^{-1}$ (Armbrust 2000).

Biodegradation:

$k = 0.014 \text{ d}^{-1}$ in soil at 28°C (Miles et al. 1979; quoted, Klečka 1985)
 $k = 0.008\text{--}0.025 \text{ d}^{-1}$ in soil at 25°C (Getzin 1981; quoted, Klečka 1985)
 $k = (-0.000945 \text{ to } -0.00243) \text{ h}^{-1}$ in nonsterile sediment and $k = (-0.000562 \text{ to } -0.00151) \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and also $k = (-0.00109 \text{ to } -0.00231) \text{ h}^{-1}$ in nonsterile water and $k = (-0.00144 \text{ to } -0.00197) \text{ h}^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988)
 $t_{1/2} = 39\text{--}51$ d in loamy and clay soils under anaerobic conditions, $t_{1/2} = 150\text{--}200$ d in anaerobic pond sediments (Racke 1993)
 $k(\text{aerobic}) = 9.47 \times 10^{-4} \text{ h}^{-1}$ for exposure analysis (Armbrust 2000).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

elimination $t_{1/2} = 3.3$ d in channel catfish (Barron et al. 1991)

$k_1 = 7000 \pm 2000$ L kg⁻¹ d⁻¹ (guppy, lipid-based modeling data, Deneer 1993)

$k_2 = (0.40 \pm 0.11)$ d⁻¹ (guppy, lipid-based modeling data, Deneer 1993)

$k_1 = (26 \pm 8.0) \times 10^3$ L kg⁻¹ d⁻¹ (stickleback, lipid-based lab data, Deneer 1994).

$k_2 = (1.2 \pm 0.4)$ d⁻¹ (stickleback, lipid-based lab data, Deneer 1994).

Half-Lives in the Environment:

Air: $t_{1/2} = 6.34$ h for the vapor phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991);
reaction rate $k = 4.77 \times 10^{-4}$ min⁻¹ in air (Paraiba et al. 1999).

Surface water: based on Henry's law constant, volatilization $t_{1/2} \sim 9.0$ d for a model river 1-meter deep, flowing 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1991);

half-lives of a 100 mL pesticide-seawater solution containing 10 g of sediment were: $t_{1/2} < 2.0$ d, indoor at 25°C with 12-h photo-period white fluorescent light, $t_{1/2} = 4.6$ d, outdoor-light (stoppered, Pyrex flasks exposed to ambient sunlight with temperature 22–45°C), $t_{1/2} = 7.1$ d, outdoor-dark (foil-covered flasks) and $t_{1/2} = 24$ d in an estuary (Schimmel et al. 1983; quoted, Montgomery 1993)

$t_{1/2} = 120$ d in water at pH 6.1, 20°C (quoted, Lartiges & Garrigues 1995);

reaction rate $k = 3.80 \times 10^{-4}$ min⁻¹ in water (Paraiba et al. 1999).

Ground water:

Sediment: $t_{1/2} = 24$ d in 10 g untreated sediment/100 mL of a pesticide-seawater solution and $t_{1/2} > 28$ d in 10 g sterile sediment/100 mL of a pesticide-seawater solution (Schimmel et al. 1983)

$t_{1/2} = 150$ –200 d in anaerobic pond sediments (Racke 1993)

reaction rate $k = 2.85 \times 10^{-5}$ min⁻¹ in sediment (Paraiba et al. 1999)

First-order degradation $k = 0.034$ d⁻¹ with $t_{1/2} = 20.3$ d under aerobic conditions, $k = 0.003$ d⁻¹ with $t_{1/2} = 223$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.029$ d⁻¹ with $t_{1/2} = 23.7$ d under aerobic conditions, $k = 0.012$ d⁻¹ with $t_{1/2} = 57.6$ d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: $t_{1/2} = 17.0$ wk in sterile sandy loam and $t_{1/2} < 1.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 2.5$ wk in nonsterile organic soil (Miles et al. 1979);

$t_{1/2} = 12$ and 24 wk in a silt loam and clay loam, $t_{1/2} = 24$ wk while in sterilized soils; however, temperature also had noticeable effects on decomposition as $t_{1/2} = 25$, 13, and 6 wk for soil samples incubated at 15, 25, and 35°C, respectively (Getzin 1981a; quoted, Montgomery 1993);

hydrolysis $t_{1/2} = 8$ d in Sultan silt loam (Getzin 1981b; quoted, Montgomery 1993);

$t_{1/2} = 80$ –100 d slowly degraded in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);

$t_{1/2} = 63$ d from screening model calculations (Jury 1987b);

persists in soil for 60–120 d (Worthing & Hance 1991);

Selected field $t_{1/2} = 30$ d (Wauchope et al. 1992; quoted, Dowd et al. 1993; Richards & Baker 1993; Hornsby et al. 1996);

$t_{1/2} = 30$ d (Pait et al. 1992);

Field dissipation $t_{1/2} = 39$ –51 d in loamy and clay soils under anaerobic conditions; and aerobic solid degradation $t_{1/2} = 5$ –141 d (Racke 1993)

$t_{1/2}$ = of 60–120 d (Tomlin 1994)

Dissipation $t_{1/2} \leq 7$ d when applied to dry soils or the soil surface ($t_{1/2} = 7$ –14 d); and $t_{1/2} = 30$ –60 d when incorporated into the soil profile (Racke et al. 1996)

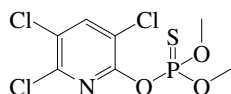
First order rate constants for photolytic decline in sandy soil: $k = 2.91 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 240$ h irradiated in moisture-maintained, $k = 2.06 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 340$ h, irradiated in air-dried $k = 1.67 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 420$ h in dark control moist and $k = 0.99 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 700$ h in dark control air-dried sandy soil from Sauk County, WI. The photolytic $k = 8.43 \times 10^{-4}$ h⁻¹ with $t_{1/2} = 820$ h in moist soil, $k = 1.07 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 650$ h in dry soil. The contribution of moisture to irradiated metabolism $k = 1.24 \times 10^{-3}$ h⁻¹ with $t_{1/2} = 560$ h, but for dark control system for $k = 6.78 \times 10^{-4}$ h⁻¹ with $t_{1/2} = 1020$ h (Graebing & Chib 2004)

Biota: $t_{1/2} = 335$ h clearance from fish (Neely 1980);

biochemical $t_{1/2} = 63$ d from screening model calculations (Jury et al. 1987b);

elimination $t_{1/2} \sim 3.3$ d in channel catfish (Barron et al. 1991)

18.1.1.16 Chlorpyrifos-methyl



Common Name: Chlorpyrifos-methyl

Synonym: Reldan

Chemical Name: *O,O*-dimethyl *O*-3,5,6-trichloro-2-pyridyl phosphorothioate

Uses: insecticide

CAS Registry No: 5598-13-0

Molecular Formula: $C_7H_7Cl_3NO_3PS$

Molecular Weight: 322.534

Melting Point ($^{\circ}C$):

43 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.666 (mp at $43^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.76	($20^{\circ}C$, shake flask-GC, Chiou et al. 1977)
0.40	(Spencer 1982)
4.0	(Kenaga 1980a, b, Kenaga & Goring 1980)
3.2	($20^{\circ}C$, shake flask, Bowman & Sans 1983b)
4.0	($24^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)
4.0	(selected, 20 – $25^{\circ}C$, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

5.63×10^{-3}	(Spencer 1982, Hartley & Kidd 1987; Tomlin 1994)
5.60×10^{-3}	(selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.31	(shake flask-GC, Chiou et al. 1977)
4.17	(Kenaga 1980a; Kenaga & Goring 1980)
3.29, 4.30	(Rao & Davidson 1980)
4.30	(shake flask-concn ratio-GC; Bowman & Sans 1983b)
4.31	(recommended, Sangster 1993)
3.99	(HPLC-RT correlation, Sicbaldi & Finizio 1993)
4.24	(Tomlin 1994)
4.31	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.98	(fish, static water, Kenaga & Goring 1980)
2.45, 2.36	(calculated-solubility, K_{ow} , Kenaga 1980b)
1.98	(fish, microcosm conditions, Garten & Trabalka 1983)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.52 (soil, Kenaga 1980a; Kenaga & Goring 1980)
- 3.30 (soil, calculated, Kanga 1980b)
- 3.76 (soil, Sabljic 1987)
- 3.48 (estimated, soil, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 3.52 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 3.52; 3.36, 3.49 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constant and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: under goes rapid photodecomposition in UV light (Spencer 1982).

Photooxidation:

Hydrolysis: relatively stable under neutral conditions, but hydrolyzed by acids (pH 4–6) and, more readily by alkalis (pH 8–10), $t_{1/2} = 3$ d at pH 8 (Tomlin 1994)

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air:

Surface water: estimated $t_{1/2} \sim 38$ d in buffered water at pH 6 (Spencer 1982);
relatively stable under neutral conditions, but hydrolyzed by acids (pH 4–6) and, more readily by alkalis (pH 8–10), $t_{1/2} = 3$ d at pH 8 (Tomlin 1994).

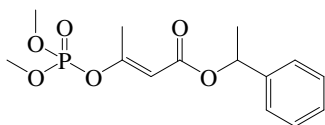
Ground water:

Sediment:

Soil: field $t_{1/2} = 7$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
 $t_{1/2} = 1.5$ and 33 d depending upon soil type and microbial activity (Tomlin 1994).

Biota:

18.1.1.17 Crotoxyphos



Common Name: Crotoxyphos

Synonym: Ciodrin, Ciovap, Cyodrin, Cypona EC, Decrotox, Duo-kill, Duravos, ENT 24717, Volfazol

Chemical Name: dimethyl(*E*)-1-methyl-2-(1-phenyl-ethoxycarbonyl)vinyl phosphate

Uses: insecticide

CAS Registry No: 7700-17-6

Molecular Formula: C₁₄H₁₉O₆P

Molecular Weight: 314.271

Melting Point (°C): liquid

Boiling Point (°C):

135 (at 0.03 mmHg, Montgomery 1993)

Density (g/cm³ at 20°C):

1.2 (Spencer 1982)

1.19 (25°C, Montgomery 1993)

Molar Volume (cm³/mol):

264.1 (calculated-density)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

1000 (Günther et al. 1968)

1000 (Melnikov 1971; Spencer 1973, 1982;)

1000 (Martin & Worthing 1977; Worthing & Walker 1987; Montgomery 1993)

Vapor Pressure (Pa at 25°C or as indicated):

0.0019 (20°C, Khan 1980)

0.00187, 0.0052, 0.013 (20, 30, 40°C, Spencer 1982)

0.0019 (20°C, Montgomery 1993)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.00063 (20–25°C, calculated-P/C, Montgomery 1993)

0.00060 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

3.00 (Callahan et al. 1979)

2.23 (Kenaga 1980)

3.30 (shake flask, Log P Database, Hansch & Leo 1987)

3.30 (selected, Sangster 1993)

3.30 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.10 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC}:

2.23 (soil, Hamaker & Thompson 1972; Kenaga & Goring 1980)

2.00, 1.70 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)

2.23 (Montgomery 1993)

2.00 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

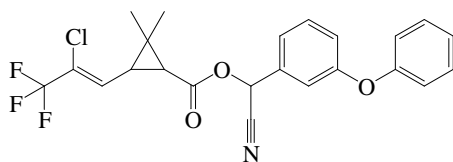
2.00; 2.07, 2.59 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Surface water: biodegradation $t_{1/2} = 7.5$ d at pH 9 and $t_{1/2} = 22.5$ d at pH 2 from river die-away tests (Konrad & Chester 1969; quoted, Scow 1982).

18.1.1.18 Cyhalothrin



Common Name: Cyhalothrin

Synonym: Grenade, cyhalothrine

Chemical Name: (*RS*)- α -cyano-3-phenoxybenzyl(*Z*)-(1*RS*,3*RS*)-(2-chloro-3,3,3-trifluoropropyl)-2,2-dimethylcyclopropanecarboxylate

Uses: insecticide

CAS Registry No: 68085-85-8

Molecular Formula: $C_{23}H_{19}ClF_3NO_3$

Molecular Weight: 449.850

Melting Point ($^{\circ}C$):

yellow to brown viscous oil (technical, Hartley & Kidd 1987; Tomlin 1994)

Boiling Point ($^{\circ}C$):

187–190/0.2 mmHg (Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3):

1.25 (25 $^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated):

< 1.0 (Worthing & Walker 1983)

0.003 (20 $^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987)

0.004 (20 $^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated):

$\sim 1.0 \times 10^{-6}$ (20 $^{\circ}C$, Hartley & Kidd 1987)

0.001×10^{-3} (20 $^{\circ}C$, Tomlin 1994)

1.90×10^{-5} (40 $^{\circ}C$, Knudsen effusion method, Goodman 1997)

$\log(P/Pa) = 13.47 - 5723/(T/K)$ (Antoine eq., measured range 45–85 $^{\circ}C$, Goodman 1997)

1.51×10^{-5} (P^S , GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.02 (HPLC-RT correlation, Hu & Leng 1992)

6.80 (20 $^{\circ}C$, Tomlin 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

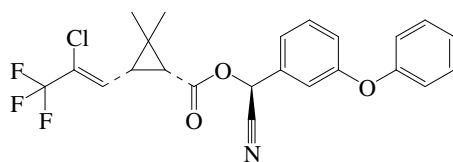
Environmental Fate Rate Constants, k , and Half-Lives. $t_{1/2}$:

Hydrolysis: slowly hydrolysed in sunlight at pH 7–9, more rapidly at pH >9 (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} \sim 4$ –12 wks (Hartley & Kidd 1987; Tomlin 1994)

18.1.1.19 Lambda-cyhalothrin



Common Name: lambda-cyhalothrin

Synonym: lambda-cyhalothrin

Chemical Name: equal quantities of (*S*)- α -cyano-3-phenoxybenzyl(*Z*)-(1*R*,3*R*)-3-(2-chloro-3,3,3-trifluoropropyl)-2,2-dimethylcyclopropanecarboxylate and (*S*)- α -cyano-3-phenoxybenzyl(*Z*)-(1*S*,3*S*)-3-(2-chloro-3,3,3-trifluoropropyl)-2,2-dimethylcyclopropanecarboxylate

Uses: insecticide

CAS Registry No: 91465-08-6

Molecular Formula: $C_{23}H_{19}ClF_3NO_3$

Molecular Weight: 449.850

Melting Point ($^{\circ}C$):

49.2 (Hartley & Kidd 1987; Tomlin 1994; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

1.33 ($25^{\circ}C$, Tomlin 1994)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.579 (mp at $49.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.005 ($20^{\circ}C$, pH 6.5, Hartley & Kidd 1987)

0.005, 0.004 (pH 6.5 in purified water, pH 5.0 in buffered water Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

2.0×10^{-7} ($20^{\circ}C$, Hartley & Kidd 1987)

2.0×10^{-7} , 2.0×10^{-4} (20 , $60^{\circ}C$, Tomlin 1994)

$7.80 \times 10^{-6*}$ ($40^{\circ}C$, Wollerton & Husband 1988, quoted in Goodman 1997)

$19 \times 10^{-6*}$ ($40^{\circ}C$, Knudsen effusion method, measured range 40 – $80^{\circ}C$, Goodman 1997)

1.88 (extrapolated-Antoine eq., Goodman 1997)

$\log(P/kPa) = 13.47 - 5723/(T/K)$; temp range 40 – $80^{\circ}C$ (Antoine eq., Knudsen effusion, Goodman 1997)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.0 ($20^{\circ}C$, Tomlin 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment: t_{1/2} ~ 20 d in water-sediment mixture in sunlight (Tomlin 1994).
- Soil: t_{1/2} ~ 4–12 wk (Hartley & Kidd 1987; Tomlin 1994)
- Biota:

TABLE 18.1.1.19.1
Reported vapor pressures of lambda-cyhalothrin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$		(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)		
Wollerton & Husband 1988		Goodman 1997		
quoted in Goodman 1997		Knudsen effusion		
t/°C	P/Pa	t/°C	P/Pa	
40	7.8×10^{-6}	40	1.9×10^{-5}	
50	4.0×10^{-5}	50	4.7×10^{-5}	
60	1.9×10^{-4}	60	1.7×10^{-4}	
70	8.2×10^{-4}	70	6.5×10^{-4}	
80	3.2×10^{-3}	80	2.0×10^{-3}	
		eq. 1	P/Pa	
		A	13.47	
		B	5723	

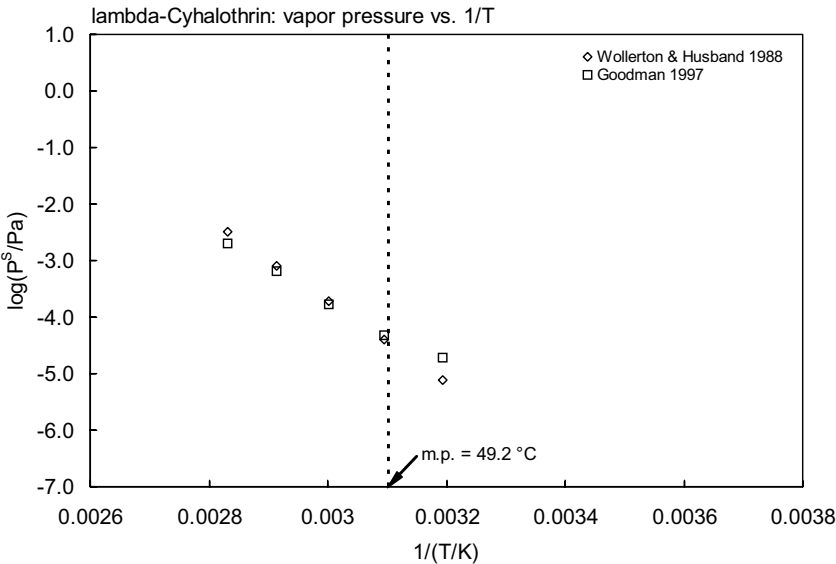
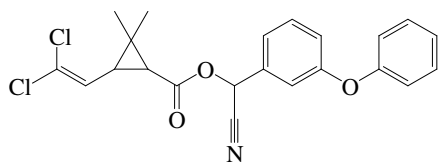


FIGURE 18.1.1.19.1 Logarithm of vapor pressure versus reciprocal temperature for lambda-cyhalothrin.

18.1.1.20 Cypermethrin



Common Name: Cypermethrin

Synonym: Agrothrin, Ambush C, Barricade, CCN 52, Cymbush, Cyperkill, Demon, FMC 30980, Folcord, Imperator, Kafil Super, Polytrin, Ripcord, Sherpa, Stocade, Toppel

Chemical Name: cyano(3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclo-propanecarboxylate; (*RS*)- α -cyano-3-phenoxybenzyl(1*RS*,3*RS*;1*RS*,3*SR*)-3(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-carboxylate

Uses: nonsystemic insecticide with contact and stomach action to control a wide range of insects in fruits, vegetables, vines, potatoes, cucurbits, capsicums, cereals, maize, soybeans, cotton, coffee, coca, rice, pecans, ornamentals and forestry, etc.; also used to control flies in animal houses and mosquitoes, cockroaches, houseflies and other pests in public health.

CAS Registry No: 52315-07-8

Molecular Formula: $C_{22}H_{19}Cl_2NO_3$

Molecular Weight: 416.297

Melting Point ($^{\circ}C$):

70 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.23 (Tomlin 1994)

1.25 (Milne 1995)

Molar Volume (cm^3/mol):

457.7 (calculated-Le Bas method at normal boiling point)

335.7 (calculated-density)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.362 (mp at $70^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.041 (shake flask-GC, Coats & O'Donnell-Jefferey 1979)

0.005–0.01 (Stephenson 1982)

0.010 ($20^{\circ}C$, Hartley & Kidd 1987)

0.01–0.2 ($21^{\circ}C$, Worthing & Walker 1987)

0.004 (20 – $25^{\circ}C$, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

0.004 (Montgomery 1993)

0.004 (at pH 7, Tomlin 1994)

0.009 ($20^{\circ}C$, selected, Siebers & Mattusch 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

8.7×10^{-7} (Barlow 1978)

4.3×10^{-7} (gas saturation, Grayson et al. 1982)

$<1.3 \times 10^{-5}$ (Spencer 1982)

5.1×10^{-10} ($70^{\circ}C$, Hartley & Kidd 1987)

2.4×10^{-6} (GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990)

1.9×10^{-7} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.9×10^{-7} ($20^{\circ}C$, extrapolated, Montgomery 1993)

2.3×10^{-7} ($20^{\circ}C$, Tomlin 1994)

2.75×10^{-6} ; 2.4×10^{-6} ; 1.86×10^{-6} ; 1.15×10^{-6} (liquid P_L , GC-RT correlation; quoted lit. values, Donovan 1996)

2.3×10^{-6} ($20^{\circ}C$, selected, Siebers & Mattusch 1996)

3.23×10^{-6} (solid P^S , converted from P_L by GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$) at 25°C or as indicated:

0.0199	(20–25°C, calculated-P/C, Montgomery 1993)
0.0194	(20–25°C, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
0.080	(selected, Siebers & Mattusch 1996)
0.0195	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.47	(shake flask-GC, Coats & O'Donnell-Jefferey 1979)
5.90	(Schimmel et al. 1983)
5.2 ± 0.6	(<i>cis</i> -form, HPLC-RT correlation, Muir et al. 1985)
5.0 ± 0.6	(<i>trans</i> -form, HPLC-RT correlation, Muir et al. 1985)
6.60	(Montgomery 1993)
4.47, 6.0	(quoted, Sangster 1993)
6.60	(Tomlin 1994)
6.60	(Milne 1995)
6.05, 6.05	(α -, β -isomer, Hansch et al. 1995)
5.56, 6.35, 5.60	(RP-HPLC correlation, ClogP, calculated-S, Finizio et al. 1997)
5.62	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$:

2.99	(activated sludge, Freitag et al. 1984)
3.52, 2.62, 2.99	(algae, golden ide, activated sludge, Freitag et al. 1985)
1.73–2.34	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.63–2.39	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.49–2.05	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
1.53–2.38	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.84–2.59	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.68–2.02	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
2.89	(<i>Oncorhynchus mykiss</i> , Muir et al. 1994; quoted, Devillers et al. 1996)
2.92	(<i>Oncorhynchus mykiss</i> , Muir et al. 1994; quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{oc}$:

2.36	(<i>cis</i> -form, silt, K_p on 24% DOC, Muir et al. 1985)
2.57	(<i>cis</i> -form, clay, K_p on 56% DOC, Muir et al. 1985)
2.59	(<i>trans</i> -form, silt, K_p on 10% DOC, Muir et al. 1985)
5.00	(soil, 20–25°C, estimated, Wauchope et al. 1992; quoted, Lohninger 1994; Hornsby et al. 1996)
4.0–4.53	(Montgomery 1993)
5.54	(sediments, Maund et al. 2002)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 5$ d in river water (Tomlin 1994).

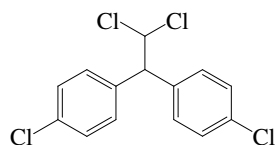
Ground water:

Sediment:

Soil: estimated field $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

18.1.1.21 DDD



Common Name: DDD

Synonym: dichloro diphenyl dichloroethane; *p,p'*-DDD; Dilene; ENT 4225; ME 1700; NCI-C00475; Rhothane; *p,p'*-TDE; TDE; tetrachlorodiphenylethane

Chemical Name: 1,1-dichloro-2,2-bis(4-chlorophenyl)ethane; 1,1'-(2,2-dichloroethylidene)bis[4-chlorobenzene]

Uses: degradation product of DDT used as insecticide.

CAS Registry No: 72-54-8 (*p,p'*-DDD or DDD); 53-10-0 (*o,p'*-DDD)

Molecular Formula: C₁₄H₁₀Cl₄

Molecular Weight: 321.041

Melting Point (°C):

109.5 (Ballschmiter & Wittlinger 1991; Kühne et al. 1995; Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

312.6 (calculated-LeBas method at normal boiling point)

246.4 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.96 (DSC method, Plato & Glasgow 1969)

27.313 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

81.17 (Plato & Glasgow 1969; Hinckley et al. 1990)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.148 (mp at 109.5°C)

Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.002 (shake flask-LSC, Metcalf et al. 1973)

0.005, 0.015, 0.09* (shake flask-GC with particle sizes: 0.01, 0.05, 5.0 micron, Biggar & Riggs 1974)

0.24 (*p, p'*-DDD shake flask-GC, *o, p'*-DDD with particle sizes: 0.05 micron, Biggar & Riggs 1974)

0.060, 0.10, 0.25, 0.315 (shake flask-GC, *o, p'*-DDD at 15, 25, 35, 45°C with particle sizes: 5.0 micron or less, Biggar & Riggs 1974)

0.020 (generator column-GC/ECD, Weil et al. 1974)

0.005 (Martin & Worthing 1977)

0.09, 0.10 (quoted, *p,p'*-, *o,p'*-DDD, Callahan et al. 1979)

0.004 (shake flask-nephelometry, Hollifield 1979)

0.10 (20°C, selected, *o,p'*-DDD, Suntio et al. 1988)

0.16 (Agency for Toxic Substances & Disease Registry 1988; quoted, Burmaster et al. 1991)

0.020 (20–25°C, selected, Hornsby et al. 1996)

0.050; 0.010, 0.0035 (quoted; predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

log [S_L/(mol/L)] = 0.2910 – 1442/(T/K) (liquid, Passivirta et al. 1999)

0.90, 0.738 (*p,p'*-DDD, supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

2.52 × 10⁻⁴ (30°C, *o, p'*-DDD, gas saturation-vapor density-GC, Spencer & Cliath 1972; Spencer 1975)

1.36 × 10⁻⁴ (30°C, *p, p'*-DDD, gas saturation-GC, Spencer & Cliath 1972; Spencer 1975)

1.63 × 10⁻³, 6.24 × 10⁻⁴ (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)

4.34 × 10⁻⁴ (supercooled liquid P_L, converted from literature P_S with ΔS_{fus} Bidleman 1984)

- 1.00×10^{-4} (20°C, selected, Suntio et al. 1988)
 2.00×10^{-4} (20°C, *o,p'*-, selected, Suntio et al. 1988)
 4.35×10^{-4} , 9.84×10^{-4} (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 1.63×10^{-3} , 1.10×10^{-3} (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log(P_L/Pa) = 12.49 - 4622/(T/K)$ (supercooled liquid, GC-RT correlation, Hinckley et al. 1990; quoted, Passivirta et al. 1999)
 1.33×10^{-4} (20–25°C, estimated, Hornsby et al. 1996)
 9.69×10^{-4} , 1.13×10^{-4} , 9.16×10^{-5} (*p,p'*-DDD, supercooled liquid P_L : calculated, GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 $\log(P_S/Pa) = 16.23 - 6062/(T/K)$ (solid, *p,p'*-DDD, Passivirta et al. 1999)
0.00097, 0.0023 (*p,p'*-DDD, supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry's Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):

- 2.18 (calculated-P/C, Yoshida et al. 1983)
0.27 (Agency for Toxic Substances & Disease Registry 1988; quoted, Burmaster et al. 1991)
0.64 (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
9.00 (calculated-P/C, Ballschmiter & Wittlinger 1991)
0.669 (*p,p'*-DDD, wetted wall column-GC, Altschuh et al. 1999)
 $\log[H/(Pa \text{ m}^3/\text{mol})] = 12.20 - 3168/(T/K)$ (*p,p'*-DDD, Passivirta et al. 1999)
0.67, 0.50 (*p,p'*-DDD, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 5.99 (O'Brien 1975)
6.02 (Ernst 1977)
6.02 (Veith & Morris 1978; Veith et al. 1979)
5.69 (Hansch & Leo 1979)
5.99, 6.08 (*p,p'*-, *o,p'*-DDD, Callahan et al. 1979)
6.00 (Kenaga & Goring 1980)
5.19 (RP-HPLC-RT correlation, Chin et al. 1986)
5.00 (RP-HPLC-RT correlation, De Kock & Lord 1987)
 6.217 ± 0.031 (*p,p'*-DDD, shake flask/slow-stirring method, De Bruijn et al. 1989)
6.02 (recommended, Sangster 1993)
4.82 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
6.22 (recommended, Hansch et al. 1995)
4.87 (*o,p'*-, RP-HPLC-RT correlation, Finizio et al. 1997)
6.02 (*p,p'*-DDD, calculated, Passivirta et al. 1999)
6.22, 6.33 (*p,p'*-DDD, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficients, $\log K_{OA}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 8.90 (*p,p'*-DDD, calculated- K_{ow}/K_{aw} , Wania & Mackay 1996)
9.45 (*p,p'*-DDD, calculated, Finizio et al. 1997)
10.11*, 10.27 (*p,p'*-DDD, gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
 $\log K_{OA} = -5.193 + 4610/(T/K)$, temp range: 5–35°C (*p,p'*-DDD, gas saturation-GC, Shoeib & Harner 2002)
10.10, 10.03 (*p,p'*-DDD, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, $\log BCF$:

- 4.92, 3.92 (*Gambusia*, *Physa*, Metcalf et al. 1973)
3.96 (mussel, Ernst 1977)
4.72 (fathead minnow, Veith et al. 1979)
4.09 (calculated-S, Kenaga 1980)
4.11 (calculated-S or K_{ow} , Kenaga & Goring 1980)
3.30 (*Triaenodes tardus*, Belluck & Felsot 1981)

- 4.34, 4.42 (mussel, oyster; calculated- K_{OW} , Zaroogian et al. 1985)
 4.68 (oyster, Zaroogian et al. 1985; quoted, Hawker & Connell 1986)
 2.85–4.29 (benthic macroinvertebrates, Reich et al. 1986)
 4.81 (calculated-S and K_{OW} , Isnard & Lambert 1988)
 –1.90 (beef biotransfer factor $\log B_b$, correlated- K_{OW} from Fries et al. 1969, Travis & Arms 1988)
 –2.52 (milk biotransfer factor $\log B_m$, correlated- K_{OW} from Fries et al. 1969, Travis & Arms 1988)
 0.301 (earthworms, quoted, Menzie et al. 1992)
 –0.456, –0.745, –0.602 (earthworms, field/lab. estimated, field leaf litter, calculated-modeled, Menzie et al. 1992)
 4.68 (calculated- $\log K_{OW}$ as per Mackay 1982, this work)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.91 (calculated-S, Kenaga 1980)
 4.63 (calculated-S or K_{OW} , Kenaga & Goring 1980;)
 5.86 (calculated-S, Mill et al. 1980; quoted, Adams 1987)
 5.89 (estimated-QSAR & SPARC, Kollig 1993)
 5.00 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: aquatic half-life of a few days to about a month (summarized data, Callahan et al. 1979).

Photolysis: aquatic $t_{1/2} > 150$ d (summarized data, Callahan et al. 1979).

Oxidation: aquatic $t_{1/2} \sim 22$ yr (summarized data, Callahan et al. 1979);

photooxidation $t_{1/2} = 13.3$ –133 h in air, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

$t_{1/2} \sim 570$ d at pH 9 and $t_{1/2} = 190$ yr at pH 5 (summarized data, Callahan et al. 1979);

$t_{1/2} = 28$ yr at pH 7 and 25°C, calculated from measured neutral and base catalyzed hydrolysis constants of $(2.8 \pm 0.9) \times 10^{-6} \text{ h}^{-1}$ and $5.2 \text{ M}^{-1} \text{ h}^{-1}$ (Ellington et al. 1987, 1988, 1989; quoted, Howard et al. 1991);
 rate constant $k = 2.5 \times 10^{-2} \text{ yr}^{-1}$ at pH 7 and 25°C (Kollig 1993).

Biodegradation: aqueous aerobic $t_{1/2} = 2$ –15.6 yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 70$ –294 d, based on anaerobic flooded soil die-away study data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 52.9 \text{ h}^{-1}$; $k_2 = 0.0058 \text{ h}^{-1}$ (mussel, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: $t_{1/2} = 17.7$ –177 h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 2$ –15.6 yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991)

dehydrochlorination rate constant $k = 5.0 \times 10^{-2} \text{ h}^{-1}$ with $t_{1/2} = 13.9$ h for 1.0 ppm *p,p'*-DDD and $k = 0.76 \times 10^{-2} \text{ h}^{-1}$ with $t_{1/2} = 96.3$ h for *o,p'*-DDD both at $21 \pm 2^\circ\text{C}$ and pH 12.8 (in 0.1 N NaOH solution) (Choi & Chen 1976)

estimated $t_{1/2} = 45$ d for surface waters in case of a first order reduction process may be assumed (Zoeteman et al. 1980)

Ground water: $t_{1/2} = 1680$ –270,000 h, based on anaerobic flooded soil die-away study data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991) and observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 2$ –15.6 yr, based on observed rates of biodegradation of DDT in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991);

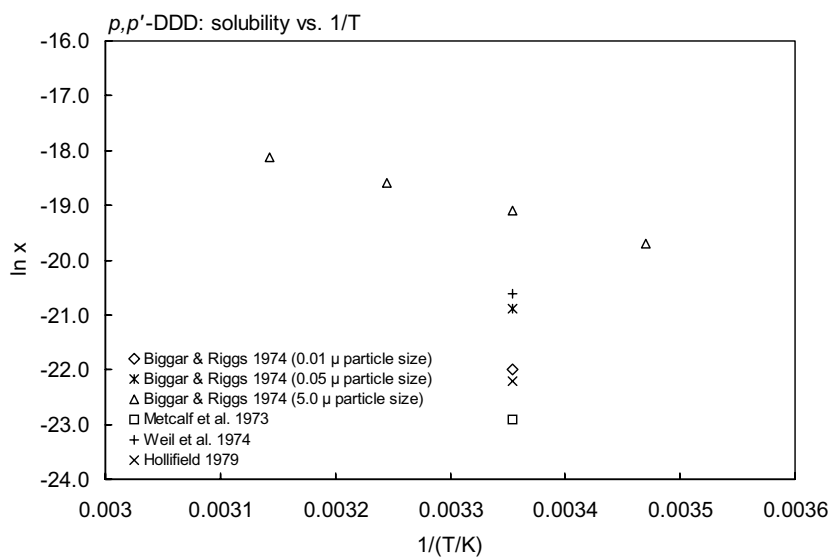
estimated field $t_{1/2} \sim 1000$ d (20–25°C, Hornsby et al. 1996).

Biota: $t_{1/2} = 119$ h in mussel (Ernst 1977).

TABLE 18.1.1.21.1

Reported aqueous solubilities and octanol-air partition coefficients of DDD at various temperatures

Aqueous solubility						log K _{OA}	
<i>p,p'</i> -DDD			<i>o,p</i> -DDD			<i>p,p'</i> -DDD	
Biggar & Riggs 1974			Biggar & Riggs 1974			Shoeib & Harner 2002	
shake flask-GC			shake flask-GC			generator column-GC/MS	
t/°C	S/g·m ⁻³	S/g·m ⁻³	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	log K _{OA}
particle size	0.01μ	0.05μ	5.0μ	particle size	5.0μ		
15	—	—	0.050	15	0.060	5	11.287
25	0.005	0.015	0.090	25	0.100	15	11.238
35	—	—	0.150	35	0.280	20	10.286
45	—	—	0.240	45	0.315	25	10.110
						35	9.870
						log K _{OA} = A + B/(T/K)	
						A	-5.193
						B	4610
						enthalpy of phase change	
						ΔH _{OA} /(kJ mol ⁻¹) = 80.1	

FIGURE 18.1.1.21.1A Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *p,p'*-DDD.

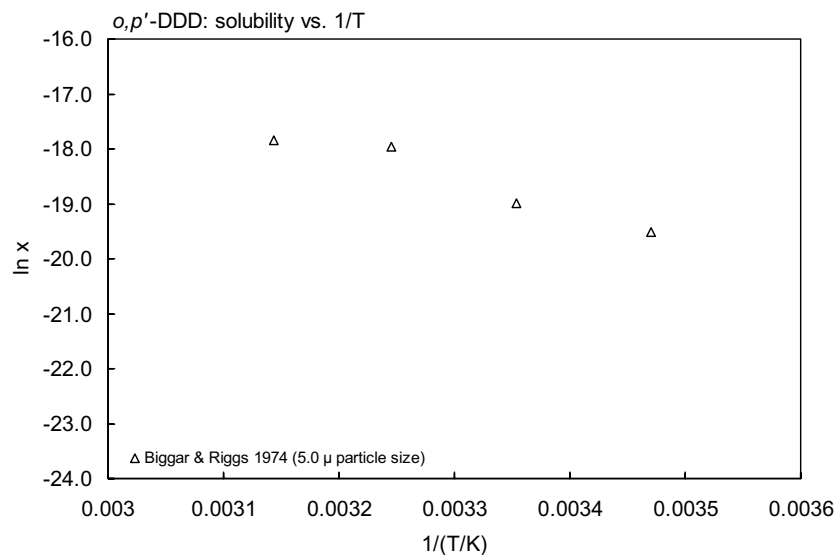


FIGURE 18.1.1.21.1B Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *o,p'*-DDD.

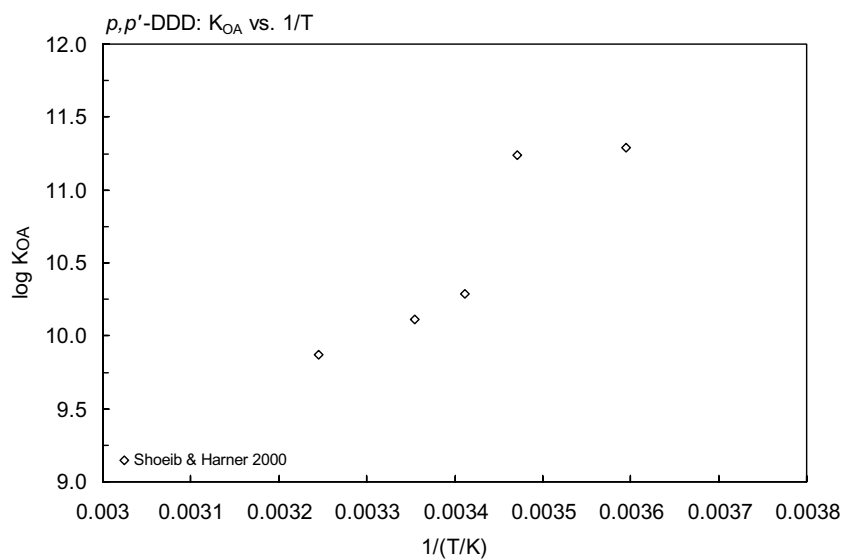
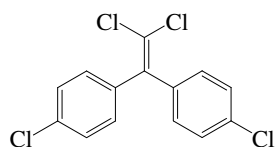


FIGURE 18.1.1.21.2 Logarithm of K_{OA} versus reciprocal temperature for *p,p'*-DDD.

18.1.1.22 DDE



Common Name: DDE (*p,p'*-DDE; *o,p'*-DDE)

Synonym: 4,4'-DDE, DDE; 2,4-DDE

Chemical Name: 1,1-dichloro-2,2-bis(*p*-chlorophenyl)-ethylene

CAS Registry No: 72-55-9 (*p,p'*-DDE); 3424-82-6 (*o,p*-DDE)

Molecular Formula: $C_{14}H_8Cl_4$

Molecular Weight: 319.0

Melting Point ($^{\circ}C$):

89 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

305.2 (calculated-Le Bas method at normal boiling point)

243.1 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.543 (*o,p'*-DDE, DSC method, Plato & Glasgow 1969)

24.267 (*p,p'*-DDE, DSC method, Plato & Glasgow 1969)

Entropy of fusion, ΔS_{fus} (J/mol K):

67.0 (Hinckley et al. 1990; Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K, F: 0.236 (mp at $89^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

p,p'-DDE

0.0013 (shake flask-LSC, Metcalf et al. 1973, 1975)

0.12* (shake flask-GC for particles 5μ - or less, measured range $15-45^{\circ}C$, Biggar & Riggs 1974)

0.014 (generator column-GC/ECD, Weil et al. 1974)

0.040 ($20^{\circ}C$, shake flask-GC, Chiou et al. 1977; Freed et al. 1977)

0.065 (shake flask-nephelometry, Hollifield 1979)

0.0079 (Kenaga & Goring 1980)

0.0017 ($30^{\circ}C$, semimicro gas-saturation method, Westcott et al. 1981)

0.0011, 0.006 (generator column-GC, HPLC-RT correlation, Swann et al. 1983)

$\log [S_L/(mol/L)] = 0.173 - 1263/(T/K)$ (liquid, Passivirta et al. 1999)

0.00012 ± 0.00010 (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)

0.258, 0.252 (supercooled liquid: derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

o,p-DDE

0.140 (shake flask-GC for particles 5 - or less, Biggar & Riggs 1974)

0.0013 (Zepp et al. 1978)

0.10 (selected, Suntio et al. 1988; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

p,p'-DDE

8.65×10^{-4} ($30^{\circ}C$, gas saturation-vapor density-GC, Spencer & Cliath 1972)

9.87×10^{-4} (GC-RT correlation, Westcott & Bidleman 1981)

1.73×10^{-4} ($30^{\circ}C$, gas saturation-GC, Westcott et al. 1981)

8.66×10^{-4} (selected, Yoshida et al. 1983)

2.70×10^{-3} , 2.09×10^{-3} (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)

2.55×10^{-3} (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)

1.73×10^{-3} (20°C, supercooled liquid value, Bidleman et al. 1986)
 7.50×10^{-5} (10°C, estimated, McLachlin et al. 1990)
 0.00225, 0.00334 (supercooled liquid values, GC-RT correlation, Hinckley et al. 1990)
 2.33×10^{-3} , 3.34×10^{-3} (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 2.58×10^{-3} , 1.87×10^{-3} (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log(P_L/Pa) = 12.79 - 4554/(T/K)$ (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
 5.13×10^{-4} , 1.82×10^{-3} (supercooled liquid values at 10°C, 20°C, Cotham & Bidleman 1992)
 4.36×10^{-3} (supercooled liquid value, quoted, Majewski & Capel 1995)
 2.27×10^{-3} , 2.78×10^{-3} ; 5.45×10^{-4} (supercooled liquid P_L : calculated; GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)
 $\log(P_S/Pa) = 16.29 - 5816/(T/K)$ (solid, Passivirta et al. 1999)
 0.0033, 0.0034 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

o,p-DDE

8.21×10^{-4} (30°C, gas saturation-vapor density-GC, Spencer & Cliath 1972)
 8.27×10^{-4} (Callahan et al. 1979, Mabey et al. 1982)
 8.67×10^{-4} (isomer unspecified, estimated, Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations):

27.4 (Levins 1981; quoted, Tucker et al. 1983)
 0.78 (estimated-group method per Hine & Mookerjee 1975)
 6.89 (calculated-P/C, Mabey et al. 1982)
 124 (gas stripping-GC, Atlas et al. 1982)
 19.59 (calculated-P/C, Yoshida et al. 1983)
 7.95 (calculated-P/C, Suntio et al. 1988)
 1.25 (10°C, calculated-P/C, McLachlin et al. 1990)
 34.0 (calculated-P/C, Ballschmiter & Wittlinger 1991)
 120, 370 (23°C), 7.95 (20°C) (quoted, Iwata et al. 1993)
 7.95 (20–25°C, calculated-P/C, Majewski & Capel 1995)
 4.214 (*p,p'*-DDE, wetted wall column-GC, Altschuh et al. 1999)
 $\log(H/(Pa \text{ m}^3/\text{mol})) = 12.62 - 3291/(T/K)$ (*p,p'*-DDE, Passivirta et al. 1999)
 4.2, 4.2 (*p,p*-DDE, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.80 (*o,p*-DDE, O'Brien 1975)
 4.28 (correlated, Metcalf et al. 1975)
 5.69 (*p,p'*-DDE, O'Brien 1975)
 5.83 (*p,p'*-DDE, HPLC-RT correlation, Veith et al. 1979a)
 5.69 (HPLC-RT correlation, Veith et al. 1979b)
 5.77 (Kenaga & Goring 1980)
 5.89 (HPLC-RT correlation, McDuffie 1981)
 5.63 (RP-HPLC-RT correlation, Swann et al. 1983)
 5.89 (estimated-HPLC/MS correlation, Burkhard et al. 1985)
 6.51 (HPLC-RT correlation, Webster et al. 1985)
 6.29 (RP-HPLC correlation, Chin et al. 1986)
 6.09 (RP-HPLC correlation, De Kock & Lord 1987)
 6.956 ± 0.011 (*p,p'*-DDE, shake flask/slow stirring method, De Bruijn et al. 1989; received highest ranking from Pontolillo & Eganhouse 2001)
 6.51 (recommended, Sangster 1993)
 5.78 (RP-HPLC correlation, Sicbaldi & Finizio 1993)
 6.96 (recommended, Hansch et al. 1995)
 5.43 (*o,p'*-, RP-HPLC correlation, Finizio et al. 1997)
 6.65 (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
 6.96, 6.93 (*p,p'*-DDE, LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition coefficient, $\log K_{OA}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 8.40 (*p,p'*-DDE, calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
- 9.45 (*p,p'*-DDE, calculated, Finizio et al. 1997)
- 9.53*, 9.676 (*p,p'*-DDE, gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
- $\log K_{OA} = -7.49 + 5116/(T/K)$; temp range: 5–35°C (*p,p'*-DDE, gas saturation-GC, Shoeib & Harner 2002)
- 9.69, 9.70 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, $\log BCF$:

- 4.44, 4.29 (*Gambusia*, *Physa*, Metcalf et al. 1973)
- 4.05, 4.56, 4.77, 4.08 (alga, snail, mosquito, fish, Metcalf et al. 1975)
- 4.71 (fathead minnows, 32-d exposure, Veith et al. 1979; Veith & Kosian 1983)
- 3.80 (calculated-S or K_{OW} , Kenaga & Goring 1980)
- 4.71, 4.37 (quoted exptl, calculated- K_{OW} , Mackay 1982)
- 5.95 (microorganism-water: calculated- K_{OW} , Mabey et al. 1982)
- 3.34–4.00 mean 4.00; 4.26–4.15 mean 4.15 (*p,p'*-DDE, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
- 4.91, 4.08; 7.25 (*p,p'*-DDE, rainbow trout: kinetic BCF, steady-state BCF, Lake Ontario field BCF, Oliver & Niimi 1985)
- 3.70–5.32 (*p,p'*-DDE, benthic macroinvertebrates, Reich et al. 1986)
- 3.70–5.32 (*o,p'*-DDE, benthic macroinvertebrates, Reich et al. 1986)
- 4.13 (azalea leaves, Bacci & Gaggi 1987)
- 6.01 (*p,p*-DDE, Connell et al. 1988)
- 7.48 (Azalea leaves, Bacci et al. 1990)
- 1.025; -0.824; -0.602 (earthworms: quoted; field/lab. estimated; calculated-modeled, Menzie et al. 1992)
- 4.95, 6.05 (rainbow trout: wet wt basis, lipid wt basis, *p,p'*-DDE, Geyer et al. 2000)
- >4.78, >5.76 (fathead minnow, 32-d uptake: wet wt basis, lipid wt basis, *p,p'*-DDE, Geyer et al. 2000)

Bioaccumulation Factor, $\log BAF$:

- 8.35 (rainbow trout, Thomann 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.48 (calculated-S or K_{OW} , Kenaga & Goring 1980;)
- 6.64 (sediment, calculated- K_{OW} , Mabey et al. 1982)
- 4.70, 5.17 (quoted, calculated-MCI χ , Sabljic 1984)
- 6.00, 5.30 (*p,p'*-DDE, field data of sediment trap material, calculated- K_{OW} , Oliver & Charlton 1984)
- 3.70 (soil, estimated, Hornsby et al. 1996)
- 4.82 (av. lit. value, Gerstl 1990)
- 4.82 (*p,p'*-DDE, soil, calculated- MCI χ , Sabljic et al. 1995)
- 4.85 (*p,p'*-DDE, soil, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: midday $t_{1/2} = 5$ h in hydrocarbon media (Zepp et al. 1976)

$t_{1/2} = 1.5$ d under sunlight in water (Mansour & Feicht 1994).

Oxidation:

Hydrolysis: the first-order rate constant $k = 1.4 \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$ and the hydrolytic $t_{1/2} > 120$ yr in water at 27°C (Wolfe et al. 1977);

hydrolytic $t_{1/2} = 120$ yr at pH 7 and 25°C of 120 yr and a rate constant $k = 6.6 \times 10^{-7} \text{ h}^{-1}$ (Callahan et al. 1979, Mabey et al. 1982).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 170.0 \text{ d}^{-1}$; $k_2 = 0.021 \text{ d}^{-1}$ (*p,p'*-DDE, rainbow trout, Oliver & Niimi 1985)

$k_2 = 0.950 \text{ yr}^{-1}$ (*Larus argentatus*, Norstrom et al. 1986)
 $k_1 = 20800 \text{ d}^{-1}$; $k_2 = 0.020 \text{ d}^{-1}$ (*Oligochaetes*, Connell et al. 1988)
 $k_2 = 0.0004 \text{ h}^{-1}$ (azalea leaves, Paterson et al. 1991)
 $k_2 = 0.0030 \text{ h}^{-1}$ (midge *C. riparius*, water only system, Lydy et al. 1992)
 $k_2 = 0.0046 \text{ h}^{-1}$ (midge *C. riparius*, screened, Lydy et al. 1992)
 $k_2 = 0.0080 \text{ h}^{-1}$ (midge *C. riparius*, 3% organic carbon, Lydy et al. 1992)
 $k_2 = 0.0046 \text{ h}^{-1}$ (midge *C. riparius*, 15% organic carbon, Lydy et al. 1992)

Half-Lives in the Environment:

Air: atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: midday $t_{1/2} = 5 \text{ h}$ in hydrocarbon media (Zepp et al. 1976)

hydrolytic $t_{1/2} > 120 \text{ yr}$ in water at 27°C (Wolfe et al. 1977);

estimated $t_{1/2} = 690 \text{ d}$ in surface waters in case of first order reduction process, and estimated $t_{1/2} > 300 \text{ d}$ in lakes in the Netherlands (Zoeteman et al. 1980);

photolysis $t_{1/2} = 1.5 \text{ d}$ under sunlight in water (Mansour & Feicht 1994).

Ground water:

Sediment:

Soil: field $t_{1/2} = 1000 \text{ d}$ (estimated, Hornsby et al. 1996);

$t_{1/2} > 20 \text{ yr}$, very persistent (Geyer et al. 2000)

$t_{1/2} = 40.9$ and 17.2 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).

Biota: elimination $t_{1/2} = 340 \text{ d}$ (*p,p'*-DDE, rainbow trout, Oliver & Niimi 1985);

$t_{1/2} = 264 \text{ d}$ in herring gulls compared to literature average $t_{1/2} = 300 \text{ d}$ for birds (Norstrom et al. 1986);

elimination $t_{1/2} = 2230 \text{ h}$ (Azalea leaves, Bacci & Gaggi 1987);

$t_{1/2} = 231 \text{ h}$ in the midge (*Chironomus riparius*) under varying sediment conditions (water only system with no sediment), $t_{1/2} = 150 \text{ h}$ (midge screened from the sediment), $t_{1/2} = 87 \text{ h}$ (midge screened from 3% organic carbon sediment), $t_{1/2} = 99 \text{ h}$ (midge screened from 3% organic carbon sediment) (Lydy et al. 1992).

TABLE 18.1.1.22.1

Reported aqueous solubilities of DDE at various temperatures

<i>p,p'</i> -DDE				<i>o,p'</i> -DDE			
Biggar & Riggs 1974				Biggar & Riggs 1974			
shake flask-GC				shake flask-GC			
t/°C	S/g·m ⁻³	S/g·m ⁻³	S/g·m ⁻³	t/°C	S/g·m ⁻³	S/g·m ⁻³	S/g·m ⁻³
particle size	0.01μ	0.05μ	5.0μ	particle size	0.01μ	0.05μ	5.0μ
15			0.055	15			
25	0.010	0.040	0.120	25	0.015	0.040	0.140
35			0.235	35			
45			0.450	45			

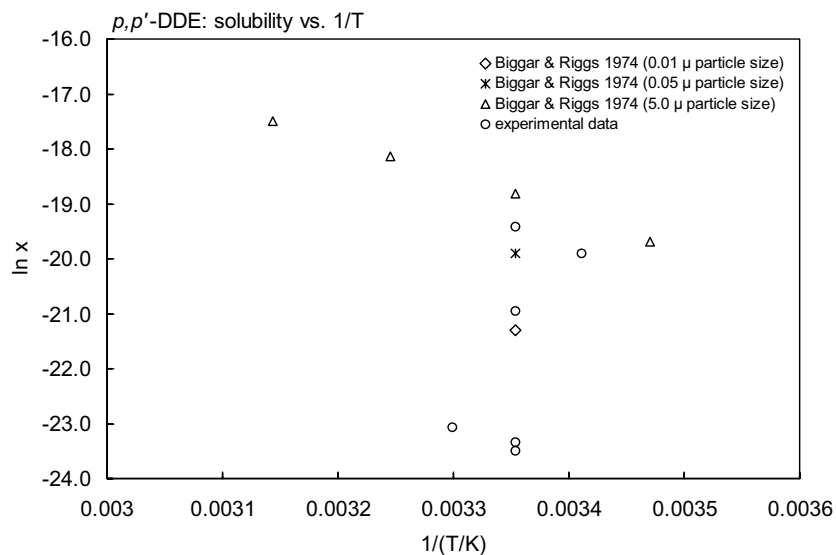


FIGURE 18.1.1.22.1A Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *p,p'*-DDE.

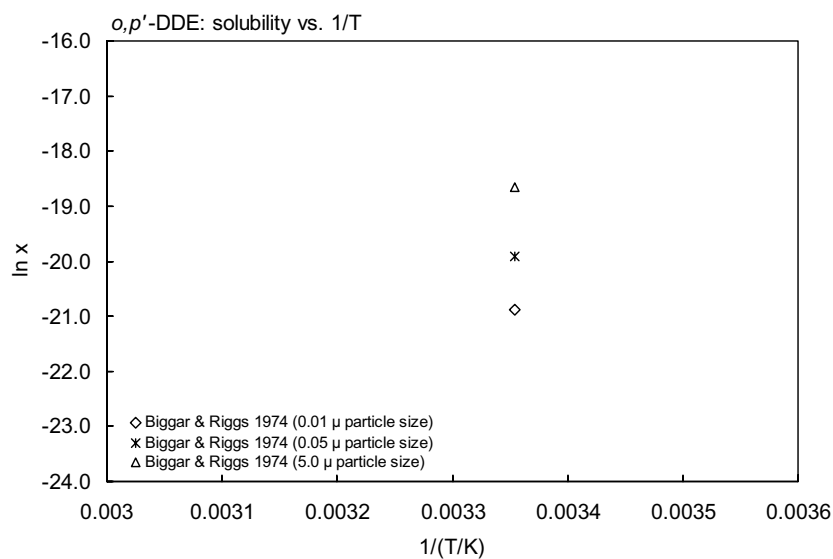
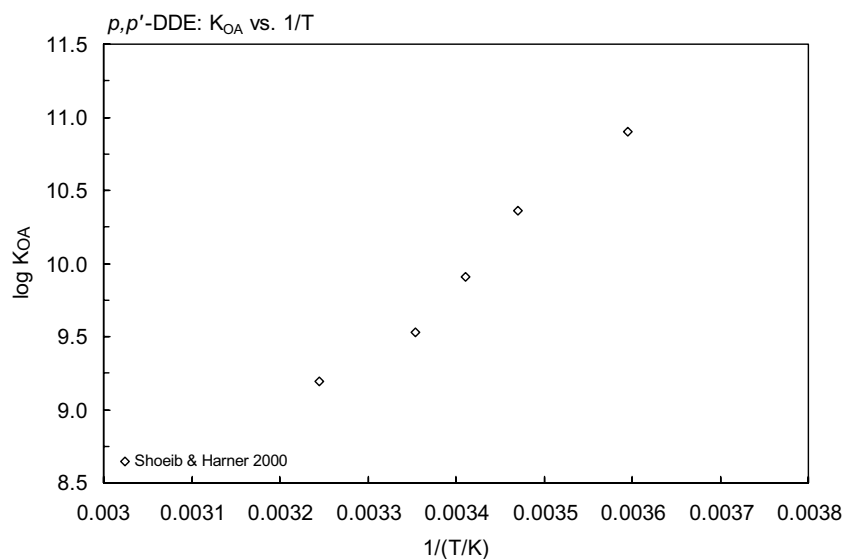


FIGURE 18.1.1.22.1B Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *o,p'*-DDE.

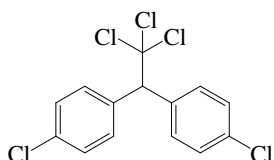
TABLE 18.1.1.22.2

Reported octanol-air partition coefficient of *p,p'*-DDE at various temperaturesShoeib & Harner 2002
generator column-GC/MS

t/°C	log K _{OA}
5	10.905
15	10.361
20	9.906
25	9.530
35	9.196
log K _{OA} = A + B/(T/K)	
A	-7.492
B	5116
enthalpy of phase change	
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 98.0$	

FIGURE 18.1.1.22.2 Logarithm of K_{OA} versus reciprocal temperature for *p,p'*-DDE.

18.1.1.23 DDT



Common Name: DDT

Synonym: Agritan, Anofex, Arkotine, Azotox, Bosan supra, Bovidermol, Cesarex, chlorophenoethane, Chlorophenothanum, Chlorophenotoxum, Citox, Clofenotan, Dedelo, Deoval, Devol, Detox, Detoxan, Dibovan, Dichophane, dichlorodiphenyltrichloroethane, Didigam, Didimac, Dodat, Dykol, ENT 1506, Estonate, Genitox, Gesafid, Gesapon, Gesarex, Gesarol, Guesarol, Gyron, Havero-extra, Ivoran, Ixodex, Kopsol, Mutoxin, Neocid, Parachlorocidum, PEBI, Pentachlorin, Pentech, *p,p'*-DDT, 4,4'-DDT, Rukseam, Santobane, Zeidane, Zerdane

Chemical Name: 1,1,1-trichloro-2,2-bis-(4-chlorophenyl)-ethane; 1,1'-(2,2,2-trichloroethylidene)-bis(4-chlorobenzene)

Uses: persistent nonsystemic insecticide with contact and stomach action to control mosquitoes for the eradication of malaria but is now prohibited and displaced with less persistent insecticides on crop application.

CAS Registry No: 50-29-3 (*p,p'*-DDT, DDT), 789-02-6 (*o,p'*-DDT)

Molecular Formula: $C_{14}H_9Cl_5$

Molecular Weight: 354.486

Melting Point ($^{\circ}C$):

108.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

260 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.55 (Hadaway et al. 1970; Kenaga 1972)

Molar Volume (cm^3/mol):

250 (calculated-density, Chiou 1985)

333.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.196 (*o,p'*-DDT, DSC method, Plato & Glasgow 1969)

26.36 (*p,p'*-DDT, DSC method, Plato & Glasgow 1969)

26.284 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

69.036 (Plato & Glasgow 1969)

70.29 (Hinckley et al. 1990)

72.8 (*p,p'*-DDT, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F:

0.147 (assuming $\Delta S_{fus} = 56$ J/mol K., Mackay et al. 1986)

0.130 ($20^{\circ}C$, assuming $\Delta S_{fus} = 56$ J/mol K, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0002–0.001 ($15^{\circ}C$, shake flask-bioassay, Richards & Cutkomp 1946)

0.0374 (shake flask-radiometric method, measured range 2 – $37.5^{\circ}C$, Babers 1955)

≤ 0.0012 (shake flask-radiometric method, Bowman et al. 1960)

0.035 (shake flask-colorimetric, Lipke & Kearns 1960)

0.0012 (Stephen & Stephen 1963)

0.0016 (99% pure DDT isomers plus DDE at rm. temp., shake flask-GC, Robeck et al. 1965)

0.0034 (Biggar et al. 1966)

0.0017 (ultracentrifugation-GC, Biggar et al. 1967)

0.0012–0.0374 (Günther et al. 1968)

0.0017*, 0.006*, 0.025* (shake flask-GC, *p,p'*-DDT, particle size: 0.01, 0.05, 5.0μ , Biggar & Riggs 1974)

0.004, 0.012, 0.085* (shake flask-GC, *o,p'*-DDT, particle size: 0.01, 0.05, 5.0 μ size or less, Biggar & Riggs 1974)
 0.0055 (generator column-GC/ECD, Weil et al. 1974)
 0.0017 (Martin & Worthing 1977)
 0.0010 (shake flask-GC, Paris et al. 1977)
 0.004 (shake flask-nephelometry, Hollifield 1979)
 0.0012 (Hartley & Graham-Bryce 1980)
 0.040 (shake flask-HPLC, Ellgehausen et al. 1981)
 0.0645 (shake flask-GC, Chiou et al. 1982)
 0.0023 (generator column-GC, Swann et al. 1983)
 0.020 (RP-HPLC-RT correlation, Swann et al. 1983)
 0.0031–0.0034 (Verschuere 1983)
 0.0045 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
 0.030 (RP-HPLC-RT correlation, Chin et al. 1986)
 0.0054 (24°C, shake flask-GC/ECD, Chiou et al. 1986)
 0.0055 (shake flask-GC, Chiou et al. 1991)
 0.001–0.0055 (Montgomery 1993)
 0.0055 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 $\log [S_L/(\text{mol/L})] = -0.195 - 1454/(T/K)$ (liquid, Passivirta et al. 1999)
 0.00023 ± 0.00010 (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
 0.0956, 0.149 (*p,p'*-DDT, supercooled liquid S_L : derivation of literature-derived value LDV, final-adjusted value FAV, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.0×10^{-5} * (*p,p'*-DDT, 20°C, effusion manometer, measured range 0–100°C, Balson 1947)
 $\log (P/\text{mmHg}) = 14.191 - 6160/(T/K)$, temp range 66–100°C (Antoine eq., effusion, Balson 1947)
 $\log (P/\text{mmHg}) = 13.778 - 6010/(T/K)$; temp range 50–90°C (Antoine eq., effusion, Dickinson 1947)
 0.001973 *, 0.002027 * (*p,p'*-DDT, 50.1°C, gas saturation-spec., measured range 50.1–90.2°C, Dickinson 1956)
 3.30×10^{-5} (interpolated exptl. data of Balson 1947, Spencer & Cliath 1970; Ballschmiter & Wittlinger 1991)
 3.33×10^{-5} (20°C, partition coefficient, Atkins & Eggleton 1971)
 2.53×10^{-5} (20°C, Melnikov 1971; Spencer 1973, 1982; Callahan et al. 1979, Mabey et al. 1982)
 2.03×10^{-5} * (20°C, *p,p'*-DDT, 30°C, gas saturation-GC, measured range 20–40°C, Spencer & Cliath 1972)
 $\log (P/\text{mmHg}) = 14.24 - 6176/(T/K)$; temp range 20–40°C (*p,p'*-DDT, 30°C, gas saturation-GC, Antoine eq., Spencer & Cliath 1972; Spencer 1975)
 7.37×10^{-4} (*o,p'*-DDT, 30°C, gas saturation-GC, Spencer & Cliath 1972; Spencer 1975)
 2.50×10^{-5} (20°C, Hartley & Graham-Bryce 1980; Worthing & Hance 1991)
 5.73×10^{-5} * (*p,p'*-DDT, gas saturation-HPLC/liquid scintillation spectrometry, measured range 20–80°C, Rothman 1980)
 2.00×10^{-5} (20–25°C, Weber et al. 1980)
 1.50×10^{-4} (20°C, GC, Seiber et al. 1981)
 6.0×10^{-4} , 1.12×10^{-3} (*o,p'*-DDT 25, 30°C, capillary GC-RT correlation, Westcott & Bidleman 1981)
 1.17×10^{-3} (*o,p'*-DDT, 30°C, semi-micro gas-saturation-GC, Westcott et al. 1981)
 4.30×10^{-5} (estimated-relative volatilization rate, Dobbs & Cull 1982)
 2.67×10^{-3} , 2.67×10^{-5} (20°C, calculated values, Grain 1982)
 $2.01 \times 10^{-5} - 2.8 \times 10^{-5}$ (gas saturation, Jaber et al. 1982)
 1.96×10^{-5} (20°C, evaporation rate at 20–60°C, Gückel et al. 1982)
 4.31×10^{-5} (20°C, relative loss rate, Dobbs & Cull 1982)
 1.61×10^{-3} , 1.28×10^{-3} (*o,p'*-DDT, P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
 1.33×10^{-3} (*o,p'*-DDT, supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)
 8.30×10^{-4} , 4.70×10^{-4} (*p,p'*-DDT, P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
 3.16×10^{-4} (*p,p'*-DDT, supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)
 2.48×10^{-5} (20°C, GC-RT correlation, Kim 1985)
 1.73×10^{-4} (20°C, supercooled liquid value, Bidleman et al. 1986)
 2.50×10^{-5} (Hartley & Kidd 1987; Tomlin 1994)
 1.33×10^{-3} , 1.83×10^{-3} (*o,p'*-DDT, supercooled liquid P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)

- 1.614×10^{-3} , 1.035×10^{-3} (*o,p'*-DDT, P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log (P_L/Pa) = 12.77 - 4626/(T/K)$ (*o,p'*-DDT, supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
 3.16×10^{-4} , 5.12×10^{-4} (*p,p'*-DDT, supercooled liquid P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 8.30×10^{-4} (*p,p'*-DDT, P_{GC} by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
 $\log (P_L/Pa) = 13.02 - 4865/(T/K)$ (*p,p'*-DDT, GC-RT correlation, supercooled liquid, Hinckley et al. 1990)
 6.92×10^{-5} , 2.69×10^{-4} , 9.33×10^{-4} (supercooled liquid values at 10°C, 20°C, 30°C, calculated from Hinckley et al. 1990; Cotham & Bidleman 1992)
 2.27×10^{-8} (20°C, Montgomery 1993)
 2.53×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 1.715×10^{-5} * (*p, p'*-DDT 20°C, gas saturation-GC/ECD, measured range 0–40°C, Wania et al. 1994)
 $\log (P/Pa) = 16.62 - 6276/(T/K)$, temp range 0–40°C (Antoine eq., gas saturation, Wania et al. 1994)
 1.05×10^{-4} (supercooled liquid P_L , GC-RT correlation; Donovan 1996)
 5.01×10^{-4} (supercooled liquid P_L , Wania & Mackay 1996)
 4.39×10^{-4} , 4.27×10^{-4} , 3.78×10^{-5} (supercooled liquid P_L , calculated; GC-RT correlation; solid P_S converted from P_L with fugacity ratio F , Passivirta et al. 1999)
 $\log (P_S/Pa) = 16.62 - 6276/(T/K)$ (solid, quoted from Wania et al. 1994, Passivirta et al. 1999)
 $\log (P_L/Pa) = 12.82 - 4823/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
 $\log (P_L/Pa) = (12.38 \pm 0.48) - (4665 \pm 166)/(T/K)$; $\Delta S_{fus} = 70.9 \text{ J mol}^{-1} \text{ K}^{-1}$ (*p,p'*-DDT, supercooled liquid, summary of literature exptl. data, Bidleman et al. 2003)
0.00056, 0.00048 (*p,p'*-DDT, supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
 $\log (P_L/Pa) = -4666/(T/K) + 12.40$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 1.30 (measured, Atkins & Eggleton 1971)
3.94 (calculated-P/C, Mackay & Leinonen 1975)
6.02 (20–25°C, calculated, Thibodeaux 1979)
7.48 (20°C, volatilization rate, Burkhard & Guth 1981)
7.29 (calculated-P/C, Levins 1981)
5.30 (calculated-P/C, Mackay & Shiu 1981)
1.60 (calculated-P/C, Mabey et al. 1982)
3.85 (calculated-P/C, Thomas 1982)
0.466 (estimated-group method per Hine & Mookerjee 1975, Tucker et al. 1983)
4.96 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
1.63 (calculated-P/C, Caron et al. 1984)
1.31 (calculated-P/C, Mackay et al. 1986)
4.96, 8.18 (calculated-P/C, Taylor & Glotfelty 1988)
2.36 (20°C, calculated-P/C, Suntio et al. 1988)
1.28, 1.33 (22–24°C, fog chamber-concn. ratio-GC/ECD, Fendinger et al. 1989)
0.862 (23°C, wetted-wall column-GC/ECD, Fendinger et al. 1989, 1990)
0.16 (0°C, selected, Cotham & Bidleman 1991)
2.90 (calculated-P/C, Calamari et al. 1991)
6.0 (calculated-P/C, Ballschmiter & Wittlinger 1991)
1.55 (calculated-bond contribution method, Meylan & Howard 1991)
1.31, 0.86 (25°C, 24°C, Iwata et al. 1993)
1.31 (23°C, quoted, Montgomery 1993)
0.843 (*p,p'*-DDT, wetted wall column-GC, Altschuh et al. 1999)
 $\log (H/(\text{Pa m}^3/\text{mol})) = 13.02 - 3369/(T/K)$ (Passivirta et al. 1999)
1.1, 1.1 (*p,p'*-DDT, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.98 (shake flask, Kapoor et al. 1973; Lu & Metcalf 1975)
6.19 (calculated, O'Brien 1975)

- 6.36 (shake flask-GC, Chiou et al. 1982)
- 4.89 (Wolfe et al. 1977; Callahan et al. 1979)
- 5.98 (Kenaga & Goring 1978, 1980; Kenaga 1980b)
- 6.19 (shake flask-GC, Freed et al. 1979)
- 3.98–6.19 (Hansch & Leo 1979)
- 6.36 (shake flask, Karickhoff et al. 1979)
- 5.75 (HPLC-RT correlation, Veith et al. 1979b, 1980; Veith & Kosian 1983)
- 6.69 (Belluck & Felsot 1981)
- 5.94 (shake flask-GC/LC, Ellgehausen et al. 1981)
- 5.55 (HPLC- k' correlation, McDuffie 1981)
- 6.38 (HPLC-RT correlation, Hammers et al. 1982)
- 5.10 \pm 0.1 (radioactive analysis method, Platford et al. 1982)
- 5.60 (shake flask-GC, Platford 1982, 1983)
- 5.90 (average of shake flask values, Eadsforth & Moser 1983)
- 6.12 (average of HPLC-RT correlation, Eadsforth & Moser 1983)
- 6.20 (Elgar 1983)
- 5.44 (shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
- 6.40 (HPLC-RV correlation, Garst 1984)
- 5.44 (estimated-HPLC/MS; Burkhard et al. 1985)
- 6.22 (HPLC-RT correlation, Brooke 1986)
- 6.06 (RP-HPLC-RT correlation, Chin et al. 1986)
- 6.21 (HPLC-RT correlation, Eadsforth 1986)
- 6.19 (RP-HPLC correlation, De Kock & Lord 1987)
- 6.51 (HPLC-RT correlation, Liu & Leng 1988)
- 6.914 \pm 0.030 (p,p' -, shake flask/slow-stirring method, De Bruijn et al. 1989; received highest ranking from Pontolillo & Eganhouse 2001)
- 6.307 \pm 0.045; 6.914 \pm 0.030 (shake flask-UV/GC/HPLC, BRE value, RITOX value, inter-laboratory studies, Brooke et al. 1990; received highest ranking from Pontolillo & Eganhouse 2001)
- 4.89–6.91 (Montgomery 1993)
- 5.50 (RP-HPLC correlation, Sicbaldi & Finizio 1993)
- 6.36 (recommended, Sangster 1993)
- 8.3064 (o,p' -DDT, calculated-UNIFAC group-interaction, Chen et al. 1993)
- 6.91 (recommended, Hansch et al. 1995)
- 5.65 (o,p' -DDT, RP-HPLC-RT correlation, Finizio et al. 1997)
- 5.50 (p,p' -DDT, RP-HPLC-RT correlation, Finizio et al. 1997)
- 6.50 (p,p' -DDT, quoted lit., calculated, Passivirta et al. 1999)
- 6.65 (mean literature value-basic statistics for uncensored original data, Pontolillo & Eganhouse 2001)
- 6.28, 6.39 (p,p' -DDT, LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 10.09, 9.22 (p,p' -DDT, generator column-GC/ECD, calculated- K_{OW}/K_{AW} , Harner & Mackay 1995)
- 8.70 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
- 9.93 (p,p' -DDT, calculated, Finizio et al. 1997)
- 9.66* (o,p' -DDT, gas saturation-GC/MS, measured range 5–35°C, Shoeib & Harner 2002)
- $\log K_{OA} = -11.291 + 6266/(T/K)$, temp range 5–35°C (o,p' -DDT, gas saturation-GC, Shoeib & Harner 2002)
- 9.879*, 9.816 (p,p' -DDT, gas saturation-GC/MS, calculated, measured range 5–45°C, Shoeib & Harner 2002)
- $\log K_{OA} = -5.63 + 4603/(T/K)$, temp range 5–35°C (p,p' -DDT, gas saturation-GC, Shoeib & Harner 2002)
- 9.81, 9.73 (p,p' -DDT, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, $\log BCF$:

- 5.31–6.23 (earthworms, Wheatley & Hardman 1968)
- 2.42 (*Cylindrotheca closterium*, Keil & Priester 1969)
- 4.40; 4.90; 4.40 (*Syracosphaera carterae*; *Amphidarium cartaria*; *Tholassiosira fluviatilus*, Cox 1970)
- 4.00 (pinfish, Hansen & Wilson 1970)
- 4.58 (Atlantic croaker, Hansen & Wilson 1970)

- 3.94 (soft clam, Butler 1971)
- 4.20–4.36 (*Daphnia magna* over concn. gradient 8 µg/L to 1.1 mg/L, Crosby & Tucker 1971)
- 5.00 (*Daphnia magna* at water level 80 ng/L, Johnson et al. 1971)
- 4.27 (*Daphnia magna*, wet wt. basis, Crosby & Tucker 1971)
- 4.45 (*Daphnia magna*, wet wt. basis, Johnson et al. 1971;)
- 4.08–4.60 (fishes, Menzie 1972)
- 4.93, 4.54 (*Gambusia, Physa*, Metcalf et al. 1973)
- 4.68 (oyster, Parrish 1974)
- 4.79 (*Ankistrodesmus*, Neudorf & Khan 1975)
- 3.52–3.63, 3.11–3.43 (bacteria, algae, Wolfe et al. 1977)
- 3.14 (trout muscle, Branson 1978)
- 4.47 (fathead minnow, 32-d exposure, Veith et al. 1979b, 1980)
- 4.72 (bluegill sunfish-kinetic value, Bishop & Maki 1980)
- 4.79, 4.93 (fish: flowing water, static water; Kenaga 1980a,b; Kenaga & Goring 1980)
- 4.35; 4.43 (calculated-S, calculated-K_{OC}, Kenaga 1980a)
- 0.045 (average beef fat diet, Kenaga 1980b)
- 4.15 (pulex, Kenaga & Goring 1980)
- 4.11 (algae, estimated, Baughman & Paris 1981)
- 2.95–3.03; 3.02–3.13 (*Rhodotorulus solani, Alfafa tissue*, Baughman & Paris 1981)
- 2.10 (*Triaenodes tardus*, Belluck & Felsot 1981)
- 5.38 (calculated-K_{OW}, Briggs 1981)
- 5.11 (selected, Schnoor & McAvoy 1981, Schnoor 1992)
- 4.36, 4.15, 4.43 (estimated-S, calculated-K_{OW}, calculated-K_{OC}, Bysshe 1982)
- 4.47, 4.43 (fish: quoted, correlated, Mackay 1982)
- 4.37 (mussels, quoted average, Geyer et al. 1982)
- 6.90 (microorganism-water, Mabey et al. 1982)
- 2.30, 4.08 (trout, pinfish, Verschueren 1983)
- 4.71 (15°C, rainbow trout, Davies & Dobbs 1984)
- 5.00 (25°C, fathead minnow-steady state, Davies & Dobbs 1984)
- 4.15 (activated sludge, Freitag et al. 1984)
- 3.97, 3.46, 4.15 (algae, fish, activated sludge, Klein et al. 1984)
- 3.97, 3.28, 4.15 (algae, golden ide, activated sludge, Freitag et al. 1985)
- 4.97 (*Oncorhynchus mykiss*, Muir et al. 1985)
- 3.91, 3.08 (rainbow trout: kinetic, steady-state, Oliver & Niimi 1985)
- 4.47, 4.56 (oyster, calculated-K_{OW} & models, Zaroogian et al. 1985)
- 3.24–5.00 (*p,p'*-DDT, benthic macroinvertebrates, Reich et al. 1986)
- 3.44–5.71 (*o,p'*-DDT, benthic macroinvertebrates, Reich et al. 1986)
- 4.08 (*Selenastrum capricornutum*, Mailhot 1987)
- 6.50 (zooplankton, chum salmon; Kawano et al. 1988)
- 1.55 (beef biotransfer factor log B_b, correlated-K_{OW} from Radeleff et al. 1952 & Kenaga 1980, Travis & Arms 1988)
- 2.62 (milk biotransfer factor log B_m, correlated-K_{OW} from Fries et al. 1969; Saha 1969 & Whiting et al. 1973, Travis & Arms 1988)
- 1.80 (vegetation, correlated-K_{OW} from Beall & Nash 1972 & Voerman & Besemer 1975, Travis & Arms 1988)
- 5.28, 7.64 (dry leaf, wet leaf, Bacci et al. 1990)
- 4.47, 4.30 (quoted, calculated, Banerjee & Baughman 1991)
- 4.72 (selected, Chessells et al. 1992)
- 0.155, –1.0 (earthworms, quoted, field/lab., Menzie et al. 1992)
- 1.0, –0.602 (earthworms, field leaf litter, calculated-model, Menzie et al. 1992)
- 4.81, 4.86, 4.95, 4.99 (*Oncorhynchus mykiss*, Muir et al. 1994)
- 4.05, 2.85, 3.70 (algae *Selenastrum capricornutum*, water flea *Daphnia magna*, catfish *Ictalurus melas*, wet wt. basis, Wang et al. 1996)
- 3.97, 4.81 (algae *Chlorella*: wet wt basis, dry wt basis, *p,p'*-DDT, Geyer et al. 2000)

- 4.45, 6.45 (*Daphnia*: wet wt basis, lipid wt basis, *p,p'*-DDT, Geyer et al. 2000)
 5.14, 7.06 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, *p,p'*-DDT, Geyer et al. 2000)
 4.97, 6.67 (rainbow trout: wet wt basis, lipid wt basis, *p,p'*-DDT, Geyer et al. 2000)
 >4.57, >5.55 (fathead minnow, 10.5% lipid, 28-d: wet wt basis, lipid wt basis, *o,p'*-DDT, Geyer et al. 2000)

Bioaccumulation Factor BAF:

- 1.27 (bioaccumulation factor log BAF, adipose tissue in male Albino rats, Berdanier & de Dennis 1977)
 4.20; 3.539; 3.35 (log BF-bioaccumulation factor of algae; catfish; daphnids, Ellgehausen et al. 1980)
 5.10 (fish, reported as log BAF_w, LeBlanc 1995)

Sorption Partition Coefficient, log K_{OC}:

- 5.38 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980; Karickhoff 1981)
 3.93 (sediment, Wolfe et al. 1977)
 5.38 (calculated-K_{OW}, Kenaga 1980)
 5.16 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
 5.38 (Kenaga & Goring 1980; quoted, Hodson & Williams 1988)
 5.18 (average 3 soils, HPLC-RT correlation, McCall et al. 1980)
 5.39 (average soils/sediments, Rao & Davidson 1980)
 5.20, 5.18, 5.18; 5.18 (commerce soil, Tracy soil, Catlin soil; average soil, McCall et al. 1980)
 5.00 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
 5.62; 6.81, 5.80 (estimated-S; estimated-S and mp, calculated-K_{OW}, Karickhoff 1981)
 6.59 (calculated-K_{OW}, Mabey et al. 1982)
 5.38 (soil, Thomas 1982; quoted, Nash 1988)
 5.20 (Pavlou & Weston 1983, 1984)
 5.18, 4.64 (soil slurry method, HPLC-RT correlation, Swann et al. 1983)
 5.38 (soil, Jury et al. 1984; quoted, Mackay & Stiver 1991)
 5.38, 5.33 (soil: quoted, calculated-MCI χ , Sabljic 1984)
 5.61 (Caron et al. 1984)
 5.39 (soil, estimated, Karickhoff 1985)
 6.00 (best estimate at low sediment concn., Karickhoff 1985)
 5.11–5.45 (Aldrich humic acid, Landrum et al. 1984)
 4.28–4.66 (natural water, Landrum et al. 1984)
 5.61 \pm 0.11 (Chiou et al. 1987; quoted, Chin et al. 1991)
 6.03 (predicted-K_{OW}, Chiou et al. 1987)
 5.39 (selected, Elzerman & Coates 1987)
 3.94 (calculated-MCI χ , Gerstl & Helling 1987)
 5.38 (soil, screening model calculations, Jury et al. 1987a,b; Jury & Ghodrati 1989)
 5.38, 5.34 (quoted, calculated- MCI χ , Bahnick & Doucette 1988)
 5.63 (RP-HPLC-k' correlation, cyanopropyl column, Hodson & Williams 1988)
 4.09 (calculated-K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
 5.15–6.26 (Montgomery 1993)
 6.59 (estimated-QSAR and SPARC, Kollig 1993)
 6.30 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 5.31 (soil, calculated-MCI χ , Sabljic et al. 1995)
 5.63; 5.34 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 5.17 (*p,p'*-DDT, soil, estimated-general model, Gramatica et al. 2000)
 6.08 (*p,p'*-DDT, average values for sediments OC \geq 0.5%, Delle Site 2001)
 5.63, 5.54 (*p,p'*-DDT, soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)
 5.20 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

Sorption Partition Coefficient, log K_{OM}:

- 5.14 (exptl., Briggs 1981)
 4.24 (calculated-Parachor, Briggs 1981)
 4.88 – 5.41 (Mingelgrin & Gerstl 1983)
 5.69, 5.59, 5.69 (average soil, sediment, soil and sediment, Gerstl & Mingelgrin 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 3.7$ d for water depth of 1 m (Mackay & Wolkoff 1973);

$t_{1/2} = 73.9$ h (Mackay & Leinonen 1975, Branson 1978);

initial rate constant $k = 6.9 \times 10^{-4} \text{ h}^{-1}$ and predicted rate constant $k = 1.2 \times 10^{-3} \text{ h}^{-1}$ from soil with $t_{1/2} = 578$ h;

$t_{1/2}(\text{calc}) = 45$ h from water (Thomas 1982);

half-flux values times, 0.3 d from field study, 0.3–12 d from microagroecosystem, >80–1000 d from laboratory data (Nash 1983).

Photolysis: midsummer direct photolysis $k = 8.5 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} > 227000$ h in water, $t_{1/2} = 280000$ h in hydrocarbon media; midday $t_{1/2} > 460000$ h (52.5 yr) average over all seasons in water at latitude 40°N , daily average direct photolysis $t_{1/2} > 150$ yr (12-h days) in water in the Central U.S. (Zepp et al. 1976)

using fungus and either 254 or 300 nm UV light, more than 97% initial added amounts were metabolized in 3 wk of incubation (Katayama & Matsumura 1991).

Oxidation: $t_{1/2} = 22$ yr, estimated first-order half-life in aquatic environment (Callahan et al. 1979)

$k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, $k = 3600 \text{ M}^{-1} \text{ h}^{-1}$ for RO_2 (Mabey et al., 1982)

photooxidation $t_{1/2} = 17.7$ –177 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

photooxidation $t_{1/2} = 168$ –8400 h in water, based on measured rate of photooxidation in two natural waters under sunlight for 7 d and 56 d (Howard et al. 1991)

Hydrolysis: $k(\text{alkaline}) = 9.90 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C corresponds to $t_{1/2} = 81$ d at pH 9, $k(\text{neutral}) = 1.9 \times 10^{-9} \text{ s}^{-1}$ corresponds to $t_{1/2} = 12$ yr in 5% acetonitrile-water at pH 5 and 27°C (Wolfe et al. 1977b)

$k(\text{alkaline}) = 9.90 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at pH 9, $k(\text{neutral}) = 1.9 \times 10^{-9} \text{ s}^{-1}$ for $1 \times 10^{-8} \text{ M}$ in water at 27°C (Harris 1982)

$k = 1.57 \times 10^{-4} \text{ h}^{-1}$ at pH 7 (Neely & Blau 1985)

$k = 6.0 \times 10^{-2} \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993).

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 2$ –15.6 yr based on observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 16$ –100 d, based on anaerobic flooded soil die-away data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991)

$t_{1/2} = 3837$ d (Hamaker 1972; quoted, Jury et al. 1983, 1984, 1987a, b, Jury & Ghodrati 1989)

$k = 0.00013 \text{ d}^{-1}$ from soil incubation studies, and $k = 0.0035 \text{ d}^{-1}$ from flooded soil incubation studies in anaerobic system both by die-away test (Rao & Davidson 1980; quoted, Scow 1982)

$t_{1/2}(\text{aq. aerobic}) = 2$ –15.6 yr, based on aerobic degradation in soil; $t_{1/2}(\text{aq. anaerobic}) = 16$ –100 d, based on anaerobic flooded soil die-away study data (Howard et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.002, 0.0007 \text{ h}^{-1}$ (algae, daphnids, Ellgehausen et al. 1980)

$k_2 = 0.052 \text{ d}^{-1}$ (catfish, Ellgehausen et al. 1980)

$k_1 = 170 \text{ d}^{-1}$; $k_2 = 0.0021 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1 = 818 \text{ d}^{-1}$; $k_2 = 0.009 \text{ d}^{-1}$ (rainbow trout, Muir et al. 1985)

$k_2 = 8.60 \text{ yr}^{-1}$; $k_2 = 4.50 \text{ yr}^{-1}$ (*P. hoyi*, Evans et al. 1991)

$k_1 = 20609 \text{ d}^{-1}$; $k_2 = 1.845 \text{ d}^{-1}$ (algae *Selenastrum capricornutum*, Wang et al. 1996)

$k_1 = 135.6 \text{ d}^{-1}$; $k_2 = 0.191 \text{ d}^{-1}$ (water flea *Daphnia magna*, Wang et al. 1996)

$k_1 = 9.761 \text{ d}^{-1}$; $k_2 = 0.002 \text{ d}^{-1}$ (catfish *Ictalurus melas*, Wang et al. 1996)

Half-Lives in the Environment:

Air: $t_{1/2} = 17.7$ –177 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Howard et al. 1991; Mortimer & Connell 1995);

half-lives for ΣDDT in the Great Lake's atmosphere. $t_{1/2} = 17.0 \pm 6.8$ yr at Eagle Harbor, $t_{1/2} = 8.2 \pm 1.4$ yr at Sleeping Bear Dunes and $t_{1/2} = 7.1 \pm 1.0$ yr at Sturgeon Point (Buehler et al. 2004).

Surface water: dehydrochlorination rate constant $k = 1.75 \times 10^{-2} \text{ h}^{-1}$ for 1 ppm *p,p'*-DDT and $k = 1.65 \times 10^{-2} \text{ h}^{-1}$ for 1 ppm *o,p'*-DDT both at $21 \pm 2^\circ\text{C}$ and pH 12.8, in 0.1 N NaOH solution (Choi & Chen 1976);

degradation $t_{1/2} = 8$ yr in water at 27°C (Wolfe et al. 1977);

midsummer direct photolysis $t_{1/2} > 227000$ h in water, $t_{1/2} = 280000$ h in hydrocarbon media; midday $t_{1/2} > 460000$ h (52.5 yr) average over all seasons in water at latitude 40°N , daily average direct photolysis $t_{1/2} > 150$ yr (12-h days) in water in the Central U.S. (Zepp et al. 1976)

- $t_{1/2} = 73.9$ h for a pond 1 m deep (Branson 1978);
 $t_{1/2} = 168\text{--}8400$ h, based on measured rate of photooxidation in two natural waters under sunlight for 7 d and 56 d (Callahan et al. 1979; quoted, Howard et al. 1991; Mortimer & Connell 1995);
 estimated $t_{1/2} = 110$ and 56 d for o,p- and p,p-DDT, respectively, in surface waters in case of first order reduction process may be assumed in the Netherlands (Zoeteman et al. 1980)
 degradation $t_{1/2} \sim 10$ yr average from the loss rates in Lake Michigan (Bierman & Swain 1982).
 Ground water: $t_{1/2} = 16$ d to 31.3 yr, based on anaerobic flooded soil die-away data for two flooded soils (Castro & Yoshida 1971; quoted, Howard et al. 1991) and observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991).
 Sediment: $t_{1/2} = 3$ to 5 yr (Bierman & Swain 1982); $t_{1/2} = 21$ yr (conversion of p,p'-DDT to p,p'-DDE in sediment, Oliver et al. 1989); $t_{1/2} = 78800$ h (quoted mean value from Howard et al. 1991, Mortimer & Connell 1995).
 Soil: $t_{1/2} = 2\text{--}15.6$ yr, based on observed rates of biodegradation in aerobic soils under field conditions (Lichtenstein & Schultz 1959; Stewart & Chisholm 1971; quoted, Howard et al. 1991);
 average $t_{1/2} \sim 12$ yr in 3 different soils for ~ 50 ppm in soil (Nash & Woolson 1967);
 estimated persistence of 4 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);
 field $t_{1/2} = 173$ d when incorporated into soil (Willis et al. 1971; quoted, Nash 1983);
 microagroecosystem $t_{1/2} > 50$ d with open cotton canopy (quoted, Nash 1983);
 persistence of more than 36 months (Wauchope 1978);
 $t_{1/2} > 50$ d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988);
 estimated first-order $t_{1/2} = 14.6$ yr from biodegradation rate constant $k = 0.00013\text{ d}^{-1}$ from soil incubation studies and $t_{1/2} = 198$ d from rate constant $k = 0.0035\text{ d}^{-1}$ from flooded soil incubation studies in anaerobic system both by die-away test (Rao & Davidson 1980; quoted, Scow 1982);
 very persistent in soils with $t_{1/2} > 100$ d (Willis & McDowell 1982);
 microagroecosystem $t_{1/2} > 50$ d in moist fallow soil (Nash 1983);
 $t_{1/2} = 3837$ d from screening model calculations (Jury et al. 1984, 1987a, b; Jury & Ghorati 1989);
 $t_{1/2} = 173$ d from field study, $t_{1/2} > 50$ d from microagroecosystem, $t_{1/2} = 116$ d from laboratory data (Nash 1985);
 $t_{1/2} = 3800$ d (Jury et al. 1987; quoted, Montgomery 1993);
 reaction $t_{1/2} = 3837$ d and overall $t_{1/2} =$ in soil 9.4 yr (Mackay & Stiver 1991);
 estimated field $t_{1/2} = 2000$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
 $t_{1/2} = 14.0$ and 12.0 yr for control and sludge-amended Luddington soils, respectively, for o,p'-DDT, and
 $t_{1/2} = 11.8$ and 10.5 yr for control and sludge-amended Luddington soils, respectively, for p,p'-DDT (Meijer et al. 2001).
 Biota: field $t_{1/2} = 15$ d in fruit leaves (Decker et al. 1950; quoted, Nash 1983);
 microagroecosystem $t_{1/2} = 29$ d in cotton leaves (Nash & Harris 1977; quoted, Nash 1983);
 $t_{1/2} = 915$ h from fish compared with calculated value of $t_{1/2} = 517$ h from regression (Neely 1980);
 $t_{1/2} = 0.70$ h in algae, $t_{1/2} = 3.65$ d in catfish and $t_{1/2} = 315$ h in daphnids (Ellgehausen et al. 1980);
 $t_{1/2} = 340$ d in rainbow trout (Oliver & Niimi 1985);
 biochemical $t_{1/2} = 3837$ d (Jury et al. 1987a, b; Jury & Ghodrati 1989);
 biological $t_{1/2} = 77$ d for trout, $t_{1/2} = 31$ d for salmon, $t_{1/2} = 4$ d for catfish (Niimi 1987).

TABLE 18.1.1.23.1
Reported aqueous solubilities of DDT at various temperatures

<i>p,p'</i> -DDT				<i>o,p'</i> -DDT			
Biggar & Riggs 1974				Biggar & Riggs 1974			
shake flask-GC				shake flask-GC			
t/°C	S/g·m ⁻³	S/g·m ⁻³	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
particle size	0.01μ	0.05μ	5.0μ	particle size	0.01μ	0.05μ	5.0μ
15	0.001	0.0025	0.017	15			0.050
25	0.0017	0.006	0.025	25	0.004	0.012	0.085
35	0.0026	0.013	0.037	35			0.135
45	0.0039	0.0275	0.045	45			0.200

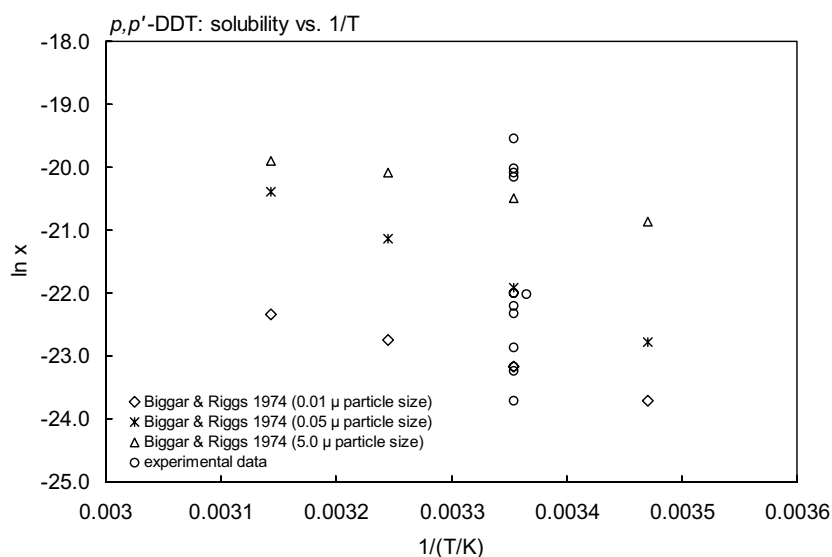


FIGURE 18.1.1.23.1A Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *p,p'*-DDT.

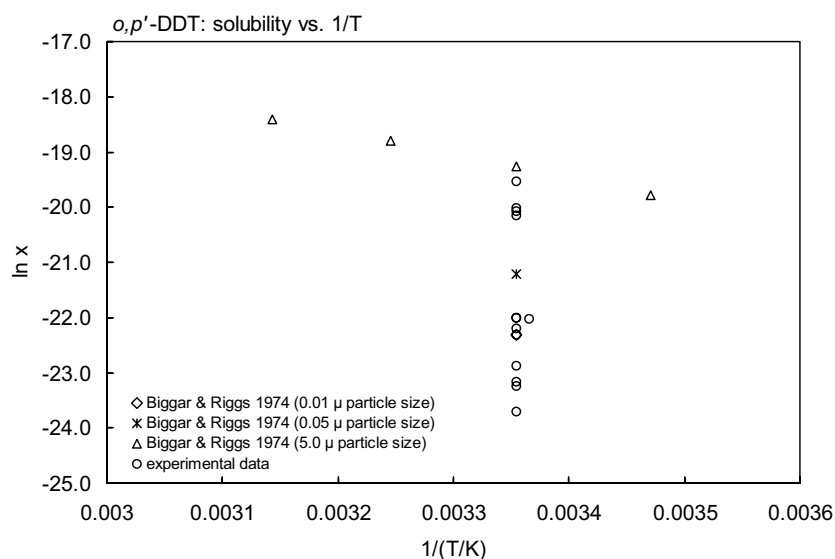


FIGURE 18.1.1.23.1B Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *o,p'*-DDT.

TABLE 18.1.1.23.2

Reported vapor pressures of DDT at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Balson 1947		Dickinson 1956		Spencer & Cliath 1972		Rothman 1980	
effusion manometer		gas saturation-spec.		gas saturation-GC		radiotracer transpiration	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
<i>p,p'</i> -DDT		<i>p,p'</i> -DDT		<i>p,p'</i> -DDT		<i>p,p'</i> -DDT	
0	5.87×10^{-7}	71.0	0.01947	20	2.03×10^{-5}	20	2.93×10^{-5}
10	3.60×10^{-6}	71.0	0.02586	30	9.68×10^{-5}	25	5.73×10^{-5}
20	2.00×10^{-5}	71.0	0.02733	40	4.43×10^{-4}	30	1.24×10^{-4}
30	9.60×10^{-5}	70.7	0.02706			40	5.33×10^{-4}
40	4.27×10^{-4}	70.7	0.02640	eq. 1	P/mmHg	50	2.0×10^{-3}
50	1.77×10^{-3}	70.7	0.02680	A	14.24	60	6.40×10^{-3}
60	4.00×10^{-3}	71.3	0.02973	B	6176	70	0.020
70	0.0231	71.3	0.02893			80	0.060
80	0.0301	50.1	0.001973	<i>o,p'</i> -DDT			
90	0.224	50.1	0.002027	30	7.37×10^{-4}	$\Delta H_{\text{sub}} = 100.6 \text{ kJ/mol}$	
100	0.640	60.1	0.007106				
		60.1	0.006999				
		60.1	0.007199				
eq. 1	P/mmHg	80.4	0.08053				
A	14.191	80.4	0.07666				
B	6160	80.4	0.07879				
temp range: 66–100 $^{\circ}\text{C}$		80.4	0.07599				
		88.8	0.2039				
		88.8	0.1933				
		90.2	0.2200				
		90.2	0.2346				
		eq. 1	P/mmHg				
		A	13.778				
		B	6010				

TABLE 18.1.1.23.2 (Continued)

2.

Westcott et al. 1981		Westcott & Bidleman 1981		Wania et al. 1994	
gas saturation-GC		capillary GC-RT correlation		gas saturation-GC/ECD	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
<i>o,p'</i> -DDT					
30	1.17 × 10 ⁻³	<i>o,p'</i> -DDT		<i>p,p'</i> -DDT	
		25	6.0 × 10 ⁻⁴	0	5.003 × 10 ⁻⁷
		30	1.12 × 10 ⁻³	10	2.531 × 10 ⁻⁶
				20	1.715 × 10 ⁻⁵
		<i>p,p'</i> -DDT		30	8.180 × 10 ⁻⁵
		30	1.87 × 10 ⁻³	40	3.846 × 10 ⁻⁴
				eq. 1	P/Pa
				A	16.62
				B	6276
				for temp range 0–40°C	
				enthalpy of sublimation:	
				ΔH _{sub} = 120.2 kJ/mol	

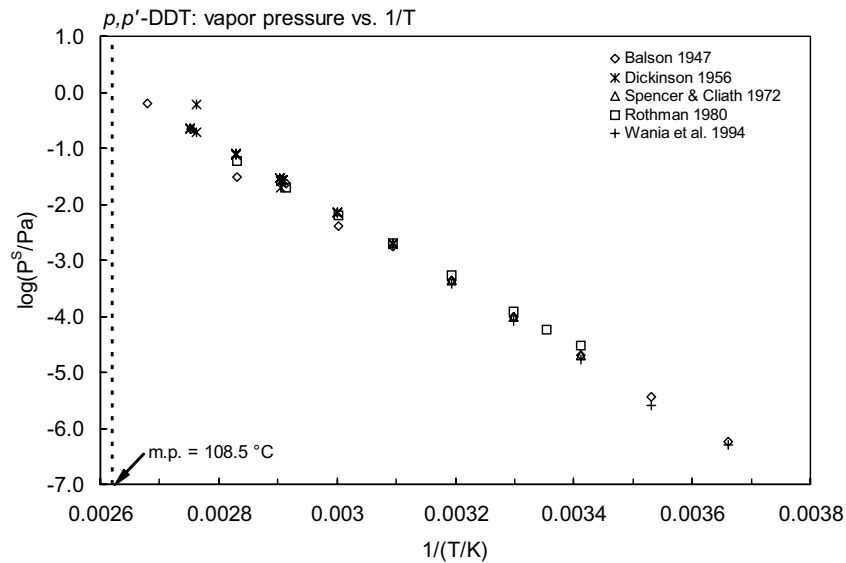
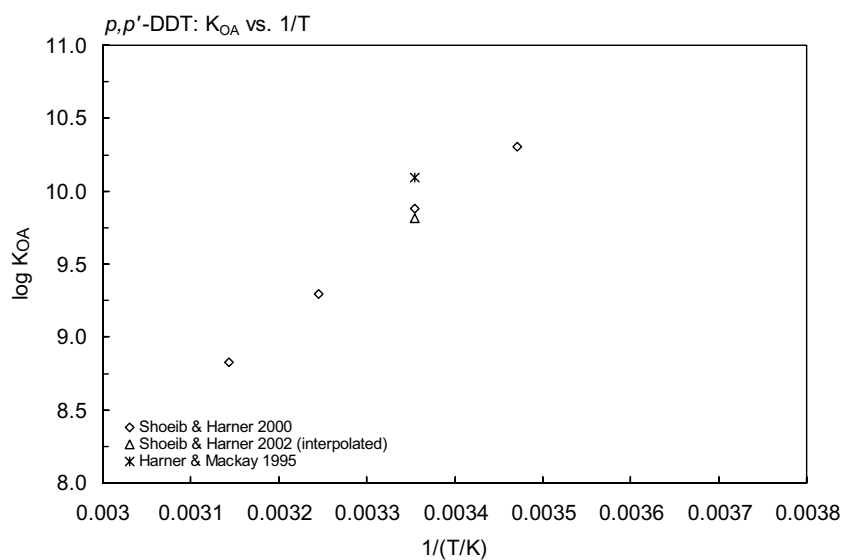


FIGURE 18.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for *p,p'*-DDT.

TABLE 18.1.1.23.3

Reported octanol-air partition coefficients of DDT at various temperatures

<i>p,p'</i> -DDT				<i>o,p'</i> -DDT	
Harner & Mackay 1995		Shoeib & Harner 2002		Shoeib & Harner 2002	
generator column-GC/MS		generator column-GC		generator column-GC	
t/°C	log K _{OA}	t/°C	log K _{OA}	t/°C	log K _{OA}
15		15	10.307	5	10.905
25	10.09	25	9.879	15	10.455
35		35	9.295	20	9.881
45		45	8.824	25	9.660
		25	9.816	35	9.1959
log K _{OA} = A + B/(T/K)		log K _{OA} = A + B/(T/K)		log K _{OA} = A + B/(T/K)	
A	-3.20	A	-5.63	A	-11.291
B	3954	B	4603	B	6266
enthalpy of phase change		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 88.1$		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 87.9$	
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 75.7$					

FIGURE 18.1.1.23.3A Logarithm of K_{OA} versus reciprocal temperature for *p,p'*-DDT.

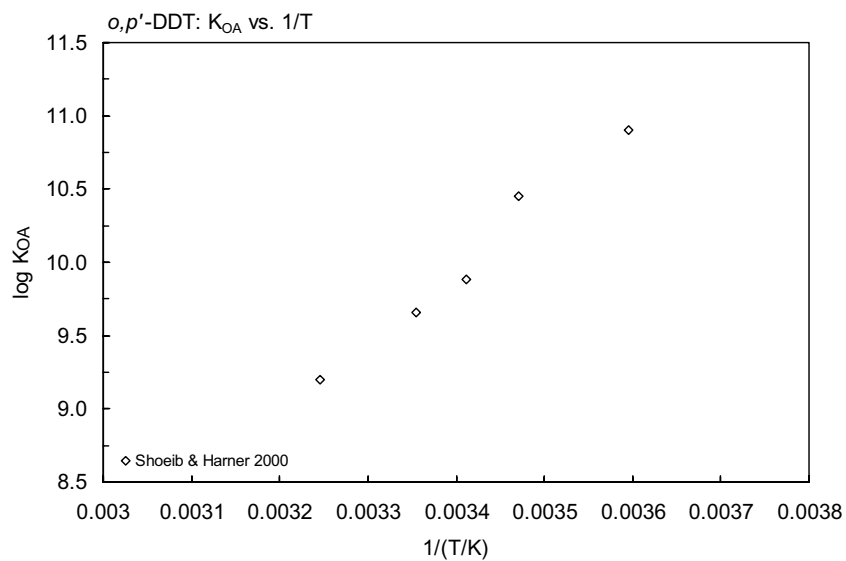
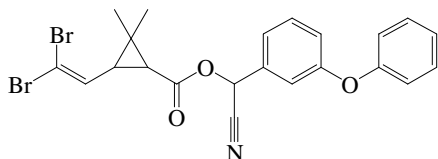


FIGURE 18.1.1.23.3B Logarithm of K_{OA} versus reciprocal temperature for *o,p'*-DDT.

18.1.1.24 Deltamethrin



Common Name: Deltamethrin

Synonym: Decis, K-Othrin, Butoss, RU 22074, Cislin, Crackdown

Chemical Name: *S*- α -cyano-3-phenoxybenzyl (1*R*,3*R*)-3-(2,2-dibromovinyl)-2,2-dimethyl cyclopropan-1-carboxylate

CAS Registry No: 52918-63-5

Uses: insecticide (pyrethroid)

Molecular Formula: $C_{22}H_{19}Br_2NO_3$

Molecular Weight: 505.199

Melting Point ($^{\circ}C$):

98–101 (Hartley & Kidd 1987)

98–102 (Tomlin 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

0.55 ($25^{\circ}C$, bulk density, Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F :

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

<0.002 ($20^{\circ}C$, Hartley & Kidd 1987)

<0.0002 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

2.0×10^{-6} (Hartley & Kidd 1987)

$<1.33 \times 10^{-5}$ (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

12.6 (gas stripping-LSC, Muir et al. 1985a)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.20 (HPLC-RT correlation, Muir et al. 1985b)

6.20 (shake flask, Log P Database, Hansch & Leo 1987)

6.21 (HPLC-RT correlation, Hu & Leng 1992)

6.20 (recommended, Sangster 1993)

4.60 (Tomlin 1994)

6.20 (recommended, Hansch et al. 1995)

5.74 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.53–3.0 (fathead minnows, Muir et al. 1985a)

2.06–2.48 (chironomid larvae, Muir et al. 1985b)

2.62, 2.70 (*Oncorhynchus mykiss*, flow-through condition, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

3.66–4.21 (Tomlin 1994)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 9$ d in soil (Tomlin 1994).

Oxidation:

Hydrolysis: more stable in acidic than in alkaline media with $t_{1/2} = 2.5$ d at pH 9 and 25°C (Tomlin 1994).

Biodegradation: microbial degradation half-life are, $t_{1/2}(\text{aerobic}) = 21\text{--}25$ d, $t_{1/2}(\text{anaerobic}) = 31\text{--}36$ d in laboratory;
 $t_{1/2} < 23$ d in field (Tomlin 1994)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 2\text{--}4$ d in water of small outdoor ponds (Muir et al. 1985);

more stable in acidic than in alkaline media with $t_{1/2} = 2.5$ d at pH 9 and 25°C (Tomlin 1994).

Ground water:

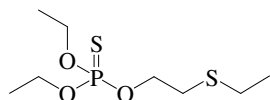
Sediment:

Soil: undergoes microbial degradation within 1–2 wk (Hartley & Kidd 1987)

microbial degradation half-life are, $t_{1/2}(\text{aerobic}) = 21\text{--}25$ d, $t_{1/2}(\text{anaerobic}) = 31\text{--}36$ d in laboratory; $t_{1/2} < 23$ d in field; photolysis $t_{1/2} = 9$ d (Tomlin 1994).

Biota:

18.1.1.25 Demeton



Common Name: Demeton

Synonym: Bayer 8169, Demeton-O, E-1059, mercaptophos, Systox-O

Chemical Name: *O,O*-diethyl-*O*-(2-ethylthioethyl)phosphorothioate mixture with *O,O*-diethyl-*S*-(2-ethylthioethyl)-phosphorothioate

Uses: insecticide to control sucking insects and mites in a wide range of crops, including fruit, nuts, vegetables, ornamentals, and field crops; also used as acaricide.

CAS Registry No: 8065-48-3, 298-03-3 demeton-O, systox-O
126-75-0 demeton-S, systox-S

Molecular Formula: $C_8H_{19}O_3PS_2$

Molecular Weight: 258.339

Melting Point ($^{\circ}C$):

pale yellow oil (Hartley & Kidd 1987)

Boiling Point ($^{\circ}C$):

123 (Khan 1980)

92–93 (at 0.15 mmHg, Hartley & Kidd 1987)

Density (g/cm^3 at $20^{\circ}C$):

1.119 ($25^{\circ}C$, Spencer 1982)

1.119–1.132 (Hartley & Kidd 1987)

Molar Volume (cm^3/mol):

264.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

60 ($20^{\circ}C$, Kenaga 1980a)

60 ($22^{\circ}C$, Khan 1980; Worthing & Walker 1983)

100 (20 – $25^{\circ}C$, Willis & McDowell 1982)

60 (rm. temp., Spencer 1982; Hartley & Kidd 1987)

60 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0973, 0.0987 ($30^{\circ}C$, demeton-O, demeton-S, Eichler 1965)

0.00331, 0.0347 ($20^{\circ}C$, demeton-O, demeton-S, Melnikov 1971)

0.00373, 0.0347 ($20^{\circ}C$, demeton-O, demeton-S, Hartley & Graham-Bryce 1980)

0.0331 (Khan 1980)

0.033 ($20^{\circ}C$, Spencer 1982)

0.0167, 0.00707 ($20^{\circ}C$, demeton-O, demeton-S, GC-RT correlation, Kim 1985)

0.034 ($20^{\circ}C$, Hartley & Kidd 1987)

0.030 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.1333 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.130 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

1.79 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{oc} :

2.66 (soil, calculated-S, Kenaga 1980)

1.85 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

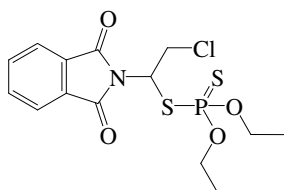
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Oxidation: calculated rate constant $k = 128 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor phase reaction with hydroxyl radical in air (Winer & Atkinson 1990).

Half-Lives in the Environment:

Soil: selected field $t_{1/2} = 15 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

18.1.1.26 Dialifor



Common Name: Dialifor

Synonym: dialiphos, Torak

Chemical Name: *S*-(2-chloro-(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)ethyl) *O,O*-diethyl phosphorodithioate

CAS Registry No: 10311-84-9

Uses: insecticide/acaricide

Molecular Formula: $C_{14}H_{17}ClNO_4PS_2$

Molecular Weight: 393.846

Melting Point ($^{\circ}C$):

68 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.379 (mp at $68^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.18 (Chiou et al. 1977; Kenaga 1980b)

< 1.0 (Hartley & Kidd 1987)

0.18 (room temp., Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

0.133 ($35^{\circ}C$, Hartley & Kidd 1987)

1.08×10^{-7} ($20^{\circ}C$, Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.142 ($20^{\circ}C$, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.69 (shake flask-GC, Chiou et al. 1977; quoted, Rao & Davidson 1980; Sangster 1993)

4.69 (Montgomery 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.21 (calculated, Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{OC}$:

4.04 (soil, calculated, Kenaga 1980b)

4.05 (Montgomery 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} = 14\ h$ at $20^{\circ}C$ and pH 7.4, $t_{1/2} = 1.8\ h$ at $37.5^{\circ}C$ and pH 7.4 (Montgomery 1993).

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} = 14$ h at 20°C and pH 7.4, $t_{1/2} = 1.8$ h at 37.5°C and pH 7.4 (Montgomery 1993).

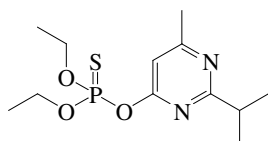
Ground water:

Sediment:

Soil:

Biota: rapidly eliminated in animal (Hartley & Kidd 1987).

18.1.1.27 Diazinon



Common Name: Diazinon

Synonym: Alfa-Tox, AG-500, Basudin, Bazinon, Bazuden, Ciazinon, Dacutox, Dassitox, Dazzel, Desapon, Dianon, Diater, Diaterr-fos, Diazitol, Diazide, Diazol, Dicid, Dimpylate, Dipofene, Dizinon, Dyzol, ENT 19507, Flytrol, G 301, Gardentox, Geigy 24480, Kayazinon, Kayazol, NA 2763, Nedicisol, Neocidol, Nipsan, Nucidol, Sarolex, Spectracide

Chemical Name: *O,O*-diethyl *O*-2-isopropyl-6-methylpyrimidin-4-yl phosphorothioate; *O,O*-diethyl-*O*-(2-isopropyl-6-methyl 4-pyrimidinyl) phosphorothioate; *O,O*-diethyl 2-isopropyl-4-methylpyrimidinyl-6-thiophosphate

Uses: nonsystemic insecticide to control flies, aphids and spider mites in soil, fruit, vegetables and ornamentals; also used as acaricide.

CAS Registry No: 333-41-5

Molecular Formula: $C_{12}H_{21}N_2O_3PS$

Molecular Weight: 304.345

Melting Point ($^{\circ}C$):

colorless oil (Hartley & Kidd 1987; Tomlin 1994)

Boiling Point ($^{\circ}C$):

125 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

83–84 (at 0.0002 mmHg, Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.11 (Worthing & Hance 1991)

1.116–1.118 (Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

320.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

< 2.5 (Albert 1963; Perrin 1989; Somasundaram et al. 1991; Montgomery 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

87.5 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

40 (Spencer 1973, 1982; Martin & Worthing 1977; Worthing 1979, Worthing & Walker 1987)

40 (Wauchope 1978; Briggs 1981; Burkhard & Guth 1981; Kanazawa 1989)

68.8 ($22^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983a, b)

40 (Hartley & Graham-Bryce 1980)

40 ($22^{\circ}C$, Khan 1980)

40.5 (20 – $25^{\circ}C$, shake flask-GC, Kanazawa 1981)

40 ($20^{\circ}C$, Windholz 1983)

40 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

60 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

53.5, 43.7 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

52.36, 103.8 (supercooled liquid S_L : literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0187 (Margot & Stammbach 1964)

0.0111 ($20^{\circ}C$, Wolfdietrich 1965)

0.0112 ($20^{\circ}C$, Melnikov 1971)

- 0.0161 (gas saturation, Heiber & Szelagiewicz 1976)
 0.020 (gas saturation method, measured range 32–73°C, Marti 1976)
 $\log(P/\text{mmHg}) = 11.46 - 4569.55/(T/K)$, temp range 32–73°C (Marti 1976)
 0.0187 (Worthing 1979)
 0.019 (20°C, Hartley & Graham-Bryce 1980)
 0.0187 (Khan 1980)
 0.00971 (20°C, volatilization rate, Burkhard & Guth 1981)
 0.00236–0.00469 (20°C, GC, Seiber et al. 1981)
 0.0109* (gas saturation-GC, measured range 25.3–45.0°C, Kim et al. 1984)
 $\log(P/\text{mmHg}) = 9.3871 - 4014.67/(T/K)$; temp range 25.3–45°C (gas saturation, Kim et al. 1984)
 0.0064 (20°C, extrapolated-Clausius-Clapeyron eq. with vapor pressures at several temp, Kim et al. 1984)
 0.0024 (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
 9.7×10^{-5} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)
 0.014* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
 $\log(P_L/\text{Pa}) = 13.482 - 4571.2/(T/K)$; measured range 32.4–140°C (liquid, gas saturation-GC, Rordorf 1989)
 0.020 (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
 0.008 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.0113 (20°C, Montgomery 1993)
 0.012 (20°C, Tomlin 1994)
 0.0123 (liquid P_L , GC-RT correlation, Donovan 1996)
 0.011 (gradient GC method; Tsuzuki 2000)
 0.011; 0.0339, 0.0513 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)
 0.014, 0.0073 (supercooled liquid P_L : literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.074 (20°C, volatilization rate, Burkhard & Guth 1981)
 0.0114 (calculated, Adachi et al. 1984)
 0.124 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
 0.0114 (23°C, wetted-wall column-GC/ECD, Fendinger & Glotfelty 1988)
 0.0669 (20°C, calculated-P/C, Suntio et al. 1988)
 0.1438 (calculated-P/C, Taylor & Glotfelty 1988)
 0.0138, 0.0101 (22–24°C, fog chamber-GC/ECD: drain water, cyclone water, Fendinger et al. 1989)
 0.007 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
 0.0114 (20°C, calculated-P/C, Montgomery 1993)
 0.0406 (calculated-P/C, this work)
 0.0338* (20°C, gas stripping-GC/MS, measured range 283–301 K, Feigenbrugel et al. 2004)
 $H'/(M \text{ atm}^{-1}) = (7.2 \pm 0.5) \times 10^{-15} \exp[(11900 \pm 700)/(T/K)]$; temp range 283–310 K (Arrhenius eq., gas stripping-GC/MS, Feigenbrugel et al. 2004)
 0.0108, 0.0216 (literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.02 (Rao & Davidson 1980)
 3.11 (shake flask-UV, Lord et al. 1980)
 3.11 (20°C, shake flask-UV, Briggs 1981)
 3.14 (shake flask-GC, Kanazawa 1980, 1981)
 3.81 (shake flask-GC, Bowman & Sans 1983b)
 1.92 (Veith & Kosian 1983)
 3.02 (shake flask, Log P Database, Hansch & Leo 1987)
 3.02–3.81 (Montgomery 1993)
 3.70 (RP-HPLC-RT correlation, Saito et al. 1993)
 3.58 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
 3.30 (Tomlin 1994)

- 3.81 (recommended, Hansch et al. 1995)
- 3.58 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 4.23 (RP-HPLC-RT correlation, Nakamura et al. 2001)
- 3.81 (literature-derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, log K_{OA} :

- 8.87 (final adjusted value FAV, Muir et al. 2004)

Bioconcentration Factor, log BCF:

- 2.39 (motsugo, Kanazawa 1975)
- 1.54 (fish in flowing water, Alison & Hermanutz 1977)
- 2.18, 1.56 (topmouth gudgeon, silver crucian carp, Kanazawa 1978, 1981)
- 1.81; 1.24 (carp; guppy, Kanazawa 1978)
- 0.69, 1.23, 0.77 (crayfish, red snail, pond snail, Kanazawa 1978)
- 1.83; 0.954 (fish; invertebrates, Kanazawa 1978)
- 1.89 (calculated-S, Kenaga 1980)
- 2.75 (earthworms, Lord et al. 1980)
- 2.08, 1.80 (carp, rainbow trout, Seguchi & Asaka 1981)
- 1.41, 0.477 (loach, shrimp, Seguchi & Asaka 1981)
- 1.81; 1.24; 2.18 (carp; guppy; topmouth gudgeon, Veith & Kosian 1983)
- 2.32 (topmouth gudgeon, Kanazawa 1983)
- 2.30 (sheepshead minnow, Zarogian et al. 1985)
- 1.46 (Isnard & Lambert 1988)
- 0.59 (vegetation, correlated- K_{OW} , Nash 1974)
- 2.39 (willow shiner, Tsuda et al. 1989; Tsuda et al. 1992)
- 1.81, 2.08 (carp, De Bruijn & Hermens 1991)
- 1.38, 1.81, 1.81 (loach, motsugo, rainbow trout, De Bruijn & Hermens 1991)
- 2.16–2.33 (sheepshead minnow, De Bruijn & Hermens 1991)
- 1.56, 2.18 (silver crucian carp, topmouth gudgeon, De Bruijn & Hermens 1991)
- 2.18, 1.79 (pale chub, ayu sweetfish, calculated-field data, Tsuda et al. 1992)
- 3.20 (eel, Sancho et al. 1993)
- 2.02 (killifish *Oryzias latipes*, after 24–72 h exposure, Tsuda et al. 1995)
- 1.34, 1.45 (*Oryzias latipes*, Tsuda et al. 1995; quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC} :

- 2.76 (calculated-S as per Kenaga & Goring 1978, Kenaga)
- 2.93 (Rao & Davidson 1980)
- 2.28, 2.40 (average of 3 soils, 1 sediment, Sharom et al. 1980)
- 2.36 (soil, sorption isotherm, converted from reported log K_{OM} of 2.12, Briggs 1981)
- 2.36 (estimated, Lyman et al. 1982; quoted, Howard 1991; Lohninger 1994)
- 2.93 (screening model calculations, Jury et al. 1987b; Jury & Ghodrati 1989)
- 2.40 (average of 2 soils, Kanazawa 1989)
- 2.12, 3.27 (reported, estimated as log K_{OM} , Magee 1991)
- 2.75, 3.13 (soil, quoted exptl., calculated- χ and fragment contribution, Meylan et al. 1992)
- 3.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.76 (soil, average value, Dowd et al. 1993)
- 3.00–3.27 (Montgomery 1993)
- 2.75 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 2.75, 3.05 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 2.74, 2.64, 2.90 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
- 3.12–3.16 (sediments from San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization: mostly dissipated through volatilization with $t_{1/2} = 19$ d from soil (Glottfelty et al. 1990).

Photolysis: calculated $t_{1/2} = 15$ d for photolysis in an aqueous buffer solution at pH 7 and 25°C under UV light for 24 h (Burkhard & Guth 1979; quoted, Montgomery 1993);

$t_{1/2} = 41$ d without addition of humic substances; $t_{1/2} = 9$ d and $t_{1/2} = 5$ d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994)

Photodegradation ($\lambda > 290$ nm) half-lives in various diazinon aqueous solutions: $t_{1/2} \sim 1$ d river water exposed to sunlight, $t_{1/2} \sim 5$ d lake water exposed to sunlight and $t_{1/2} \sim 5.5$ d with humic acid exposed to sunlight (Mansour et al. 1997)

photolytic $k = 2.39 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 290$ h in moist sandy soil, $k = 6.62 \times 10^{-5} \text{ h}^{-1}$ with $t_{1/2} = 10500$ h in dry sandy soil; $k = 2.55 \times 10^{-3} \text{ h}^{-1}$ in moist sandy loam (Graebing & Chib 2004)

Oxidation: photooxidation $t_{1/2} = 4.1$ h in air, estimated from the vapor-phase reaction with 5×10^5 hydroxyl radicals/ m^3 in air at 25°C (Martin & Worthing 1977; quoted, Howard 1991).

$k_{\text{OH}} = 9.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K in gas phase with atmospheric lifetime of 4.1 h but reduced to .19 h at 283 K; $\log k_{\text{OH}}(\text{aq.}) = 8.2 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ in aqueous phase (Feigenbrugel et al. 2004)

Hydrolysis:

$k(\text{acid}) = 2.1 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ for acid catalyzed hydrolysis, $k(\text{neutral}) = 4.3 \times 10^{-8} \text{ M}^{-1} \text{ s}^{-1}$ for neutral hydrolysis and $k(\text{alkaline}) = 5.3 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for base catalyzed hydrolysis with 10^{-5} M in aqueous buffer (Faust & Gomaa 1972; quoted, Freed 1976; Harris 1982)

$t_{1/2} = 11.77$ h at pH 3.1, $t_{1/2} = 185$ d at pH 7.4 and $t_{1/2} = 6.0$ d at pH 10.4 in water at 20°C (Worthing & Hance 1991; Tomlin 1994)

$t_{1/2} = 11.77$ h at pH 3.1, $t_{1/2} = 185$ d at pH 7.4, $t_{1/2} = 136$ d at pH 9.0, and $t_{1/2} = 6$ d at pH 10.4 at 20°C (Montgomery 1993).

Biodegradation:

half-lives $t_{1/2} = 4.91$ d at pH 3.1 and $t_{1/2} = 185$ d at pH 7.4 from river die-away tests (Gomaa et al. 1969; quoted, Scow 1982)

$t_{1/2} = 12.5$ wk in sterile soils and $t_{1/2} < 1$ wk in nonsterile soils; $t_{1/2} = 6.5$ wk in sterile sandy loam and $t_{1/2} = 2$ wk in nonsterile sandy loam (Miles et al. 1979; quoted, Howard 1991)

$t_{1/2} = 32$ d in 0–10 cm depth of soil by 100 d leaching screening test (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989)

$k = 0.023 \text{ d}^{-1}$ with estimated first-order $t_{1/2} = 30$ d in soil incubation studies by soil die-away test (Rao & Davidson 1980; quoted, Scow 1982)

$k(\text{av.}) = 0.0193 \text{ d}^{-1}$ in silty clay with $t_{1/2} = 36$ d; and $k(\text{av.}) = 0.0245 \text{ d}^{-1}$ in sandy clay with $t_{1/2} = 28$ d (Sattar 1990)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.070 \text{ h}^{-1}$ (willow shiner, Tsuda et al. 1989)

$k_2 = 0.023 \text{ h}^{-1}$ (eel's liver, Sancho et al. 1993)

$k_2 = 0.019 \text{ h}^{-1}$ (eel's muscle, Sancho et al. 1993)

$k_2 = 0.21 \text{ h}^{-1}$ (killifish *Oryzias latipes*, Tsuda et al. 1995)

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 4.1$ h, estimated from the vapor-phase reaction with 5×10^5 hydroxyl radicals/ m^3 in air at 25°C (Martin & Worthing 1977; quoted, Howard 1991).

Surface water: photolysis $t_{1/2} = 41$ d without humic substances; $t_{1/2} = 13$ d and 5 d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994);

$t_{1/2} = 144$ d at 6°C, $t_{1/2} = 69$ d at 22°C in darkness for Milli-Q water; $t_{1/2} = 181$ d at 6°C, $t_{1/2} = 80$ d at 22°C in darkness, $t_{1/2} = 43$ d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 132$ d at 6°C, $t_{1/2} = 52$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 125$ d at 6°C, $t_{1/2} = 50$ d at 22°C in darkness, $t_{1/2} = 47$ d under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment: first-order degradation $k = 0.048 \text{ d}^{-1}$ with $t_{1/2} = 14.4$ d under aerobic conditions, $k = 0.022 \text{ d}^{-1}$ with $t_{1/2} = 31.7$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.033 \text{ d}^{-1}$ with $t_{1/2} = 21.1$ d under aerobic conditions, $k = 0.029 \text{ d}^{-1}$ with $t_{1/2} = 23.7$ d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: $t_{1/2} = 43.8$ d in sterile soil at pH 4.7 (Sethunathan & MacRae 1969; quoted, Montgomery 1993);

estimated persistence of 12 wk in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

persistence of 3 months (Wauchope 1978);

$t_{1/2}$ = 12.5 wk in sterile sandy loam and $t_{1/2}$ < 1.0 wk in nonsterile sandy loam; $t_{1/2}$ = 6.5 wk in sterile organic soil and $t_{1/2}$ = 2.0 wk in nonsterile organic soil (Miles et al. 1979);

estimated first-order $t_{1/2}$ = 30 d in soil from biodegradation rate constant k = 0.023 d⁻¹ for soil incubation studies by soil die-away test (Rao & Davidson 1980; quoted, Scow 1982);

moderate persistent in soil with $t_{1/2}$ = 20–100 d (Willis & McDowell 1982);

$t_{1/2}$ = 32 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989);

dissipation $t_{1/2}$ = 19 d in soil (Glotfelty et al. 1990);

av. degradation rate constant k = 0.0193 d⁻¹ in silty clay with $t_{1/2}$ = 36 d and average degradation rate constant k = 0.0245 d⁻¹ in sandy clay with $t_{1/2}$ = 28 d (Sattar 1990)

selected field $t_{1/2}$ = 40 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

soil $t_{1/2}$ = 65 d (Pait et al. 1992)

$t_{1/2}$ = 40 d (selected, Halfon et al. 1996)

On sandy soil: first-order rate constants for photolytic decline, k = 5.45×10^{-3} h⁻¹ with $t_{1/2}$ = 130 h irradiated in moisture-maintained soil, k = 0.84×10^{-3} h⁻¹ with $t_{1/2}$ = 830 h irradiated in air-dried soil, k = 3.06×10^{-3} h⁻¹ with $t_{1/2}$ = 230 h in dark control moist soil and k = 0.77×10^{-3} h⁻¹ with $t_{1/2}$ = 900 h in dark control air-dried sandy soil from Sauk County, WI. The photolytic k = 2.39×10^{-3} h⁻¹ with $t_{1/2}$ = 290 h in moist soil, k = 6.62×10^{-5} h⁻¹ with $t_{1/2}$ = 10500 h in dry soil. The contribution of moisture to irradiated metabolism k = 4.61×10^{-3} h⁻¹ with $t_{1/2}$ = 150 h, but for dark control system for k = 2.29×10^{-5} h⁻¹ with $t_{1/2}$ = 300 h (Graebing & Chib 2004)

On sandy loam soil: first-order rate constants for photolytic decline, k = 4.07×10^{-3} h⁻¹ irradiated in moisture-maintained soil, k = 1.07×10^{-3} h⁻¹ irradiated in air-dried soil, k = 1.52×10^{-3} h⁻¹ in dark control moist soil and no degradation in dark control air-dried sandy loam soil from Madia, CA. $t_{1/2}$ = 120 h for the first 96 h irradiation; over all $t_{1/2}$ (calc) = 200 h from 96–168 h but in dark control system $t_{1/2}$ = 460 h in moist sandy loam soil; irradiated metabolism $t_{1/2}$ = 650 h in dry sandy loam soils. Rate constants due to photolysis k = 2.55×10^{-3} h, and due to moisture k = 3.0×10^{-3} h in moist sandy loam soil (Graebing & Chib 2004)

Biota: biochemical $t_{1/2}$ = 32 d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989); excretion $t_{1/2}$ = 9.9 h by willow shiner (Tsuda et al. 1989)

$t_{1/2}$ = 25 h in eel's liver and $t_{1/2}$ = 26 h in eel's muscle (Sancho et al. 1993)

TABLE 18.1.1.27.1

Reported vapor pressures and Henry's law constants of diazinon at various temperatures

Vapor pressure				Henry's law constant	
Kim et al. 1984, Kim 1985		Rordorf 1989		Feigenbrugel et al. 2004	
gas saturation-GC		gas saturation-GC		gas stripping-GC/MS	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
25.3	0.0113	25	0.014	283.05	8.515×10^{-3}
34.9	0.0299	50	0.22	283.15	9.128×10^{-3}
45.0	0.0770	75	2.20	283.15	8.515×10^{-3}
20.0	0.0064	100	17.0	283.55	8.465×10^{-3}
25.0	0.0109	125	100	287.55	0.0138
				291.55	0.0166
				293.05	0.0281
log P = A – B/(T/K)		log P = A – B/(T/K)		293.05	0.0390
	P/mmHg		P/Pa	293.15	0.0349
A	9.3871	A	13.482	293.15	0.0375
B	4014.67	B	4571.2	293.25	0.0298
				293.25	0.0281
				295.35	0.0441
				297.55	0.0675
				299.45	0.0921
				301.45	0.101325
				ln H = A – B/(T/K)	
				H'/(M/atm)	
				A	–32.5647
				B	11900

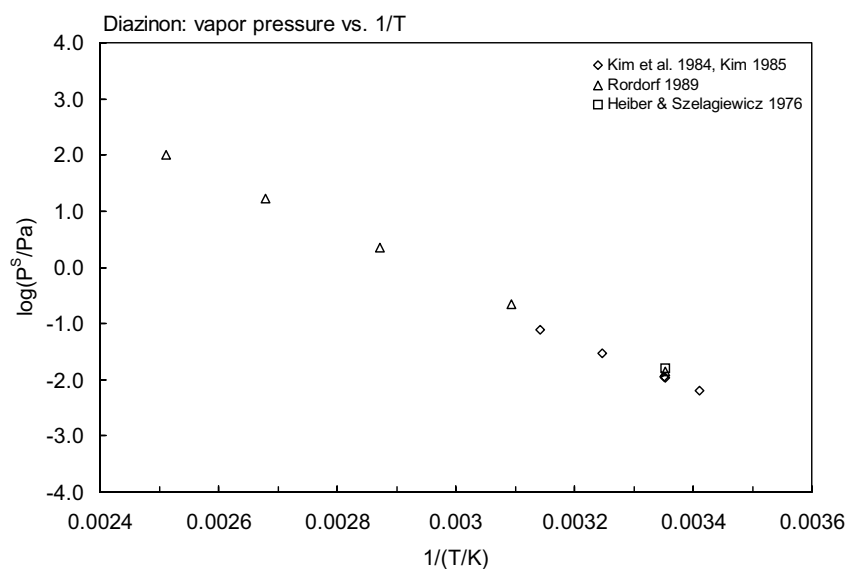


FIGURE 18.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for diazinon.

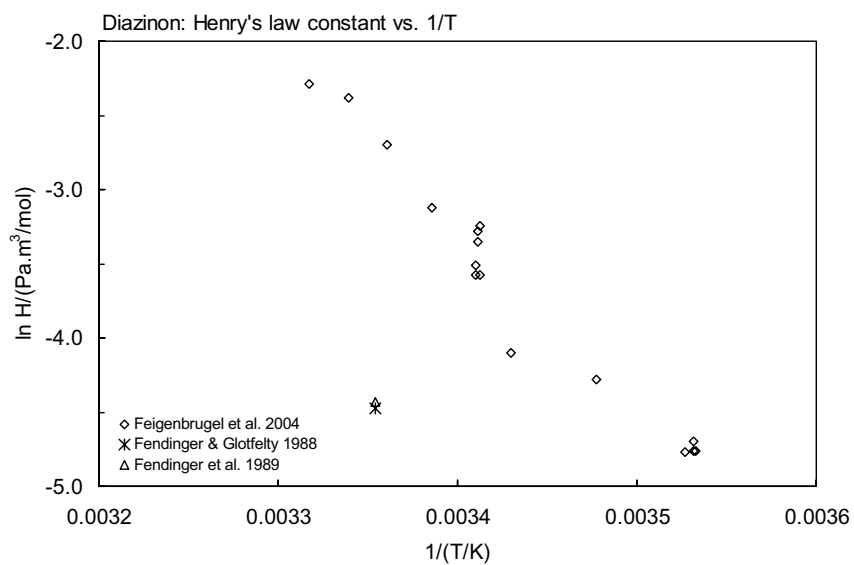
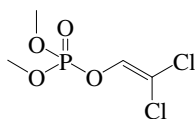


FIGURE 18.1.1.27.2 Logarithm of Henry's law constant versus reciprocal temperature for diazinon.

18.1.1.28 Dichlorvos



Common Name: Dichlorvos

Synonym: Apavap, Astrobot, Atgard, Bay 19149, Benfos, Bibesol, Brevinyl, Canogard, Cekusan, Chlorvinphos, Cyanophos, Cypona, DDVF, DDVP, Dedevap, Deriban, Derribante, Devikol, Dichlorman, Dichlorophos, Divipan, Duo-kill, Duravos, ENT 20738, Equigard, Equigel, Estrosel, Estrosol, Fecama, Fly-die, Fly fighter, Herkal, Herkol, Krecalvin, Lindan, Mafu, Mafu strip, Marvex, Mopari, NA 2783, Nerkol, Nogos, No-pest, Nuva, Nuvan, Oko, OMS 14, Phosvit, SD-1750, Szklarniak, Tap 9VP, Task, Tenac, Tetravos, UDVf, Unifos, Vapona, Vaponite, Vapora II, Verdican, Verdipor, Vinylofos, Vinylophos

Chemical Name: 2,2-dichlorovinyl-*O,O*-dimethyl phosphate; 2,2-dichloroethenyl-*O,O*-dimethyl phosphate

Uses: insecticide and fumigant to control flies, mosquitoes, and moths; also used as acaricide.

CAS Registry No: 62-73-7

Molecular Formula: $C_4H_7Cl_2O_4P$

Molecular Weight: 220.976

Melting Point ($^{\circ}C$):

colorless to amber liquid (Hartley & Kidd 1987)

Boiling Point ($^{\circ}C$):

35, 74, 117 (at 0.05, 1.0, 10 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991)

234.1 (Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.415 ($25^{\circ}C$, Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

1.420 ($25^{\circ}C$, Worthing & Hance 1991)

1.425 (Tomlin 1994)

1.440 (Montgomery 1993)

Molar Volume (cm^3/mol):

167.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

10000 (Günther et al. 1968; Melnikov 1971; Kenaga 1980a; Khan 1980; Spencer 1982)

10000 (Martin & Worthing 1977; Worthing 1979; Worthing & Walker 1987)

10000 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

16000 (Kawamoto & Urano 1989)

16000 ($20^{\circ}C$, Montgomery 1993)

10000 (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

8000 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1.60 ($20^{\circ}C$, Eichler 1965; Wolfdietrich 1965)

1.60 ($20^{\circ}C$, Melnikov 1971; Hartley & Graham-Bryce 1980; Spencer 1982; Montgomery 1993)

1.60* ($20^{\circ}C$, evaporation rate-gravimetric method, measured range 293–333 K, Gückel et al. 1973)

1.60 (Khan 1980; Brouwer et al. 1994)

$\log(P/mmHg) = 9.9081 - 3464/(T/K)$; temp range not specified (quoted from literature, Gückel et al. 1982)

0.947* ($20^{\circ}C$, evaporate rate-gravimetric method, measured range 20 – $60^{\circ}C$, Gückel et al. 1982)

7.026 (gas saturation-GC, Kim et al. 1984)

4.011 (20 , $25^{\circ}C$, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984)

- 0.67 (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
- 1.60, 3.90 (20°C, 30°C, Hartley & Kidd 1987)
- 7.0 (20°C, selected, Suntio et al. 1988)
- 0.29 (20°C, Worthing & Hance 1991)
- 0.267 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 2.10 (Tomlin 1994)
- 7.94 (gradient GC method; Tsuzuki 2000)
- 6.92; 8.51, 5.62 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.190 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.097 (calculated-P/C, Howard 1991)
- 506.5 (Montgomery 1993)
- 0.194 (calculated-P/C, this work)
- 0.0253* (gas stripping-GC/MS, measured range 10–25°C, Gautier et al. 2003)
- $\ln [H'/(M \text{ atm}^{-1})] = -28.904 + 11100/(T/K)$; temp range 283.5–298.15 K (Arrhenius eq., gas stripping-GC/MS, Gautier et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 1.40 (Leo et al. 1971; Hansch & Leo 1979)
- 2.29 (Rao & Davidson 1980)
- 1.47 (shake flask-GC, Bowman & Sans 1983)
- 1.16 (HPLC-RT correlation, Kawamoto & Urano 1989)
- 1.40–2.29 (Montgomery 1993)
- 1.73 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 1.43 (recommended, Sangster 1993)
- 1.90 (Tomlin 1994)
- 1.42 (selected, Hansch et al. 1995)
- 1.73 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.477 (calculated-S, Kenaga 1980a; quoted, Howard 1991)
- 0.097 (whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992; quoted, Devillers et al. 1996)
- < –0.30 (whole body carp, Tsuda et al. 1993)

Sorption Partition Coefficient, $\log K_{oc}$:

- 1.45 (soil, calculated-S, Kenaga 1980a; quoted, Howard 1991)
- 1.67 (correlated, Kawamoto & Urano 1989)
- 1.70 (calculated, Montgomery 1993)
- 1.48 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 1.67; 2.98, 2.04 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on the Henry's law constant, $t_{1/2} \sim 57$ d from a model river (Lyman et al. 1982; quoted, Howard 1991);

$t_{1/2} \sim 400$ yr from an model pond, which considered the effect of adsorption (Howard 1991).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate Constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

atmospheric $t_{1/2} = 320$ d, based on an estimated rate constant $k_{O_3} = 3.58 \times 10^{-20} \text{ cm}^3\cdot\text{molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with ozone of concn $7 \times 10^{11}/\text{cm}^3$ in air (Atkinson & Carter 1984; quoted, Howard 1991)

atmospheric $t_{1/2} = 2$ d, based on an estimated rate constant $k_{OH} = 9.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with hydroxyl radical of $5 \times 10^5/\text{cm}^3$ in air (Atkinson 1987; quoted, Howard 1991).

$k_{OH} = 9.4 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ with calculated tropospheric lifetime about 1.2 d at 298 K assuming an average OH concn of $1 \times 10^6 \text{ molecule/cm}^3$ (Gautier et al. 2003)

Hydrolysis: $t_{1/2} = 462$ min at pH 7 and $t_{1/2} = 30$ min at pH 8 (Montgomery 1993);

$t_{1/2} \sim 31.9$ d at pH 4, $t_{1/2} \sim 2.9$ d at pH 7, and $t_{1/2} \sim 2.0$ d at pH 9 at 22°C (Tomlin 1994)

$t_{1/2} = 3800$ d at pH 7 in natural waters (Capel & Larson 1995).

Biodegradation: the presence of active microorganisms reduced the $t_{1/2} = 0.9$ – 0.75 and 0.85 to 0.70 d in autoclaved clay and calcareous soil, respectively (Guirguis & Shafik 1975; quoted, Howard 1991);

rate constant $k(\text{aerobic}) = 0.20 \text{ d}^{-1}$ with $t_{1/2} = 3.5$ d at 20°C by aerobic activated sludge, and $k(\text{anaerobic}) = 0.20 \text{ d}^{-1}$ with $t_{1/2} = 3.5$ d at 20°C by anaerobic microorganisms (batch contacting method, Kawamoto & Urano 1990).

$t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 1$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants

Half-Lives in the Environment:

Air: $t_{1/2} = 320$ d, based on an estimated rate constant $k = 3.58 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with ozone of $7 \times 10^{11}/\text{cm}^3$ in air (Atkinson & Carter 1984; quoted, Howard 1991)

atmospheric $t_{1/2} = 2$ d, based on an estimated rate constant $k = .24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C for the vapor-phase reaction with hydroxyl radical of $5 \times 10^5/\text{cm}^3$ in air (Atkinson 1987; quoted, Howard 1991)

atmospheric transformation lifetime was estimated to be <1 d (Kelly et al. 1994)

Calculated tropospheric lifetime of 0.5 d for reaction with OH radicals, wet deposition lifetime estimated to be 5.6 d in the atmosphere by rainfall (Gautier et al. 2003)

Surface water: half-lives in lakes and rivers are reported to be approximately 4 d (Lamoreaux & Newland 1978; quoted, Howard 1991)

Biodegradation $t_{1/2} = 3.5$ d by aerobic activated sludge or anaerobic microorganisms cultivated by a an artificial sewage (Kawamoto & Urano 1990)

Biodegradation $t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 1$ d, hydrolysis $t_{1/2} = 3800$ d at pH 7 in natural waters (Capel & Larson 1995)

Ground water:

Sediment:

Soil: average degradation rate constant $k = 0.0423 \text{ d}^{-1}$ in silty clay with $t_{1/2} = 16$ d and average degradation rate constant $k = 0.0444 \text{ d}^{-1}$ in sandy clay with $t_{1/2} = 16$ d (Sattar 1990);

selected field $t_{1/2} = 0.5$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

TABLE 18.1.1.28.1

Reported vapor pressures and Henry's law constants of dichlorvos at various temperatures

Vapor pressure				Henry's law constant	
Gückel et al. 1973		Gückel et al. 1982		Gautier et al. 2003	
evaporation rate		evaporation rate		gas stripping-GC/MS	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
20	1.60	20	0.947	10	0.00322
30	4.0	40	7.30	10	0.00367
40	9.33	60	40.0	11	0.00378
50	-			12	0.00520
60	-			12	0.00504
				15	0.00209
				18	0.0109
				20	0.0151
				20	0.0163
				22.5	0.0181
				23	0.0230
				25	0.0230
				25	0.0247
				25	0.0289
				20.0	0.0253

Arrhenius expression:
 $\ln H = -(M \text{ atm}^{-1}) = -A + B/(T/K)$
A 28.904
B 11100

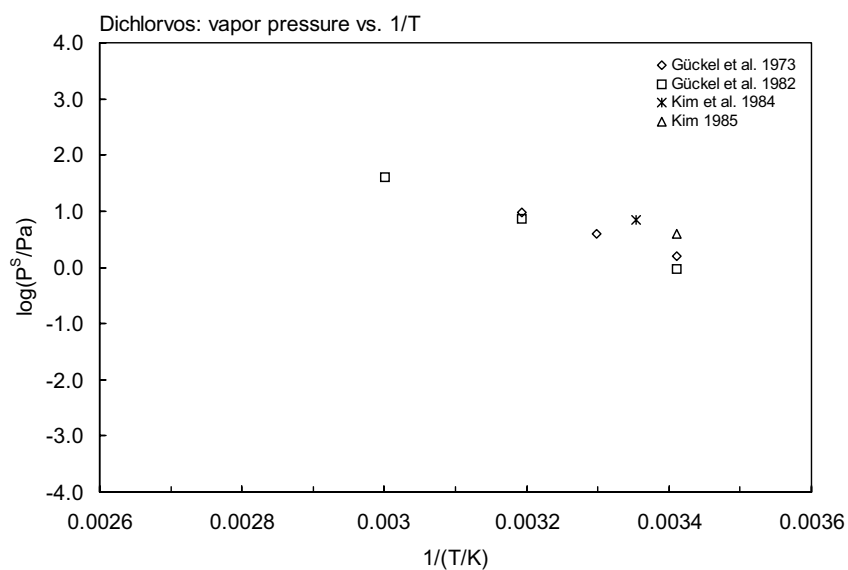


FIGURE 18.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for dichlorvos.

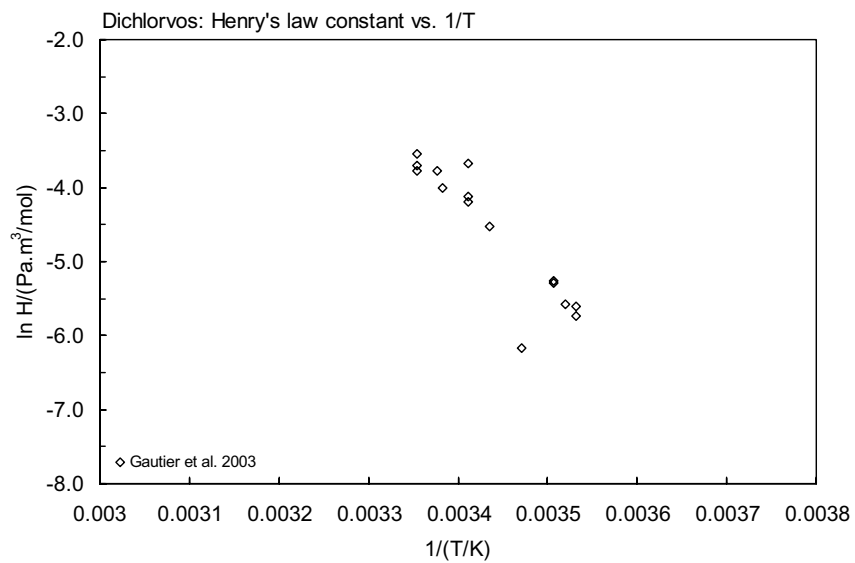
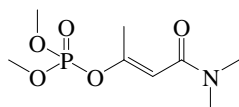


FIGURE 18.1.1.28.2 Logarithm of Henry's law constant versus reciprocal temperature for dichlorvos.

18.1.1.29 Dicrotophos



Common Name: Dicrotophos

Synonym: Bidirl, Bidrin, C 709, Cabicron, Carbomicron, CIBA 709, Diapadrin, Dicrotofos, Ektafos, ENT 24,482, Karbicon, Shell SD-3562

Chemical Name: (*E*)-2-dimethylcarbamoyl-1-methylvinyl dimethyl phosphate; (*E*)-3-(diethylamino)-1-methyl-3-oxo-1-propenyl dimethyl phosphate

Uses: contact and systemic insecticide and acaricide to control pests on rice, cotton, maize, soybeans, coffee, citrus, and potatoes.

CAS Registry No: 141-66-2 *cis*-dicrotophos

Molecular Formula: C₈H₁₆NO₅P

Molecular Weight: 237.191

Melting Point (°C): liquid

Boiling Point (°C):

130 (at 0.1 mmHg, Worthing & Hance 1991; Montgomery 1993; Milne 1995)
400 (Tomlin 1994; Milne 1995)

Density (g/cm³ at 20°C):

1.216 (Hartley & Kidd 1987)
1.216 (15°C, Merck Index 1989; Milne 1995)
1.21 (technical grade, Worthing & Hance 1991)
1.216 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm³/mol):

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Spencer 1973)
miscible (Hartley & Kidd 1987; Budavari 1989; Milne 1995)
miscible (Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)
1000000 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0115* (20°C, extrapolated, gas saturation-GC, measured range 32.3–77°C, Grayson & Fosbracey 1982)
ln (P/Pa) = 21.6 – 7631/(T/K); temp range 32.3–77°C, (Antoine eq., gas saturation-GC, Grayson & Fosbracey 1982)
0.0093 (20°C, Hartley & Kidd 1987)
0.0093 (20°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
0.0213 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C):

5.05 × 10⁻⁶ (20–25°C, calculated-P/C)

Octanol/Water Partition Coefficient, log K_{ow}:

–0.260 (calculated as per Broto et al. 1984, Karcher & Devillers 1990)
–0.49 (shake flask, Log P Database, Hansch & Leo 1987)
–0.49 (recommended, Sangster 1993)
–0.50 (Montgomery 1993)
0.0 (Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

- 1.88 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 1.04–2.27 (Montgomery 1993)
- 1.66 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.66; 1.49, 1.67 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Hydrolysis: $t_{1/2}$ = 117, 72, and 28 d in buffer solutions of pH 5, 7, and 9, respectively, at 25°C (Lee et al. 1989; quoted, Montgomery 1993);
- calculated $t_{1/2}$ = 88 d in water at 20°C at pH 5 and = 23 d at pH 9 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

- Soil: $t_{1/2}$ = 3 d in sandy loam soil (Lee et al. 1989; quoted, Montgomery 1993);
- selected field $t_{1/2}$ = 20 d (Wauchope et al. 1992; Hornsby et al. 1996).

TABLE 18.1.1.29.1
Reported vapor pressures of dicrotophos
at various temperatures

Grayson & Fosbracey 1982

gas saturation-GC	
$t/^{\circ}\text{C}$	P/Pa
32.3	0.034
33.7	0.036
41.0	0.055
45.2	0.106
51.0	0.136
60.1	0.287
65.8	0.405
69.5	0.424
77.0	0.820
30	0.0115
$\ln P = A - B/(T/K)$	
	P/Pa
A	7631
B	21.6

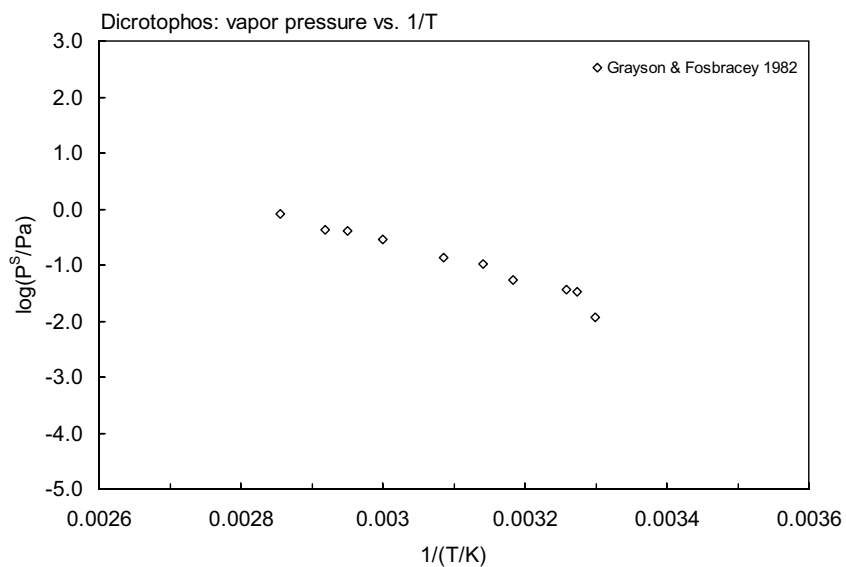
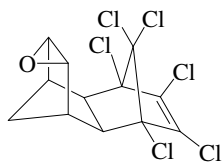


FIGURE 18.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for dicrotophos.

18.1.1.30 Dieldrin



Common Name: Dieldrin

Synonym: Aldren, Alvit, Alyran, Compound 497, Dieldrite, Dieldrix, Dorytox, ENT 16225, HEOD, Illoxol, Insectlack, Kombi-Albertan, NA 2761, NCI-C00124, Octalox, Panoram D-31, Quintox

Chemical Name: 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8, 8a-octahydroendo-1,4-*exo*-5,8-dimethano-naphthalene; 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-2,7:3,6-dimethanonaphth[2,3-b]oxirene

Uses: insecticide to control public health insect pests, termites, locusts, and tropical disease vectors.

CAS Registry No: 60-57-1

Molecular Formula: C₁₂H₈Cl₆O

Molecular Weight: 380.909

Melting Point (°C):

175.5 (Lide 2003)

Boiling Point (°C):

265, 352, 404 (estimated from structure, Tucker et al. 1983)

Density (g/cm³ at 20°C):

1.75 (Hartley & Kidd 1987; Montgomery 1993)

Molar Volume (cm³/mol):

318.2 (calculated-Le Bas method at normal boiling point)

253.6 (Ruelle & Kesselring 1997)

Dissociation Constant, pK_a:

Enthalpy of Vaporization, ΔH_v (kJ/mol):

76.6 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.4 (Rordorf 1989)

18.41 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

41.34, 48.12 (Plato 1972)

47 (Rordorf 1989)

44.77 (Hinckley et al. 1990)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 K/mol K), F:

0.026 (20°C, Suntio et al. 1988)

0.033 (Mackay et al. 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.19 (colorimetric method, Lipke & Kearns 1960)

0.25* (shake flask-GC/UV, measured range 25–45°, Richardson & Miller 1960)

0.14–0.18 (particle size of 0.04–5.0μ, shake flask-GC, Robeck et al. 1965)

0.15 (Eye 1968; quoted, Freed 1976; Jury et al. 1983,84)

0.20 (Günther et al. 1968)

0.186 (25–29°C, shake flask-GC/ECD, Park & Bruce 1968)

0.022 (Biggar & Riggs 1974)

0.195* (particle size of ≤ 5.0μ, shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)

0.022*, 0.15*, 0.195* (particle size: 0.01, 0.05 & 5.0μ; shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)

0.20 (generator column-GC/ECD, Weil et al. 1974)

0.187 (Martin & Worthing 1977; Worthing & Walker 1987)

0.10–0.25 (Wauchope 1978)

0.022	(Kenaga 1980a, b; Garten & Trabalka 1983; Isnard & Lambert 1989)
0.10	(Weber et al. 1980; Eadie & Robbins 1987)
0.468	(20–25°C, shake flask-GC, Kanazawa 1981)
0.19	(20°C, Hartley & Kidd 1987)
0.14, 0.20	(20°C, 30°C, Montgomery 1993)
0.20	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.57, 4.95	(supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
$\log [C_L/(\text{mol m}^{-3})] = -1158/(T/K) + 1.94$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)	

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.04×10^{-4}	(20°C, Porter 1964)
1.04×10^{-4} , 1.91×10^{-4} , 3.65×10^{-4}	(20, 30, 40°C, effusion method, Porter 1964 as quoted in Spencer & Cliath 1969)
2.40×10^{-5}	(Eichler 1965; Martin 1972; Melnikov 1971)
3.47×10^{-4} , 1.33×10^{-3} , 4.63×10^{-3}	(20, 30, 40°C, gas saturation method, Spencer & Cliath 1969)
6.59×10^{-4}	(calculated from vapor pressure eq. apparent vapor pressure, Spencer & Cliath 1969)
$\log (P/\text{mmHg}) = 12.07 - 5178/(T/K)$; for temp range 20–40°C (gas saturation, apparent vapor pressure, Spencer & Cliath 1969)	
6.77×10^{-4}	(gas saturation, Spencer & Cliath 1969)
3.87×10^{-4}	(20°C, partition coeff., Atkins & Eggleton 1971)
4.13×10^{-4}	(20°C, Khan 1980)
2.40×10^{-5}	(20–25°C, Weber et al. 1980)
8.90×10^{-4}	(20°C, GC, Seiber et al. 1981)
$4.20 \times 10^{-4*}$	(20°C, gas saturation-GC, extrapolated, measured range 35–75°C, Grayson & Fosbracey 1982)
$\ln (P/\text{Pa}) = 30.7 - 11285/(T/K)$; temp range 35 to 75.2°C (Antoine eq., gas saturation-GC, Grayson & Fosbracey 1982)	
0.00532, 0.0597	(P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
0.0215	(supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)
4.00×10^{-4}	(20°C, Hartley & Kidd 1987)
$7.90 \times 10^{-4*}$	(gas saturation-GC, measured range 25–125°C, Rordorf 1989)
$\log (P_S/\text{Pa}) = 14.37 - 5210.07/(T/K)$; measured range 32.4–125°C (solid, gas saturation-GC, Rordorf 1989)	
$\log (P_L/\text{Pa}) = 11.66013 - 4001.62/(T/K)$; temp range not specified (liquid, gas saturation-GC, Rordorf 1989)	
0.0215, 0.0101	(supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
0.00532, 0.0318	(P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log (P_L/\text{Pa}) = 12.46 - 4310/(T/K)$ (GC-RT correlation, supercooled liquid, Hinckley et al. 1990)	
2.37×10^{-5}	(20°C, Montgomery 1993)
4.00×10^{-4}	(20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
0.010	(supercooled liquid P_L , Wania & Mackay 1996)
3.24×10^{-4}	(liquid P_L , GC-RT correlation., Donovan 1996)
0.016, 0.014	(supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
$\log (P_L/\text{Pa}) = -3995/(T/K) + 11.62$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)	

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

4.59	(gas stripping, Atkins & Eggleton 1971)
0.02	(calculated-P/C, Mackay & Leinonen 1975)
0.0171	(20°C, calculated-P/C, Kavanaugh & Trussell 1980)
5.84	(exptl., Warner et al. 1980)
0.0456	(calculated-P/C, Levins 1981)
1.10	(20°C, Mackay & Shiu 1981)
2.94	(20°C, measured, Slater & Spedding 1981)
0.172	(estimated-group method per Hine & Mookerjee 1975, Tucker et al. 1983)
1.66	(calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
0.78	(calculated-P/C, Mackay et al. 1986)

- 0.74 (WERL Treatability Database, quoted, Ryan et al. 1988)
- 1.12 (20°C, calculated-P/C, Suntio et al. 1988)
- 1.0 (calculated-P/C, Nash 1989)
- 5.88 (Montgomery 1993)
- 1.016 (wetted wall column-GC, Altschuh et al. 1999)
- 1.0, 1.1 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{ow} :

- 2.60 (Hansch & Leo 1979)
- 5.48 (calculated, Kenaga 1980a, b)
- 6.20 (TLC-retention time correlation, Lord et al. 1980)
- 4.32 (shake flask-GC, Kanazawa 1981)
- 6.20 (20°C, shake flask-GC, Briggs 1981)
- 5.11 (HPLC-RT correlation, Hammers et al. 1982)
- 5.30 (RP-HPLC correlation, Hermens & Leeuwangh 1982)
- 5.10 (shake flask-GC, Platford 1982)
- 4.32 (Hansch & Leo 1985; Medchem Database 1988)
- 4.51, 4.49, 4.60, 4.55 (shake flask, Brooke et al. 1986)
- 4.51 (HPLC-RT correlation, De Kock & Lord 1987)
- 5.40 (shake flask/slow-stirring method, De Bruijn et al. 1989)
- 3.69–6.20 (Montgomery 1993)
- 4.76 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 5.20 (selected, Hansch et al. 1995)
- 4.76 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 5.40, 5.58 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 7.40 (calculated- K_{ow}/K_{aw} , Wania & Mackay 1996)
- 8.837*, 8.898 (gas saturation-GC/MS, calculated, measured range 5–45°C, Shoeib & Harner 2002)
- log $K_{OA} = -3.82 + 3790/(T/K)$, temp range: 5–45°C (gas saturation-GC, Shoeib & Harner 2002)
- 8.89, 8.84 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

- 3.08, 4.14, 4.69 (algae, daphnia, guppies, Reinert 1967)
- 3.65–4.69 (earthworms, Wheatley & Hardman 1968)
- 0.230 (bioaccumulation factor log BF, adipose tissue in male Albino rats, Robinson et al. 1969)
- 0.322 (bioaccumulation factor log BF, adipose tissue in male Albino rats, Walker et al. 1969)
- 3.04–3.66 (*Saccharomyces cerevisiae*, Voerman & Tammes 1969)
- 3.0–5.48 (benthic algae, Rose & McIntire 1970)
- 0.301 (bioaccumulation factor log BF, adipose tissue in male Albino rats, Baron & Walton 1971)
- 3.24 (soft clam, Butler 1971)
- 3.11, 3.54, 2.37 (*Scenedemus obliquus*, *Daphnia magna*, Reinert 1972)
- 2.37 (wet-wt. basis, *Scenedemus obliquus*, Reinert 1972)
- 3.43, 4.79, 2.66–4.60 (*Gambusia*, *Physa*, *Oedogonium sp.*, Metcalf et al. 1973)
- 4.51 (wet-wt. basis, *Ankistrodesmus*, Neudorf & Khan 1975)
- 3.39 (oyster, Mason & Rowe 1976)
- 3.20 (mussel, steady state, Ernst 1977)
- 2.30 (*Anabaena cylindrica*, Schauburger & Wildman 1977)
- 2.70; 3.26 (*Anacystis nidulans*, *Nostoc muscorum*, Schauburger & Wildman 1977)
- 2.0–4.0 (Callahan et al. 1979; quoted, Howard 1991)
- 3.76, 3.65 (fish: flowing water, static water; Kenaga 1980a, b; Kenaga & Goring 1980)
- 0.362 (average beef fat diet, Kenaga 1980b)
- 3.54 (pulex, Kenaga & Goring 1980)
- 3.62 (earthworms, Lord et al. 1980)

2.00	(<i>Triaenodes tardus</i> , Belluck & Felsot 1981)
3.65	(<i>Pseudorasbora parva</i> , flow-through conditions, Kanazawa 1981)
1.0–5.0	(selected, Schnoor & McAvoy 1981)
3.37	(mussel, quoted average, Geyer et al. 1982)
4.23–4.98	(earthworms, Gish & Hughes 1982)
4.16	(fish, correlated, Mackay 1982)
3.52	(trout, Verschueren 1983)
3.55	(clam fat, 60-d expt., Hartley & Johnson 1983)
4.10	(guppy, Davies & Dobbs 1984)
4.25	(activated sludge, Freitag et al. 1984)
3.36, 3.48, 4.25	(algae, golden ide, activated sludge, Freitag et al. 1985)
3.33, 3.29	(mussel, calculated values, Zaroogian et al. 1985)
3.33, 3.29	(oyster, calculated values, Zaroogian et al. 1985)
3.70, 3.90	(oyster, quoted from Zaroogian et al. 1985; Hawker & Connell 1986)
1.72–1.95	(human fat lipid basis, Geyer et al., 1987)
1.56–1.78	(human fat wet wt. basis, Geyer et al., 1987)
4.10	(quoted, Isnard & Lambert 1988; Howard 1991)
–2.10	(beef biotransfer factor log B_b , correlated- K_{OW} , Potter et al. 1974)
–1.97	(milk biotransfer factor log B_m , correlated- K_{OW} , Saha 1969; Wilson & Cook 1972)
–1.01	(vegetation, correlated- K_{OW} , Beall & Nash 1972; quoted, Travis & Arms 1988)
2.96–4.11	(aquatic food web, Fordham & Reagan 1991)
3.81	(fish, Fordham & Reagan 1991)
3.88	(selected, Chessells et al. 1992)
3.36, 4.06	(algae <i>Chlorella</i> : wet wt basis, dry wt basis, Geyer et al. 2000)
3.49, 5.49	(mussel <i>Mytilus edulis</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
3.54, 5.57	(<i>Daphnia</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
3.46, 5.54	(oyster <i>Crassostrea virginica</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
3.32, 5.34	(oyster <i>Crassostrea virginica</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
3.70, 5.62	(oyster <i>Crassostrea virginica</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
4.10, 5.26	(guppy female: wet wt basis, lipid wt basis, Geyer et al. 2000)
4.41, 5.41	(carp: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.32, 5.34	(oyster <i>Crassostrea virginica</i> : wet wt basis, lipid wt basis, Geyer et al. 2000)
1.69; 1.85	(human: wet wt basis, lipid wt basis, Geyer et al. 2000)
3.65; 3.66	(<i>Oncorhynchus mykiss</i> , wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

4.55	(soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
4.08	(calculated- K_{OW} , Rao & Davidson 1980)
3.87	(extrapolated from RP-TLC and reported as log K_{OM} , Briggs 1981)
4.0	(selected, Schnoor & McAvoy 1981; Schnoor 1992)
3.36–3.85	(reported as log K_{OM} , Mingelgrin & Gerstl 1983)
4.08	(soil, screening model calculations, Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989)
4.36	(calculated- K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
4.15	(soil: clay loam/kaolinite, 20°C, batch equilibrium-sorption isotherm, Kishi et al. 1990)
4.50	(sediment, Fordham & Reagan 1991)
4.10	(soil, quoted exptl., Meylan et al. 1992)
4.03	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
5.08	(estimated-QSAR and SPARC, Kollig 1993)
4.08–4.55	(Montgomery 1993)
4.08	(20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
4.55	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
4.55; 4.71	(soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)
4.90; 4.10	(soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
4.08, 4.06	(soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 1.4$ d from a model river of depth 1 m flowing at 1 m/s with a wind velocity of 3 m/s by using Henry's law constant (Lyman et al. 1982; quoted, Howard 1991).

Photolysis: rate constant $k = 4.8 \times 10^{-4} \text{ h}^{-1}$ by direct sunlight at 40° latitude (Mabey et al. 1982); using fungus and 254 nm UV, more than 90% initial added amounts were degraded in 4 weeks of incubation (Katayama & Matsumura 1991).

Oxidation: rate constant for singlet oxygen, $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ and for RO_2 radicals $k < 30 \text{ M}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982); photooxidation $t_{1/2} = 4\text{--}40.5$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

calculated tropospheric lifetimes of 1.1 d due to gas-phase reaction with OH radical (Atkinson et al. 1992).

Hydrolysis: first-order $t_{1/2} = 10.5$ yr based on a first-order rate constant $k = 7.5 \times 10^{-6} \text{ h}^{-1}$ at pH 7.0 and 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991; Montgomery 1993);

rate constant $k = 6.3 \times 10^{-2} \text{ yr}^{-1}$ at pH 7 and 25°C (Kollig 1993).

Biodegradation: aqueous aerobic $t_{1/2} = 4200\text{--}25,920$ h, based on unacclimated aerobic soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991; Howard 1991) and reported soil field test data (Kearney et al. 1969; quoted, Howard et al. 1991);

$t_{1/2} = 868$ d (Nash 1980; quoted, Jury et al. 1983);

rate constant $k = 0.013 \text{ d}^{-1}$ from soil incubation studies by die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

aqueous anaerobic $t_{1/2} = 24\text{--}168$ h, based on soil and freshwater mud grab sample data (Maule et al. 1987; quoted, Howard et al. 1991);

$t_{1/2} = 870$ d in soil by 100-d leaching screening simulation in 0–10 cm depth of soil (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 20.40 \text{ h}^{-1}$; $k_2 = 0.013 \text{ h}^{-1}$ (Ernst 1977; quoted, Hawker & Connell 1986)

$k_2 = 0.017 \text{ d}^{-1}$ (fish, Fordham & Reagan 1991)

$k_2 = 0.014 \text{ d}^{-1}$ (birds, Fordham & Reagan 1991)

Half-Lives in the Environment:

Air: $t_{1/2} = 4\text{--}40.5$ h, based on an estimated rate constant for vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991; Mortimer & Connell 1995);

calculated life-time of 1.1 d in troposphere (Atkinson et al. 1992).

Surface water: estimated $t_{1/2} \geq 300$ d in lake waters (Zoeteman et al. 1980);

$t_{1/2} = 4200\text{--}25920$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991; quoted, Mortimer & Connell 1995).

Ground water: $t_{1/2} = 24\text{--}51840$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{1/2} = 15100$ h (mean value quoted from Howard et al. 1991).

Soil: field $t_{1/2} = 49$ d in nondisked soil (Nash 1983);

$t_{1/2} \sim 7$ yr persistence in soil (Nash & Woolson 1967);

estimated persistence of 3 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

$t_{1/2} = 4200\text{--}25920$ h, based on unacclimated aerobic soil grab sample data (Castro & Yoshida 1971; quoted, Howard et al. 1991) and reported soil field test data (Kearney et al. 1969; quoted, Howard et al. 1991);

“best estimate” of 10 yr for 95% disappearance, the “true value” lies between 8.2–13.6 yr in experimental field (Freeman et al. 1975)

persistence of more than 36 months (Wauchope 1978);

first-order $t_{1/2} \sim 53.3$ d from rate constant $k = 0.013 \text{ d}^{-1}$ from soil incubation studies by die-away tests (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soils with $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982);

microagroecosystem $t_{1/2} = 19\text{--}26$ d in moist fallow soil (Nash 1983);

measured dissipation rate $k = 0.055 \text{ d}^{-1}$ (Nash 1983; quoted, Nash 1988);

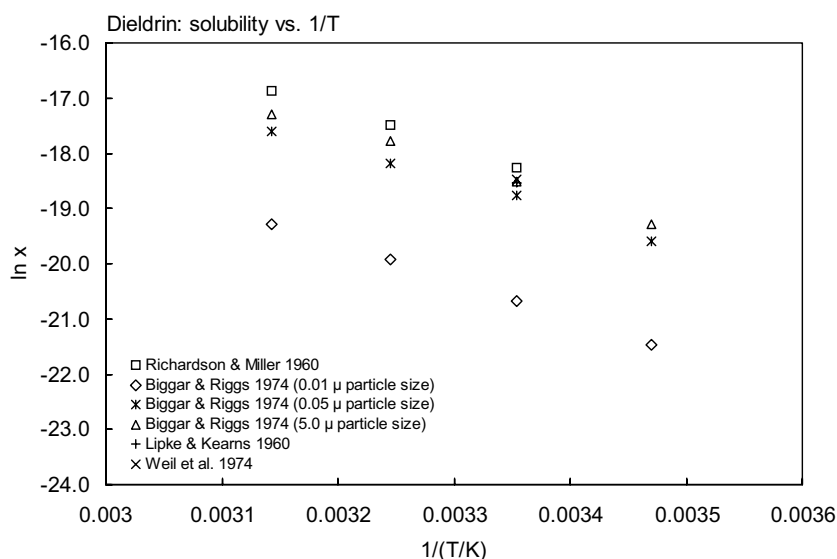
estimated dissipation rate $k = 0.034$ and 0.049 d^{-1} (Nash 1988);

biodegradation $t_{1/2} = 868$ d (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);
 $t_{1/2} > 50$ d and subject to plant uptake via volatilization (Ryan et al. 1988);
 estimated field $t_{1/2} = 1000$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
 $t_{1/2} = 5 - 9$ yr in soil (Geyer et al. 2000)
 $t_{1/2} = 21.7$ and 25 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001).
 Biota: estimated $t_{1/2} \sim 1.3$ and 10.2 d in rat's liver, and similar values estimated $t_{1/2} = 10.3$ d for the blood in rat
 and $t_{1/2} = 3$ d in adipose tissue of rat (Robinson et al. 1969);
 $t_{1/2} = 53.1$ h in mussels (Ernst 1977; quoted, Hawker & Connell 1986);
 biochemical $t_{1/2} = 868$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989)

TABLE 18.1.1.30.1

Reported aqueous solubilities and octanol-air partition coefficients of dieldrin at various temperatures

Aqueous solubility						log K_{OA}	
Richardson & Miller 1960		Biggar & Riggs 1974				Shoeib & Harner 2002	
shake flask-UV spec.		shake flask-GC				generator column-GC/MS	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	log K_{OA}
		particle size	0.01μ	0.05μ	5.0μ		
25	0.25	15	0.010	0.065	0.090	15	9.359
35	0.54	25	0.022	0.150	0.195	25	8.837
45	1.0	35	0.047	0.270	0.400	35	8.550
		45	0.090	0.480	0.650	45	8.075
						25	8.898
log $K_{OA} = A + B/(T/K)$							
A							-3.82
B							3790
enthalpy of phase change							
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 72.6$							

FIGURE 18.1.1.30.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for dieldrin.

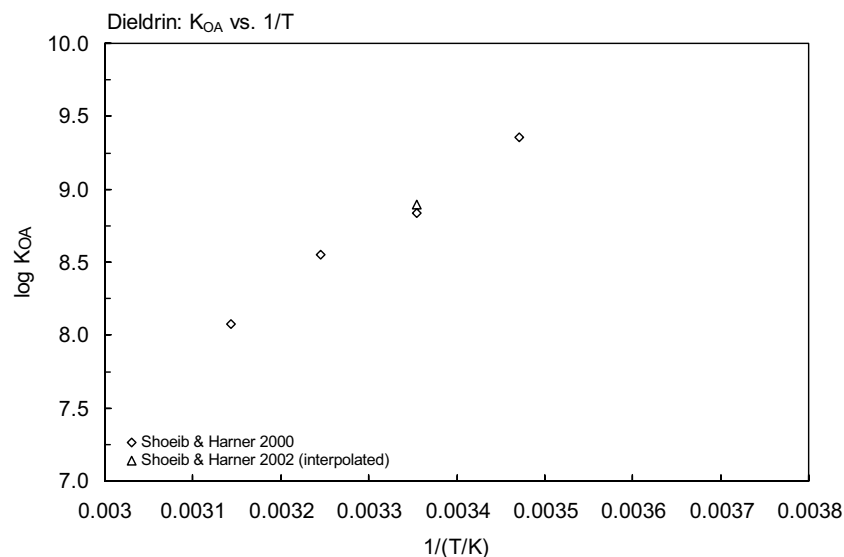


FIGURE 18.1.1.30.2 Logarithm of K_{OA} versus reciprocal temperature for dieldrin.

TABLE 18.1.1.30.2
Reported vapor pressures of dieldrin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Spencer & Cliath 1969		Grayson & Fosbracey 1982		Rordorf 1989			
gas saturation-GC		gas saturation-GC		gas saturation-GC			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
wet				set 1		set 2	
20	3.47×10^{-4}	35.0	0.0026	25	0.00079	25	0.0051
30	1.32×10^{-3}	38.2	0.0042	50	0.018	50	0.064
40	4.68×10^{-3}	51.5	0.017	75	0.25	75	0.55
dry		62.8	0.059	100	2.60	100	3.60
20	3.73×10^{-4}	70.0	0.114	125	19.0	125	18.0
30	1.35×10^{-3}	75.2	0.182				
40	4.52×10^{-3}	20	0.00042	eq. 1	P _s /Pa	eq. 1	P _S /Pa
				A	14.37	A	11.867
				B	5210.07	B	4220.71
eq.1	P/mmHg	eq. 1a	P/Pa	eq. 1	P _L /Pa	eq. 1	P _L /Pa
A	12.07	A	11285	A	11.6603	A	9.519590
B	5178	B	30.7	B	4001.62	B	3280.59
				$\Delta H_v = 76.6 \text{ kJ/mol}$		$\Delta H_v = 62.8 \text{ kJ/mol}$	

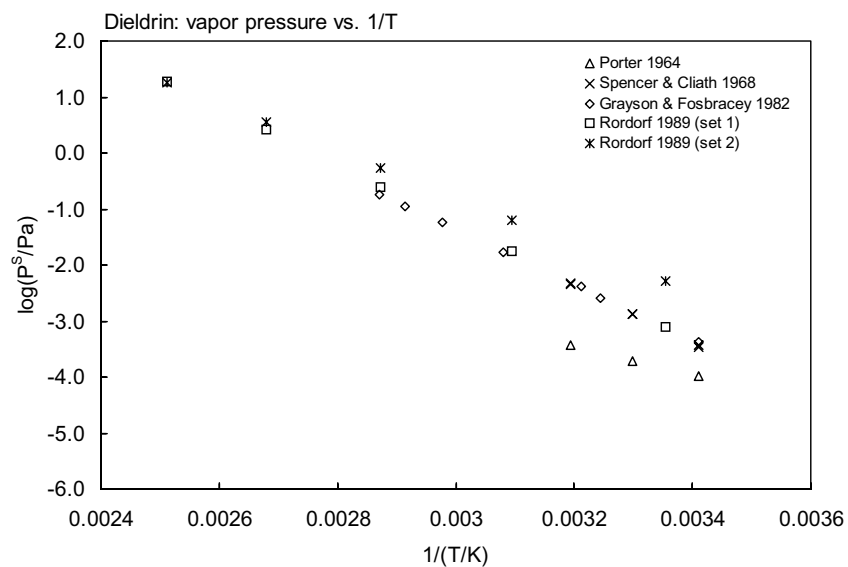
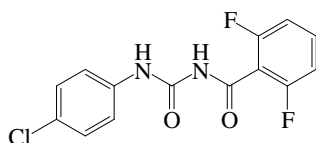


FIGURE 18.1.1.30.3 Logarithm of vapor pressure versus reciprocal temperature for dieldrin.

18.1.1.31 Diflubenzuron



Common Name: Diflubenzuron

Synonym: Deflubenzon, difluron, Dimilin, DU 112307, Duphacid, ENT 29054, OMS 1804, Largon, Micromite, PDD 60401, PH 60-40, TH-6040

Chemical Name: 1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl) urea; *N*-[[[(4-chlorophenyl)-amino]carbonyl]-2,6-difluorobenzamide

Uses: nonsystemic insecticide to control leaf-eating larvae and leaf miners in forestry, woody ornamentals and fruit trees.

CAS Registry No: 35367-38-5

Molecular Formula: $C_{14}H_9ClF_2N_2O_2$

Molecular Weight: 310.683

Melting Point ($^{\circ}C$):

230–232 (pure, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

230–232 (dec., Tomlin 1994)

239 (Lide 2003)

Boiling Point ($^{\circ}C$):

dec. on distillation (Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

288.3 (calculated-Le Bas method at normal boiling point)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.00795 (mp at $239^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.25 (Ivie et al. 1980; quoted, Belluck & Felsot 1981)

0.20 (Spencer 1982; Wauchope 1989)

0.14 ($20^{\circ}C$, Hartley & Kidd 1987; Milne 1995)

0.10 ($20^{\circ}C$, Worthing & Walker 1987, 1991)

14.0 (Montgomery 1993)

0.30 (Milne 1995)

0.08 (selected, Lohninger 1994)

0.08 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

$< 3.3 \times 10^{-5}$ ($50^{\circ}C$, Hartley & Kidd 1987)

$< 1.3 \times 10^{-5}$ (Worthing & Hance 1991)

3.33×10^{-5} ($20^{\circ}C$, Montgomery 1993)

1.20×10^{-7} (gas saturation method, Tomlin 1994)

1.20×10^{-7} (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

7.40×10^{-4} (20 – $25^{\circ}C$, calculated-P/C, Montgomery 1993)

4.70×10^{-4} (20 – $25^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.06 (Belluck & Felsot 1981)

3.88 (shake flask-UV, Sotomatsu et al. 1987)

2.12	(shake flask-UV, Nakagawa et al. 1991)
3.10	(selected, Nendza 1991)
3.29	(calculated, Montgomery 1993)
3.89	(Tomlin 1994)

Bioconcentration Factor, log BCF:

2.88	(calculated-S as per Kenaga & Goring, this work)
2.44	(calculated- K_{ow} as per Kenaga & Goring, this work)

Sorption Partition Coefficient, log K_{OC} :

3.01	(calculated, Montgomery 1993)
4.00	(average value, Dowd et al. 1993)
4.00	(20–25°C, selected, Hornsby et al. 1996)
4.06	(estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: half-lives at 20°C: $t_{1/2} > 150$ d at pH 5 and 7 and $t_{1/2} = 42$ d at pH 9 (Tomlin 1994).

$t_{1/2} > 300$ d at pH 2, $t_{1/2} = 100$ d at pH 7 and $t_{1/2} = 0.48$ d at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)

Biodegradation: $t_{1/2}$ (aerobic) = 3 d, $t_{1/2}$ (anaerobic) = 12 d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: stable at pH 5 and 7 with $t_{1/2} > 150$ d, and $t_{1/2} = 42$ d at pH 9 and 20°C (Tomlin 1994)

biodegradation $t_{1/2}$ (aerobic) = 3 d, $t_{1/2}$ (anaerobic) = 12 d, hydrolysis $t_{1/2} > 300$ d at pH 2, $t_{1/2} = 100$ d at pH 7 and $t_{1/2} = 0.48$ d at pH 12 in natural waters at 20–25°C (Capel & Larson 1995)

Ground water:

Sediment:

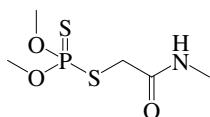
Soil: $t_{1/2} < 7$ d (Hartley & Kidd 1987; quoted, Montgomery 1993; Tomlin 1994);

$t_{1/2} = 10$ d in forest soil (Dowd et al. 1993);

field $t_{1/2} = 10$ d (20–25°C, selected, Hornsby et al. 1996).

Biota:

18.1.1.32 Dimethoate



Common Name: Dimethoate

Synonym: AC 12880, AC 18682, American Cynamid 12880, BI 58, Cekuthoate, Chemathoate, CL 12880, Cygon, Daphene, De-fend, Demos-L40, Devigon, Dimetate, Dimeton, Dimevur, ENT 24650, Ferkethion, Fip, Fortion NM, Fosfamid, Fosfotox, Fostion MM, L 395, Lurgo, NC 262, Perfekthion, Phosphamid, Rebelate, Rogodial, Rogor, Roxion, Sinoratox, Trimeton

Chemical Name: *O,O*-dimethyl *S*-methylcarbamoyl-methyl phosphorodithioate; *O,O*-dimethyl *S*-(*N*-monomethyl)carbamylmethyl dithiophosphate; 2-dimethoxyphosphinothioylthio-*N*-methylacetamide

Uses: systemic and contact insecticide to control thrips and red spider mites on many agricultural crops, sawflies on apples and plums, also wheat bulb and olive flies.

CAS Registry No: 60-51-5

Molecular Formula: C₅H₁₂NO₃PS₂

Molecular Weight: 229.258

Melting Point (°C):

51–52	(Hartley & Kidd 1987)
49.0	(Worthing & Hance 1991; Tomlin 1994; Milne 1995)
52	(Lide 2003)

Boiling Point (°C):

107	(at 0.05 mmHg, Melnikov 1971; Freed et al. 1977)
117	(at 0.1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
117	(tech. grade at 0.1 mmHg, Worthing & Hance 1991)

Density (g/cm³ at 20°C):

1.277	(65°C, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
1.281	(50°C, Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm³/mol):

205.6	(calculated-Le Bas method at normal boiling point)
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Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.43	(DSC method, Plato & Glasgow 1969)
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Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.543 (mp at 52°C)

Water Solubility (g/m³ or mg/L at 25°C at normal boiling point):

39000	(Melnikov 1971)
25000	(Martin & Worthing 1977; Worthing 1979; Kenaga 1980a)
25140	(Briggs 1981)
7000–30000	(20–25°C, selected, Willis & McDowell 1982)
> 5000	(20°C, shake flask-GC, Bowman & Sans 1983a)
25020	(20°C, shake flask-GC, Bowman & Sans 1983b)
25000	(22°C, Verschueren 1983)
25000	(21°C, Hartley & Kidd 1987; Worthing & Walker 1987, 1991; Montgomery 1993)
25120	(Kanazawa 1989)
39800	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
23300, 23800, 25000	(20°C, at pH 5, 7, 9, Tomlin 1994)
21000	(21°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

11.3 × 10 ⁻⁴	(20°C, Wolfdietrich 1965; Melnikov 1971; Khan 1980)
3.73 × 10 ⁻⁴	(20°C, vaporization rate-gravimetric method, Gückel et al. 1973)

- 11.0×10^{-4} (Worthing 1979; Hartley & Kidd 1987)
- 8.90×10^{-4} (20°C, GC, Seiber et al. 1981)
- 6.80×10^{-4} (gas saturation-GC, Kim et al. 1984, Kim 1985)
- 3.87×10^{-4} (20°C, extrapolated-Clausius-Clapeyron eq. with vapor pressures at several temperatures, Kim et al. 1984)
- 85.0×10^{-4} (20°C, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)
- 41.0×10^{-4} (20°C, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)
- 2.90×10^{-4} (20°C, Worthing & Hance 1991)
- 33.3×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 6.75×10^{-4} (20°C, Montgomery 1993)
- 11.0×10^{-4} (Tomlin 1994)
- 0.0363 (gradient GC method; Tsuzuki 2000)
- 0.0363; 0.11, 0.083 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 6.23×10^{-6} (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
- 1.10×10^{-4} (20°C, calculated-P/C, Suntio et al. 1988; quoted, Majewski & Capel 1995)
- 2.66×10^{-6} (20–21°C, calculated-P/C, Montgomery 1993)
- 1.15×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW} :

- 0.29 (Hamaker 1975; Kenaga & Goring 1980)
- 0.294 (shake flask-GC, Freed et al. 1979)
- 0.79 (20 ± 2°C, shake flask-UV, Briggs 1981)
- 0.70 (22°C, shake flask-GC, Bowman & Sans 1983)
- 0.50, 0.78 (recommended, Hansch & Leo 1985)
- 2.71 (Kanazawa 1989)
- 0.699 (Worthing & Hance 1991; Milne 1995)
- 0.51–0.78 (Montgomery 1993)
- 0.50 (recommended, Sangster 1993)
- 0.704 (Tomlin 1994)
- 0.78 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 2.00 (estimated-S, Howard 1991)

Sorption Partition Coefficient, log K_{OC} :

- 1.23 (soils, calculated, Kenaga 1980a; quoted, Howard 1991)
- 0.72 (20 ± 2°C, shake flask-UV and reported as log K_{OM} , Briggs 1981)
- 1.43 (average of 2 soils, Kanazawa 1989)
- 1.26, 1.56 (clay loam soil, Kanazawa 1989)
- 0.716 (clay soil, Kanazawa 1989;)
- 0.72, 1.47 (reported as log K_{OM} , estimated as log K_{OM} , Magee 1991)
- 1.20, 1.39 (soil, quoted exptl., calculated- χ and fragment contribution, Meylan et al. 1992)
- 1.30 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.132 (estimated-QSAR and SPARC, Kollig 1993)
- 0.96 (Montgomery 1993)
- 1.00 (estimated-chemical structure, Lohninger 1994)
- 1.21; 1.72 (sandy loam soil, sandy loam sand, Tomlin 1994)
- 1.20 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.20; 1.70, 1.85 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 0.469\text{--}4.69$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).Hydrolysis: $t_{1/2} = 0.8$ h at pH 9 and $t_{1/2} = 21$ h at pH 2 both at 70°C (Melnikov 1971; quoted, Freed et al. 1977) neutral rate constant $k = 1.7 \times 10^{-4} \text{ h}^{-1}$ with a calculated $t_{1/2} = 118$ h at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Montgomery 1993);first-order $t_{1/2} = 2822$ h, based on measured neutral and base catalyzed hydrolysis rate constants (Ellington et al. 1987; quoted, Howard et al. 1991);rate constant $k = 1.68 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993); $t_{1/2} = 12$ d at pH 9 (Tomlin 1994) $t_{1/2} = 120$ d at pH 2, $t_{1/2} = 120$ d at pH 7 and $t_{1/2} = 0.0038$ d at pH 12 in natural waters (Capel & Larson 1995)Biodegradation: aqueous aerobic $t_{1/2} = 264\text{--}1344$ h, based on river die-away test data (Eichelberger & Lichtenburg 1971; quoted, Howard et al. 1991) and soil die-away test data for two soils (Bro-Rasmussen et al. 1970; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 1056\text{--}5376$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991) $t_{1/2}(\text{aerobic}) = 11$ d, $t_{1/2}(\text{anaerobic}) = 44$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

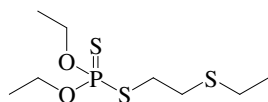
Half-Lives in the Environment:

Air: $t_{1/2} = 0.469\text{--}4.69$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).Surface water: $t_{1/2} = 264\text{--}1344$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)Biodegradation $t_{1/2}(\text{aerobic}) = 11$ d, $t_{1/2}(\text{anaerobic}) = 44$ d, hydrolysis $t_{1/2} = 120$ d at pH 2, $t_{1/2} = 120$ d at pH 7 and $t_{1/2} = 0.0038$ d at pH 12 in natural waters (Capel & Larson 1995) $t_{1/2} = 423$ d at 6°C, 193h at 23°C in darkness for Milli-Q water; $t_{1/2} = 171$ d at 6°C, $t_{1/2} = 43$ d at 22°C in darkness, $t_{1/2} = 29$ d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 173$ d at 6°C, $t_{1/2} = 29$ d at 22°C in darkness for filtered river water, pH 7.3; $t_{1/2} = 219$ d at 6°C, $t_{1/2} = 36$ d at 22°C in darkness, $t_{1/2} = 74$ d under sunlight conditions for seawater, pH 8.1 (Lartiges & Garrigues 1995).Ground water: $t_{1/2} = 528\text{--}2688$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 264\text{--}888$ h, based on soil die-away test data for two soils (Bro-Rasmussen et al. 1970; quoted, Howard et al. 1991);selected $t_{1/2} = 7.0$ d (Wauchope et al. 1992; Hornsby et al. 1996);aerobic $t_{1/2} = 2\text{--}4.1$ d in soil and photolytic $t_{1/2} = 7\text{--}16$ d on soil surface (Tomlin 1994); $t_{1/2} = 7.0$ d (selected, Halfon et al. 1996).Biota: disappearance rate and half-life from treated plants: $t_{1/2} = 2.95$ d for cabbage, $t_{1/2} = 3.40$ d for tomato leaves and $t_{1/2} = 2.40$ d for tomato fruits (Othman et al. 1987).

18.1.1.33 Disulfoton



Common Name: Disulfoton

Synonym: Di-Syston, Dimaz, Disipton, Disystox, Dithiosystox, Frumin AL, Glebofos, Solvirex

Chemical Name: *O,O*-diethyl *S*-[2-(ethylthio) ethyl] phosphorodithioate; phosphorodithioic acid, *O,O*-diethyl *S*-[2-(ethylthio)ethyl] ester

Uses: insecticide to control aphids, thrips, mealybugs, and other sucking insects, and spider mites in potatoes, vegetables, cereals, maize, sorghum, rice, soybeans, groundnuts, lucerne, clover, sugar cane, sugar beet, hops, strawberries, cotton, coffee, pineapples, tobacco, ornamentals, fruit and nut crops, and forestry nurseries; also used as acaricide.

CAS Registry No: 298-04-4

Molecular Formula: $C_8H_{19}O_2PS_3$

Molecular Weight: 274.405

Melting Point ($^{\circ}C$):

-25 (Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

62.0 (at 0.01 mmHg, Hartley & Kidd 1987)

128 (at 1 mmHg, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.144 (Hartley & Kidd 1987; Tomlin 1994)

1.14 (Worthing & Hance 1991)

Molar Volume (cm^3/mol):

282.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

66 (Günther 1968)

25 ($20^{\circ}C$, Melnikov 1971; Spencer 1973)

25 (Martin & Worthing 1977)

16.3 ($19.5^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983b)

25 ($22^{\circ}C$, Khan 1980; Worthing & Walker 1983)

15–66 (20 – $25^{\circ}C$, selected, Willis & McDowell 1982)

25 ($22^{\circ}C$, Hartley & Kidd 1987)

12 ($22^{\circ}C$, Worthing & Hance 1991)

25 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

12 ($20^{\circ}C$, Tomlin 1994)

12 ($22^{\circ}C$, Milne 1995)

29.9, 29.9 (supercooled liquid S_L : literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.024 ($20^{\circ}C$, vapor density, MacDougall & Archer 1964)

$\log(P/mmHg) = 10.20 - 4084.80/(T/K)$; temp range 10 – $40^{\circ}C$ (vapor density, MacDougall & Archer 1964)

0.024 ($20^{\circ}C$, Eichler 1965)

0.024 ($20^{\circ}C$, Melnikov 1971; Khan 1980)

0.024 (Worthing 1983)

0.0041 ($20^{\circ}C$, GC-Rt correlation, Kim et al. 1984; Kim 1985)

0.024 ($20^{\circ}C$, Hartley & Kidd 1987)

0.020 ($20^{\circ}C$, selected, Suntio et al. 1988)

- 0.024 (20°C, Worthing & Hance 1991)
- 0.020 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.013 (Tomlin 1994)
- 0.010, 0.0099 (supercooled liquid P_L : literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 0.404 (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)
- 0.22 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.101, 0.253 (10°, 20°C, Wanner et al. 1989)
- 0.090 (final adjusted value FAV, Muir et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.04 (Callahan et al. 1979)
- 3.88 (shake flask-UV, Hermens & Leeuwangh 1982)
- 4.02 (shake flask-GC, Bowman & Sans 1983b)
- 4.02 (recommended, Hansch & Leo 1985)
- 3.84 (RP-HPLC correlation, Saito et al. 1993)
- 3.95 (Tomlin 1994)
- 4.02 (recommended, Hansch et al. 1995)
- 3.95 (literature-derived value LDV, Muir et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 8.39 (final adjusted value FAV, Muir et al. 2004)

Bioconcentration Factor, $\log BCF$:

- 2.00 (calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
- 2.04 (calculated- K_{OC} , Kenaga 1980)
- 2.00, 2.83 (estimated-S, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1991)
- 2.65 (carp, Takase & Oyama 1985; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.25 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
- 2.81, 3.04, 3.72 (Hamaker & Thompson 1972)
- 2.87 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 3.20 (av. soils/sediments, Rao & Davidson 1980)
- 2.67–3.70 (reported as $\log K_{OM}$, Mingelgrin & Gerstl 1983)
- 2.90 (calculated- MCI χ , Gerstl & Helling 1987)
- 3.20 (soil, screening model calculations, Jury et al. 1987b)
- 3.36 (estimated as $\log K_{OM}$, Magee 1991)
- 3.22 (soil, quoted exptl., Meylan et al. 1992)
- 2.91 (soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
- 2.78 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.94 (estimated-QSAR and SPARC, Kollig 1993)
- 2.91 (soil, HPLC-screening method, mean value, Kördel et al. 1993, 1995)
- 3.49 (estimated-chemical structure, Lohninger 1994)
- 3.22 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 2.91; 2.91 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 3.66, 3.146, 3.11, 3.37, 4.146 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 3.417, 3.333, 3.151, 2.782, 3.127 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, HPLC- k' correlation, Gawlik et al. 2000)
- 3.22; 3.15, 3.40 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 2.92 (soil: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: gas exchange $t_{1/2}$ = of 900 d for winter and $t_{1/2}$ = 360 d for summer in Rhine River (Wanner et al. 1989).

Photolysis: photolytic $t_{1/2}$ = 1000 d for winter and $t_{1/2}$ = 100 d for summer in the Rhine River (Wanner et al. 1989); $t_{1/2}$ = 1–4 d (Tomlin 1994)

Apparent first-order rate constant phototransformation at $\lambda > 285$ nm, $k = (1.38 \pm 0.12) \times 10^{-2} \text{ h}^{-1}$ in purified water, and $k = (1.68 \pm 0.12) \times 10^{-2} \text{ h}^{-1}$ in Capot river water with $t_{1/2} \sim 40$ h (Zamy et al. 2004)

Oxidation: half-life ranged from $t_{1/2} \sim 5$ h of midday sunlight during summer to $t_{1/2} = 12$ h during winter estimated from kinetic data for oxygenation reactions photosensitized by humic substances in water exposed to sunlight (Zepp et al. 1981);

photooxidation $t_{1/2} = 0.50$ –4.80 h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order $t_{1/2} = 103$ d, based on measured overall rate constant $k = 2.8 \times 10^{-4} \text{ h}^{-1}$ at pH 7, 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991);

abiotic hydrolysis $k = 1.3 \times 10^{-7} \text{ s}^{-1}$ under neutral condition, $k = 2.0 \times 10^{-3} \text{ s}^{-1}$ under base-catalyzed condition at 20°C and hydrolysis $t_{1/2} = 170$ d at 11°C, pH 9 and $t_{1/2} = 62$ d in summer were predicted in Rhine River (Wanner et al. 1989);

$t_{1/2} = 3.04$ yr in water at pH 1–5 and at 20°C; 1.2 d at pH 7 and $t_{1/2} = 7.2$ h at pH 9 both at 70°C (Worthing & Hance 1991);

rate constant $k = 3.23 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993);

$t_{1/2} = 133$ d at pH 4, $t_{1/2} = 169$ d at pH 7, and $t_{1/2} = 131$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: $t_{1/2} < 14$ d, rapidly oxidized in soil (Szeto et al. 1983)

primary biodegradation rate constant $k = 0.2 \mu\text{g}^2 \text{ L}^2 \text{ d}^{-1}$ with $t_{1/2} = 41$ d, and the degradation $t_{1/2} = 7$ –41 d for winter and $t_{1/2} = 4$ –28 d for summer in Rhine River (Wanner et al. 1989);

aqueous aerobic $t_{1/2} = 72$ –504 h, based on aerobic soil field data and reported half-lives for soil (Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 288$ –2016 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.50$ –4.80 h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: gas exchange $t_{1/2} = 900$ d for winter, $t_{1/2} = 360$ d for summer; abiotic hydrolysis half-lives of 170 d for winter, 62 d for summer; photolytic transformation $t_{1/2} = 1000$ d for winter, $t_{1/2} = 200$ d for summer and primary biodegradation $t_{1/2} = 7$ –41 d for winter, $t_{1/2} = 8$ –28 d for summer in Rhine River under environmental conditions (Wanner et al. 1989);

overall $t_{1/2} = 72$ –504 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

$t_{1/2} \sim 40$ h upon photolysis in Capot river water (Zamy et al. 2004)

Ground water: $t_{1/2} = 144$ –1008 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: estimated persistence of 4 wk in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2} = 72$ –504 h, based on aerobic soil field data (Szeto et al. 1983; quoted, Howard et al. 1991) and reported half-lives for soil (Domsch 1984; quoted, Howard et al. 1991);

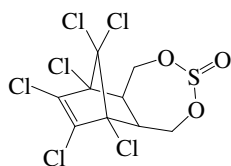
$t_{1/2} = 5$ d from screening model calculations (Jury et al. 1987b);

estimated $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996);

soil $t_{1/2} = 9$ d (Pait et al. 1992).

Biota: biochemical $t_{1/2}$ = of 5 d from screening model calculations (Jury et al. 1987b).

18.1.1.34 Endosulfan



Common Name: Endosulfan

Synonym: Benzoepin, Beosit, Bio 5462, Chlorthiepin, Crissulfan, Cyclodan, Endocel, ENT 23979, FMC 5462, Hildan, Hoe 2671, Insectophene, KOP-thiodan, Malix, NCI-C00566, Niagara 5462, OMS-570, Thifor, Thimul, Thiodan, Thiofor, Thionex, Thiosulfan, Tionel, Tiovel

Chemical Name: 1,4,5,6,7,7-hexachloro-5-norbornene-2,3-dimethyl cyclic sulfite; 1,2,3,4,7,7-hexachlorobicyclo-2,2,1-hepten-5,6-bisoxymethylene sulfite; (1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-en-2,3-ylene-bismethylene)-sulfite; 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodioxathiepine 3-oxide

Uses: insecticide for vegetable crops and also used as acaricide.

CAS Registry No: 115-29-7; 959-98-8 (α -endosulfan, endosulfan I); 33213-65-9 (β -endosulfan, endosulfan II)

Molecular Formula: $C_9H_6Cl_6O_3S$

Molecular Weight: 406.925

Melting Point ($^{\circ}C$):

70–100	(tech. grade, Worthing & Hance 1991; Milne 1995)
70–100, 108–110	(α -endosulfan, β -endosulfan, Suntio et al. 1988)
106, 207–209	(α -endosulfan, β -endosulfan, Montgomery 1993)
109.2, 213.3	(α -endosulfan, β -endosulfan, Tomlin 1994)
106, 109.2	(Milne 1995)

Boiling Point ($^{\circ}C$):

106	(at 0.7 mmHg, Hartley & Kidd 1987; Milne 1995)
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Density (g/cm^3 at $20^{\circ}C$):

1.80	(tech. grade, Tomlin 1994)
1.745	(Milne 1995; Montgomery 1993)

Molar Volume (cm^3/mol):

312.8	(calculated-Le Bas method at normal boiling point.)
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Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.22. 0.13	($20^{\circ}C$, α -, β -endosulfan, Suntio et al. 1988)
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Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ pr as indicated):

0.53	(α -endosulfan, generator column-GC, Weil et al. 1974)
0.286	(β -endosulfan, generator column-GC, Weil et al. 1974)
<1.0	(Wauchope 1978)
0.050	(Weber et al. 1980)
0.510	(α -endosulfan, $20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a)
0.45	(β -endosulfan, $20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a)
0.06–0.15	(U.S. EPA 1984; McLean et al. 1988)
0.32	($22^{\circ}C$, Hartley & Kidd 1987)
0.15	($20^{\circ}C$, selected, Suntio et al. 1988)
0.32	(α -endosulfan at $22^{\circ}C$, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
0.33	(β -endosulfan at $22^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)
0.32	(20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.53	(α -endosulfan, Montgomery 1993)
0.28	(β -endosulfan, Montgomery 1993)

- 3.75, 3.63 (α -endosulfan, supercooled liquid S_L : literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)
- 1.71, 2.56 (α -endosulfan, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)
- 32.1, 36.2 (β -endosulfan, supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated):

- 0.00133 (Martens 1972; Khan 1980)
- 0.013 (endosulfan I, Barlow 1978)
- > 0.00013 (20–25°C, Weber et al. 1980)
- 1.20 (80°C, Hartley & Kidd 1987)
- 0.0061 (endosulfan I, GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
- 0.0032 (endosulfan II, GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
- 0.0011 (20°C, selected, Suntio et al. 1988)
- 1.20 (tech. grade at 80°C, Worthing & Hance 1991)
- 2.27×10^{-5} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.00133 (Montgomery 1993)
- 8.3×10^{-5} (20°C, 2 to 1 mixture of α - and β -endosulfan, Tomlin 1994)
- 2.3×10^{-5} (selected, Halfon et al. 1996)
- 0.0061, 0.0063 (α -endosulfan, supercooled liquid P_L : literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)
- 0.0060, 0.0044 (α -endosulfan, supercooled liquid P_L : LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
- 0.0043, 0.0040 (β -endosulfan, supercooled liquid P_L : LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Henry's Law Constant (Pa·m³/mol at 25°C and reported temperature dependence equations):

- 1.09 (calculated-P/C, Mabey et al. 1982)
- 2.98 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.679, 0.0627 (endosulfan I, II, calculated, Cotham & Bidleman 1989)
- 1.135 (calculated-P/C an average of α - and β -endosulfan, Howard 1991)
- 10.23 (α -endosulfan, Montgomery 1993)
- 1.935 (β -endosulfan, calculated-P/C, Montgomery 1993)
- 6.45, 13.23 (20°C, tech. grade: distilled water, salt water 33.31%, wetted wall column-GC, Rice et al. 1997a, b)
- 6.63, 0.788 (20°C, endosulfan I, II, distilled water, wetted wall column-GC, Rice et al. 1997a, b)
- $\log K_{AW} = -876.14/(T/K) + 0.4463$; temp range: 8.3–38.2°C, (endosulfan I, distilled water, wetted-wall column-GC, Rice et al. 1997a)
- 12.89, 2.12 (20°C, endosulfan I, II, salt water 33.31%, wetted wall column-GC, Rice et al. 1997a, b)
- 8.65, 8.48; 9.31 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 171‰ and TOC 0.4–1.0 ppm, from Pt. Lookout, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
- 8.77, 8.04; 9.12 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 161‰ and TOC 0.5–0.6 ppm, from Solomons, Chesapeake Bay; estimated adjusted to salinity, Rice et al. 1997b)
- 7.14, 9.21; 8.43 (20°C, endosulfan I: microlayer, subsurface natural water of salinity 121‰, TOC 0.6 ppm, from Sandy Point, Chesapeake Bay; estimated value adjusted to salinity, Rice et al. 1997b)
- 0.719, 0.040 (α -, β -endosulfan, wetted wall column-GC, Altschuh et al. 1999)
- 6.99 (20°C, Endosulfan I, selected from literature experimentally measured data, Staudinger & Roberts 2001)
- $\log K_{AW} = 0.446 - 876/(T/K)$, (Endosulfan I, van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
- 0.715, 0.699 (α -endosulfan, literature-derived value LDV, final adjusted value FAV, Muir et al. 2004)
- 0.72, 0.70 (α -endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
- 0.040, 0.045 (β -endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW} :

- 3.55, 3.62 (α -, β -endosulfan, Ali 1978)
- 3.83 (α -endosulfan, shake flask-GC, Hermens & Leeuwangh 1982)
- 3.83 (α -endosulfan, Hansch & Leo 1985)
- 4.74, 4.78 (α -, β -endosulfan, calculated-fragment const., Noegrohati & Hammers 1992)
- 3.55, 3.62 (α -, β -endosulfan, Montgomery 1993)
- 4.74, 4.79 (α -, β -endosulfan at pH 5, Tomlin 1994)
- 3.62, 3.83 (α -, β -endosulfan, Hansch et al. 1995)
- 3.84 (Pomona-database, Müller & Kördel 1996)
- 5.09 (α -endosulfan, literature-derived value LDV, Muir et al. 2004)
- 4.74, 4.94 (α -endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)
- 4.78, 4.78 (β -endosulfan, LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:

- 8.677*, 8.638 (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
- log $K_{OA} = -5.90 + 4333/(T/K)$, temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
- 8.64 (α -endosulfan, final adjusted value FAV, Muir et al. 2004)
- 8.63, 8.49 (α -endosulfan, LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

- 3.66 (beef biotransfer factor log B_b , correlated- K_{OW} , Beck et al. 1966)
- 2.78 (α -endosulfan for mussel, Ernst 1977;)
- 1.52, –1.22 (α -, β -endosulfan, bioaccumulation factor log BF, adipose tissue in female Albino rats, Dorough et al. 1978)
- 2.63, 2.44 (α -, β -endosulfan, paddy field fish, Soon & Hock 1987)
- 1.91, 2.33 (α -, β -endosulfan, paddy field fish, Tejada 1995)
- 3.55; 3.65 (α -endosulfan for *Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 3.46 (α -endosulfan, estimated, Lyman et al. 1982; quoted, Howard 1991)
- 3.83 (β -endosulfan, calculated-S, Lyman et al. 1982; quoted, Howard 1991)
- 4.09 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 4.00 (α - or β -endosulfan, estimated-QSAR & SPARC, Kollig 1993)
- 3.31, 3.37 (α -endosulfan, β -endosulfan, calculated, Montgomery 1993)
- 4.09 (soil, α -endosulfan, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993)
- 4.09 (estimated-chemical structure, Lohninger 1994)
- 3.48–4.30 (Tomlin 1994)
- 4.09 (α -endosulfan, HPLC-screening method, Kördel et al. 1995)
- 4.09; 5.24 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 3.90 (soil, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.5$ –24.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air with a deoxygenated endosulfan analog (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order $t_{1/2} = 218$ h, based on neutral aqueous hydrolysis rate constant $k = (3.2 \pm 2.0) \times 10^{-3} \text{ h}^{-1}$ for α -Endosulfan at pH 7 and 25°C (Ellington et al. 1986, 1987, 1988; quoted, Howard et al. 1991; Montgomery 1993);

first-order $t_{1/2} = 187$ h, based on neutral aqueous hydrolysis rate constant $k = (3.7 \pm 2.0) \times 10^{-3} \text{ h}^{-1}$ for β -endosulfan at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Howard et al. 1991; Montgomery

1993); rate constant $k = 6.1 \times 10^{-2} \text{ yr}^{-1}$ for α -endosulfan at pH 7 and 25°C and rate constant $k = 8.9 \times 10^{-2} \text{ yr}^{-1}$ for β -endosulfan at pH 7 and 25°C (Kollig 1993).

$t_{1/2} = 360 \text{ d}$ at pH 2, $t_{1/2} = 9.1 \text{ d}$ at pH 7 and $t_{1/2} = 0.00029 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 48\text{--}336 \text{ h}$, based on unacclimated aerobic river die-away test data (Eichelberger & Lichtenburg 1971; quoted, Howard et al. 1991) and reported soil grab sample data (Bowman et al. 1965; quoted, Howard et al. 1991);

first-order rate constant $k = -0.00502 \text{ h}^{-1}$ in nonsterile sediment, $k = -0.00796 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point, first-order $k = -0.0157 \text{ h}^{-1}$ in nonsterile water, and $k = -0.0325 \text{ h}^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988);

first-order rate constants $k = -0.00165$ to -0.00296 h^{-1} in nonsterile sediment, $k = -0.00426$, -0.00545 h^{-1} in sterile sediment by shake-tests at Davis Bayou and first-order rate constants $k = -0.00335$ to -0.00490 h^{-1} in nonsterile water and $k = -0.0130$, -0.00866 h^{-1} in sterile water by shake-tests at Davis Bayou (Walker et al. 1988)

$t_{1/2}(\text{aerobic}) = 2 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 8 \text{ d}$ in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 12.3 \text{ h}^{-1}$; $k_2 = 0.0205 \text{ h}^{-1}$ (mussel from α -endosulfan, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: $t_{1/2} = 2.5\text{--}24.8 \text{ h}$, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air with a deoxygenated Endosulfan analog (Atkinson 1987; quoted, Howard et al. 1991);

$t_{1/2} = 9.2 \pm 4 \text{ yr}$ at Eagle Harbor in the Great Lake's atmosphere. (Buehler et al. 2004).

Surface water: persistence of up to 4 weeks in river water (Eichelberger & Lichtenberg 1971);

$t_{1/2} = 30 \text{ d}$ and 45 d for α - and β -endosulfan respectively for surface waters in case of first order reduction process may be assumed and estimated $t_{1/2} \sim 30\text{--}300 \text{ d}$ for β -endosulfan in lakes in the Netherlands (Zoeteman et al. 1980);

$t_{1/2} = 4.5\text{--}218 \text{ h}$, based on aqueous hydrolysis half-lives for both α - and β -endosulfan at pH 7 and 9 and 25°C, respectively (Ellington et al. 1987; quoted, Howard et al. 1991)

$t_{1/2} = 1.3 \text{ d}$ in rice paddy water (Tejada et al. 1993; quoted, Abdullah et al. 1997)

$t_{1/2}(\text{aerobic}) = 2 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 8 \text{ d}$, hydrolysis $t_{1/2} = 360 \text{ d}$ at pH 2, $t_{1/2} = 9.1 \text{ d}$ at pH 7 and $t_{1/2} = 0.00029 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

Ground water: estimated $t_{1/2} = 30\text{--}300 \text{ d}$ in lakes and Ground water (β -Endosulfan, Zoeteman et al. 1980);

$t_{1/2} = 4.5\text{--}218 \text{ h}$, based on aqueous hydrolysis half-lives for both α - and β -endosulfan at pH 7 and 9 and 25°C respectively (Ellington et al. 1987; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 4.5\text{--}218 \text{ h}$, based on aqueous hydrolysis half-lives for both α - and β -endosulfan at pH 7 and 9 and 25°C, respectively (Ellington et al. 1987; quoted, Howard et al. 1991);

$t_{1/2} > 50 \text{ d}$ and subject to plant uptake via volatilization (Ryan et al. 1988);

selected $t_{1/2} = 50 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 1.2 \text{ d}$ in rice soil (Tejada et al. 1993; quoted, Abdullah et al. 1997);

soil $t_{1/2} = 120 \text{ d}$ (Pait et al. 1992);

degraded in soil with $t_{1/2} = 30\text{--}70 \text{ d}$ (Tomlin 1994); 50 d (selected, Halfon et al. 1996)

$t_{1/2} = 5\text{--}7 \text{ yr}$ in soil (Geyer et al. 2000)

Biota: $t_{1/2} = 33.8 \text{ h}$ in mussels (α -endosulfan, Ernst 1977);

$t_{1/2} = 1.0 \text{ d}$ in rice leaves (Tejada et al. 1993; quoted, Abdullah et al. 1997).

TABLE 18.1.1.34.1
Reported octanol-air partition coefficients of α -endosulfan at various temperatures

Shoeib & Harner 2002
generator column-GC/MS

t/°C	log K _{OA}
5	9.7188
10	9.3591
15	9.1651
20	8.8316
25	8.6772
25	8.638

$\log K_{OA} = A + B/(T/K)$
A -5.902
B 4333

enthalpy of phase change
 $\Delta H_{OA}/(kJ\ mol^{-1}) = 83.0$

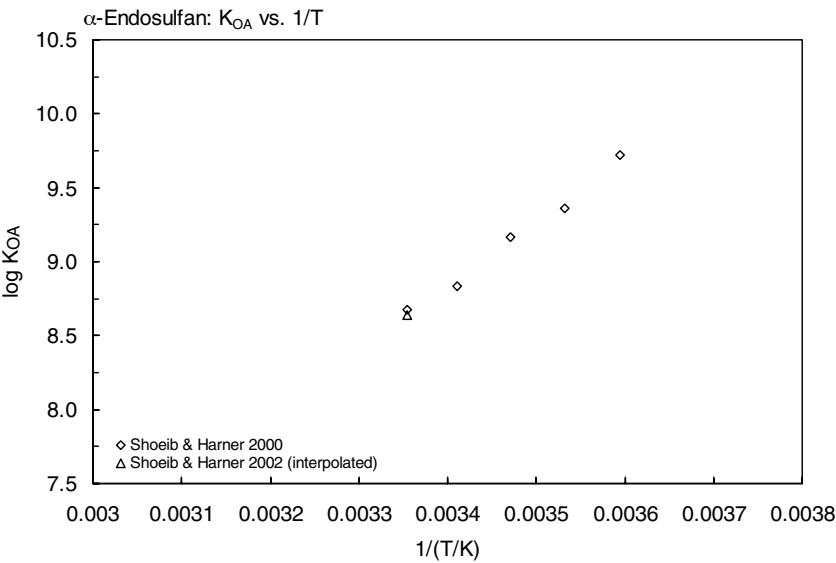
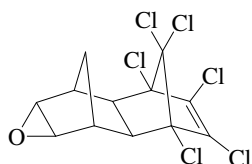


FIGURE 18.1.1.34.1 Logarithm of K_{OA} versus reciprocal temperature for α -endosulfan.

18.1.1.35 Endrin



Common Name: Endrin

Synonym: Endrex, ENT 17521, Hexadrin, Isodrin epoxidek, Mendrin, NA 2761, NCI-C00157, Nendrin, RCRA

Chemical Name: 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-*exo*-1,4-*exo*-5,8-dimethano-naphthalene

Uses: Insecticide/Avicide/Rodenticide

CAS Registry No: 72-20-8

Molecular Formula: C₁₂H₈Cl₆O

Molecular Weight: 380.909

Melting Point (°C):

226–230 (Hartley & Kidd 1987; Howard 1991)

245 (dec, Lide 2003)

Boiling Point (°C):

245 (dec. Montgomery 1993)

Density (g/cm³ at 20°C):

1.70, 1.65 (pure, technical, at 25°C, Montgomery 1993)

Molar Volume (cm³/mol):

318.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.88 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00694 (mp at 245°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.23* (shake flask-UV, measured range 25–45°C, Richardson & Miller 1960)

0.26 (rm. temp., shake flask-GC, Robeck et al. 1965)

0.23 (Günther et al. 1968)

0.25* (shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)

0.022*, 0.15*, 0.195* (particle size: 0.01, 0.05 and 5.0 μm, shake flask-GC/ECD, measured range 15–45°C, Biggar & Riggs 1974)

0.26 (generator column-GC/ECD, Weil et al. 1974)

0.10 (Weber et al. 1980)

0.024 (Bruggeman et al. 1981)

0.25 (misquoted as 0.25 μg/L from Biggar & Riggs, Howard 1991)

0.22–0.26 (Montgomery 1993)

0.23 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

15.85 (20–25°C, supercooled liquid value, Majewski & Capel 1995)

0.105, 0.000065 (predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.03, 1.14 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

log [C_L/(mol m⁻³)] = -1022/(T/K) + 0.86 (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated):

4.00 × 10⁻⁴ (20°C, Bowery 1964)

2.67 × 10⁻⁵ (Eichler 1965; Melnikov 1971; Martin 1972; Quellette & King 1977)

- 2.67×10^{-5} (20–25°C, Weber et al. 1980)
- 1.17×10^{-5} (20°C, selected exptl. value, Kim 1985)
- 2.00×10^{-5} (20°C, selected, Suntio et al. 1988)
- 9.33×10^{-5} (25°C, Montgomery 1993)
- 2.67×10^{-5} (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 1.38×10^{-3} (20–25°C, supercooled liquid value, Majewski & Capel 1995)
- 0.0052, 0.0031 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 1.8×10^{-4} (calculated-P/C, Mabey et al. 1982)
- 0.042 (Ryan et al. 1988)
- 0.033 (20°C, calculated-P/C, Suntio et al. 1988)
- 0.762 (calculated, Howard 1991)
- 0.0507 (calculated-P/C, Montgomery 1993)
- 0.644 (wetted wall column-GC, Altschuh et al. 1999)
- 0.64, 1.1 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 5.60 (calculated, Neely et al. 1974)
- 4.56 (RP-HPLC-RT correlation, Veith et al. 1979)
- 5.34 (Kenaga & Goring 1980;)
- 3.21 (Rao & Davidson 1980)
- 4.82 (Veith & Kosian 1982)
- 5.01 (HPLC-RT correlation, Eadsforth 1986)
- 5.28 (HPLC-RT correlation, Liu & Qian 1988)
- 5.195 ± 0.005 (slow-stirring method, De Bruijn et al. 1989)
- 3.21–5.34 (Montgomery 1993)
- 4.71 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 5.20 (recommended, Hansch et al. 1995)
- 4.71 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 5.20, 4.94 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section:

- 8.338*, 8.609 (gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
- $\log K_{OA} = -11.75 + 6067/(T/K)$, temp range: 5–35°C (gas saturation-GC, Shoeib & Harner 2002)
- 8.13, 8.32 (LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, $\log BCF$:

- 2.40–2.18 (bluegills, Bennett & Day 1970)
- 2.60–2.88 (channel catfish, Argyle et al. 1973)
- 3.21 (channel catfish, 55-d exposure, Argyle et al. 1973)
- 3.13, 4.69 (*Gambusia*, *Physa*, Metcalf et al. 1973)
- 3.11, 4.69, 3.66 (fish, snail, algae, Metcalf et al. 1973)
- 2.83, 2.49, 2.48 (fish, mosquitoes, *Daphnia*, 3-d expt. with no dietary routes, Metcalf et al. 1973)
- 3.43 (oyster, Mason & Rowe 1976)
- 3.28 (mussel, Ernst 1977)
- 3.24 (calculated- K_{ow} , Mackay 1982)
- 4.02; 4.18; 3.85 (flagfish, 30-d exposure; 65-d exposure; 110-d exposure, Hermanutz 1978)
- 3.70 (fathead minnow, Jarvinen & Tyo 1978)
- 3.17 (mosquito fish, 35-d exposure, Veith et al. 1979; Veith & Kosian 1983)
- 3.66 (fathead minnow, 300-d exposure, Veith et al. 1979; Veith & Kosian 1983)
- 3.66 (*Oedogonium* sp., Baughman & Paris 1981)
- 3.85–4.18 (flag fish, mosquito fish, Veith & Kosian 1983)

- 3.24, 3.18 (mussel, calculated- K_{ow} & models, Zaroogian et al. 1985)
 3.17 (fathead minnow, quoted from Veith et al. 1979, Zaroogian et al. 1985)
 3.40 (Isnard & Lambert 1988)
 3.13–4.0 (fish, quoted, Howard 1991)
 3.85 (fathead minnow, whole body, after 300-d exposure, Howard 1991)
 3.21–3.30 (channel catfish, after 41- and 55-d exposure, Howard 1991)
 4.18 (flagfish, whole body after 65-d exposure, Howard 1991)
 3.52–3.68 (sheepshead minnow, 33-d exposure for embryojuveniles, Howard 1991)
 3.40–3.81 (sheepshead minnow, adults, after 28–161 d, Howard 1991)
 2.70–3.10 (shellfish, Howard 1991)
 4.69, 3.22–3.44, 3.48 (snail, oyster, grass shrimp, mussel, Howard 1991)
 2.15–2.30 (algae, Howard 1991)
 3.83 (fish, reported as log BAF_w , LeBlanc 1996)
 3.28, 5.28 (mussel *Mytilus edulis*: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.22, 5.14 (oyster *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.44, 5.37 (oyster *Crassostrea virginica*: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.42 (clam: wet wt basis, Geyer et al. 2000)
 3.66, 5.18 (fathead minnow, uptake 300-d: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, log K_{oc} at 25°C or as indicated:

- 4.53 (calculated, Kenaga 1980, quoted, Howard 1991)
 5.36 (calculated-S, Mill et al. 1980; quoted, Adams 1987)
 4.00 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 5.00; 4.10 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 9.6$ d from a model river 1-m deep, flowing 1 m/s with a wind speed of 3 m/s, and $t_{1/2} > 14$ yr from a model pond (Howard 1991).

Photolysis:

Oxidation:

$k(aq.) = (2.7 \pm 0.7) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (Fenton reaction) at $24 \pm 1^\circ\text{C}$ and pH 2.8 (Haag & Yao 1992) with reference to $4.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of DPCP with OH radical in aqueous solution (Buxton et al. 1988; quoted, Haag & Yao 1992);

$k(aq.) = (1.3 \pm 0.4) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ (Fenton reaction) and $k = (1.1 \pm 0.2) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ (photo-Fenton reaction) for the reaction with OH radical in aqueous solution at $24 \pm 1^\circ\text{C}$ and pH 3.4 (Haag & Yao 1992) with reference to $8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction of lindane with OH radical in aqueous solution (Buxton et al. 1988; quoted, Haag & Yao 1992)

$k(aq.) < 0.02 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.4 and $23 \pm 3^\circ\text{C}$, with $t_{1/2} > 20$ d at pH 7 (Yao & Haag 1991).

Hydrolysis: $t_{1/2} = 4$ yr at least (Callahan et al. 1979).

Biodegradation: $t_{1/2} = 5$ –14 d in thick anaerobic sewage sludge (Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$-\log k_2 = 1.99$ h (oyster, Mason & Rowe 1976; quoted, Hawker & Connell 1986)

$\log k_1 = 1.5 \text{ h}^{-1}$; $-\log k_2 = 1.78$ h (mussel, Ernst 1977; quoted, Hawker & Connell 1986)

Half-Lives in the Environment:

Air: $t_{1/2} = 1.45$ h was predicted for reaction with hydroxyl radical (Howard 1991).

Surface water: $t_{1/2} > 8$ wk in river water (Eichelberger & Lichtenberg 1971);

measured $k_{O_3}(aq.) < 0.02 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.4 and $23 \pm 3^\circ\text{C}$, with $t_{1/2} > 20$ d at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil: $t_{1/2} \sim 12$ yr in Congaree sandy loam soil (Nash & Woolson 1967);
field $t_{1/2} = 63$ d for sugar cane in soil (Willis & Hamilton 1973; quoted, Nash 1983);
moderately persistent in soil with $t_{1/2} = 20\text{--}100$ d (Willis & McDowell 1982);
microagroecosystem $t_{1/2} = 33$ d in moist fallow soil (Nash 1983);
 $t_{1/2} > 50$ d in soil (Ryan et al. 1988);
selected field $t_{1/2} = 4300$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 $t_{1/2} \sim 12$ yr in soil (Geyer et al. 2000)
Biota: elimination $t_{1/2} = 24$ h (Ernst 1977, quoted, Callahan et al. 1979).

TABLE 18.1.1.35.1

Reported aqueous solubilities and octanol-air partition coefficients of endrin at various temperatures

Aqueous solubility						log K _{OA}	
Richardson & Miller 1960		Biggar & Riggs 1974				Shoeib & Harner 2002	
shake flask-UV spec.		shake flask-GC				generator column-GC/MS	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	S/g·m ⁻³	S/g·m ⁻³	t/°C	log K _{OA}
		particle size	0.01μ	0.05μ	5.0μ		
25	0.23	15	0.010	0.090	0.130	5	10.2787
35	0.38	25	0.0245	0.180	0.250	15	9.3548
45	0.51	35	0.058	0.315	0.420	20	8.6528
		45	0.120	0.518	0.625	25	8.3377
						35	8.2855
						25	8.609
						log K _{OA} = A + B/(T/K)	
						A	-11.75
						B	6067
						enthalpy of phase change	
						ΔH _{OA} /(kJ mol ⁻¹) = 84.9	

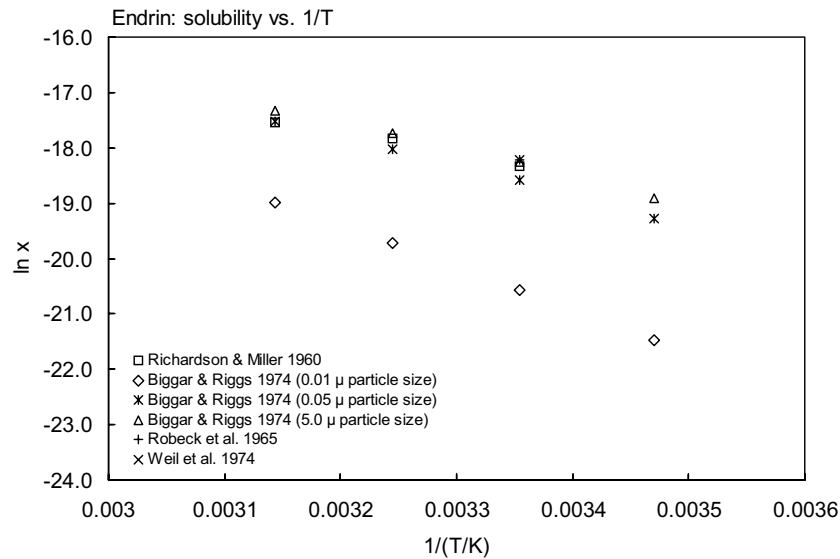


FIGURE 18.1.1.35.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for endrin.

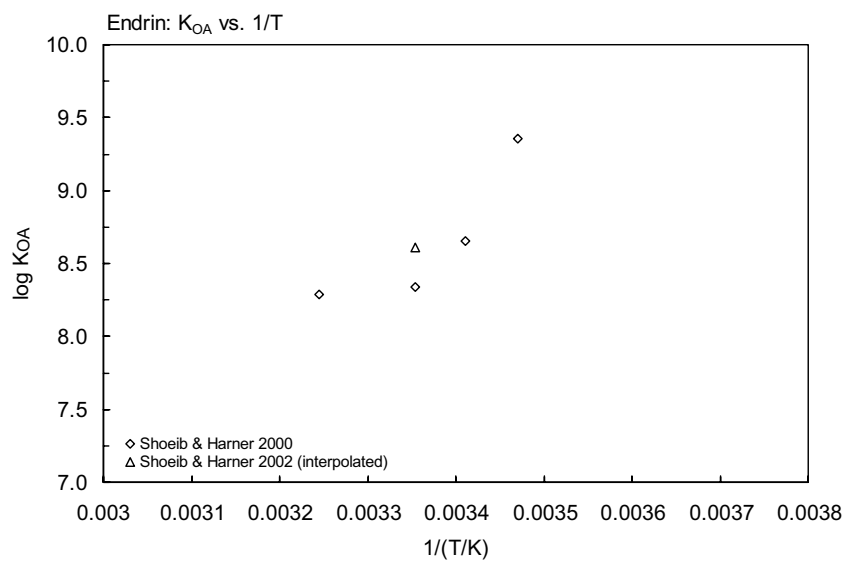
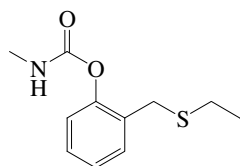


FIGURE 18.1.1.35.2 Logarithm of K_{OA} versus reciprocal temperature for endrin.

18.1.1.36 Ethiofencarb



Common Name: Ethiofencarb

Synonym: Croneton, Bay-Hox-1901

Chemical Name: α -ethylthio-*o*-tolyl methylcarbamate

CAS Registry No: 29973-13-5

Uses: insecticide

Molecular Formula: $C_{11}H_{15}NO_2S$

Molecular Weight: 225.307

Melting Point ($^{\circ}C$):

33.4 (Spencer 1982; Hartley & Kidd 1987, Montgomery 1993, Tomlin 1994)

Boiling Point ($^{\circ}C$):

decomposes on distillation (Hartley & Kidd 1987, Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.1473 (Hartley & Kidd 1987, Worthing & Walker 1987; Montgomery 1993)

1.231 ($20^{\circ}C$, Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.827 (mp at $33.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1900 ($20^{\circ}C$, Spencer 1982, Hartley & Kidd 1987, Montgomery 1993)

1820 ($20^{\circ}C$, Worthing & Walker 1987)

1800 ($20^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

6.67×10^{-4} (Spencer 1982)

0.013 ($30^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987)

4.506×10^{-4} ($20^{\circ}C$, Montgomery 1993)

0.00045, 0.00094, 0.026 (20, 25, $50^{\circ}C$, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

5.37×10^{-5} (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.98 (calculated-Montgomery 1993)

2.04 (Tomlin 1994)

4.20 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.84 (calculated, Montgomery 1993)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis: photodegradation in sunlight is very rapid (Tomlin 1994).

Oxidation:

Hydrolysis: hydrolyzed in alkaline solution (Tomlin 1994).

Biodegradation:

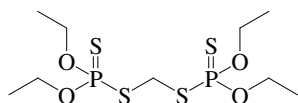
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: in isopropanol/water (1:1, 37–40°C) solutions, half-lives were $t_{1/2} = 300$ d at pH 2, $t_{1/2} = 45$ h at pH 7 and $t_{1/2} = 5$ min at pH 11.4 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994).

18.1.1.37 Ethion



Common Name: Ethion

Synonym: AC 3422, Bladan, diethion, Embathion, ENT 24105, Ethanox, Ethiol, Ethodan, Ethopaz, FMC 1240, Fosfono 50, Hylemax, Hylemox, Itopaz, KWIT, NA 2783, NIA 1240, Niagara 1240, Nialate, Vegfru fosmite

Chemical Name: bis(*S*-(dimethoxyphosphinothioyl)mercapto)methane; *O,O,O',O'*-tetraethyl-*S,S'*-methylene bis(phosphorodithioate); *O,O,O',O'*-tetraethyl-*S,S'*-methylene-bisphosphorothiolothionate

Uses: nonsystemic insecticide and acaricide used on apples.

CAS Registry No: 563-12-2

Molecular Formula: $C_9H_{22}O_4P_2S_4$

Molecular Weight: 384.476

Melting Point ($^{\circ}C$):

–12 to –15 (Montgomery 1993; Tomlin 1994; Milne 1995)

–13 (Lide 2003)

Boiling Point ($^{\circ}C$):

164–165 (at 0.3 mmHg, Hartley & Kidd 1987; Howard 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.22 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

350.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2.0 (Metcalf 1971, 1974)

0.60 (Miles 1976; Miles & Harris 1978)

1.0 (20 – $25^{\circ}C$, selected, Willis & McDowell 1982; Gerstl & Helling 1987)

1.1 ($19.5^{\circ}C$, shake flask-GC, Bowman & Sans 1983b)

1.1 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.68, 0.76 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

2.0 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0002 (Khan 1980; Merck Index 1983, 1989)

0.0002 (Worthing 1983, Worthing & Hance 1991)

0.0002 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

1.50×10^{-4} ($20^{\circ}C$, selected, Suntio et al. 1988)

3.20×10^{-4} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.58×10^{-4} (gradient GC method; quoted lit., Tsuzuki 2000)

1.58×10^{-4} ; 4.17×10^{-5} ; 1.58×10^{-4} (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.0699 (calculated-P/C, Lyman et al. 1982; quoted, Howard 1991)

0.032 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

0.0384 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{OW} :

- 5.07 (Hansch & Leo 1979)
- 5.073 (shake flask-GC, Bowman & Sans 1983b)
- 5.07 (recommended, Sangster 1993)
- 4.28, 5.07 (Montgomery 1993)
- 5.07 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 2.77 (estimated-log K_{OW} , Howard 1991)
- 2.77 (estimated-S, Howard 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 4.19 (average of 4 soils, King & McCarthy 1968)
- 4.19 (soil, Hamaker & Thompson 1972; Kenaga & Goring 1980)
- 3.81, 3.94, 4.0 (organic soil, Beverley sandy loam, Plainsfield sand, Sharom et al. 1980)
- 3.66 (calculated-MCI χ , Gerstl & Helling 1987)
- 4.19; 4.28 (reported as log K_{OM} , estimated as log K_{OM} , Magee 1991)
- 4.06, 4.12 (soil, quoted exptl., calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 4.00 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.54–4.34 (Montgomery 1993)
- 4.43 (estimated-chemical structure, Lohninger 1994)
- 4.06 (calculated-MCI χ , Sabljic et al. 1995)
- 3.70, 3.95 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 102$ d from a model river 1-m deep, flowing 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1991).

Photolysis:

Oxidation: photooxidation $t_{1/2} \sim 6.95$ h for the vapor-phase reaction with hydroxyl radicals in air (Howard 1991).

Hydrolysis: half-lives in water at 25°C and pHs of 4.5, 5.0, 6.0, 7.0 and 8.0 were 99, 63, 58, 25, and 8.4 wk, respectively (Chapman & Cole 1982; quoted, Montgomery 1993);

$t_{1/2}$ (exptl) = 20.8 wk was determined in buffered distilled water at 30°C between pH 4 and 7, $t_{1/2} = 8.9$ wk at pH 8 and $t_{1/2} = 1$ d at pH 10 (Dierberg & Pfeuffer 1983; quoted, Howard 1991);

$t_{1/2} = 390$ d at pH 9 (Tomlin 1994).

Biodegradation: $t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} = 7$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 8.0$ wk in nonsterile organic soil (Miles et al. 1979; quoted, Howard 1991);

$t_{1/2} = 24$ –26 d in both sterilized and unsterilized Florida canal water over 12 wk observation (Dierberg & Pfeuffer 1983; quoted, Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} \sim 6.95$ h for the vapor-phase reaction with hydroxyl radical in air (Howard 1991).

Surface water: $t_{1/2} = 4$ wk in river water (Eichelberger & Lichtenberg 1971).

Ground water:

Sediment:

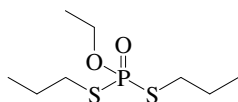
Soil: $t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} = 7$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 8.0$ wk in nonsterile organic soil (Miles et al. 1979; quoted, Howard 1991);

selected field $t_{1/2} = 150$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 90$ d in soil (Tomlin 1994).

Biota:

18.1.1.38 Ethoprop



Common Name: Ethoprop

Synonym: ethoprophos

Chemical Name: *O*-ethyl *S,S*-dipropylphosphorodithioate

CAS Registry No: 13194-48-4

Uses: insecticide/nematicide

Molecular Formula: $C_8H_{19}O_2PS_2$

Molecular Weight: 242.340

Melting Point ($^{\circ}C$): liquid

20 (Montgomery 1993)

Boiling Point ($^{\circ}C$):

86–91/0.2 mmHg (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.094 (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

700 ($20^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

750 (Worthing & Walker 1987)

700 (Montgomery 1993)

750 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0465 ($26^{\circ}C$, Hartley & Kidd 1987)

0.0465 ($20^{\circ}C$, Montgomery 1993)

0.0507 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.0161 (calculated-P/C, Montgomery 1993; Majewski & Capel 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.59 ($21^{\circ}C$, Montgomery 1993; Tomlin 1994)

3.59 (quoted, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.41–2.20 (soil, quoted values, Wauchope et al. 1992)

1.85 (soil, Wauchope et al. 1992; Hornsby et al. 1996)

1.82–2.27 (Montgomery 1993)

1.80 (soil, calculated-MCI, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

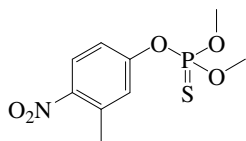
Hydrolysis: stable in water up to 100°C at pH 7, but rapidly hydrolyzed at 25°C at pH 7 (Worthing 1987; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} \sim 87$ d in humus-containing soil at pH 4.5 and $t_{1/2} = 14\text{--}28$ d in sandy loam at pH 7.2–7.3 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994);

field $t_{1/2} = 87$ d in organic soil, $t_{1/2} = 1\text{--}28$ d in sandy soil; others $t_{1/2} = 3\text{--}63$ d; recommended $t_{1/2} = 25$ d (Wauchope et al. 1992; Hornsby et al. 1996).

18.1.1.39 Fenitrothion



Common Name: Fenitrothion

Synonym: Accothion, Agria 1050, Agrothion, Arbogal, Cyfen, Cytel, Dybar, Falithion, Fenitox, Kotion, Sumithion

Chemical Name: *O,O*-dimethyl *O*-4-nitro-*m*-tolyl phosphorothioate; phosphorothioic acid *O,O*-dimethyl *O*-4-nitro-*m*-tolyl ester; *O,O*-dimethyl *O*-(3-methyl-4-nitrophenyl) phosphorothioate

Uses: insecticide to control boring, chewing and sucking insects in cereals, cotton, maize, sorghum, citrus fruit, pome fruit, stone fruit, soft fruit, vines, bananas, olives, rice, soybeans, beet, sugar cane, oilseed rape, vegetables, lucerne, coffee, cocoa, tea, tobacco, ornamentals and forestry; also used as a public health insecticide to control household insects, flies in animal houses, mosquito larvae, and locusts.

CAS Registry No: 122-14-5

Molecular Formula: $C_9H_{12}NO_5PS$

Molecular Weight: 277.234

Melting Point ($^{\circ}C$):

3.4 (Tomlin 1994)

Boiling Point ($^{\circ}C$):

164 (at 1 mmHg, Worthing & Hance 1991; Milne 1995)

140–145 (at 0.1 mmHg, dec., Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.328 (Worthing & Hance 1991; Tomlin 1994)

1.3227 ($25^{\circ}C$, Milne 1995)

Molar Volume (cm^3/mol):

229.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

7.20 (Kortum et al. 1961; Wolfe 1980)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 1.0)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

30 (Macy 1948; Hamaker 1975; Kenaga 1980; Kenaga & Goring 1980)

30 ($20^{\circ}C$, Bright et al. 1950; Melnikov 1971; Hamaker 1975)

25.2 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1979)

38.7 (20 – $25^{\circ}C$, shake flask-GC, Kanazawa 1981)

21 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

30 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

30 ($21^{\circ}C$, Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

8.0×10^{-3} ($20^{\circ}C$, Melnikov 1971)

7.2×10^{-3} ($20^{\circ}C$, Freed et al. 1979)

8.0×10^{-4} ($20^{\circ}C$, Hartley & Graham-Bryce 1980; Khan 1980)

5.5×10^{-3} (gas saturation method, Addison 1981)

5.4×10^{-3} (gas saturation-extrapolated, Addison 1981)

8.0×10^{-3} (Budavari 1989)

1.1×10^{-2} (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)

1.5×10^{-4} ($20^{\circ}C$, Worthing & Hance 1991)

1.3×10^{-4} (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

0.0180 ($20^{\circ}C$, Tomlin 1994)

0.00316 (gradient GC method, Tsuzuki 2000)

3.23×10^{-3} ; 3.47×10^{-3} ; 2.18×10^{-3} (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.0942, 0.0669 (exptl., estimated Metcalf et al. 1980)

0.0962 (calculated-bond contribution method, Meylan & Howard 1991)

0.0012 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.38 (20°C , shake flask-GC, Chiou et al. 1977)

3.30 (shake flask, Mundy et al. 1978)

3.38 (shake flask-GC, Freed et al. 1979)

3.36 (Rao & Davidson 1980)

3.44 (shake flask-GC, Kanazawa 1981, 1989)

3.397 (shake flask-GC, Bowman & Sans 1983b)

3.16 (shake flask-HPLC, Moody et al. 1987)

3.466 ± 0.003 (shake flask/slow-stirring method, De Bruijn & Hermens 1991; De Bruijn et al. 1993)

3.43 (20°C , Worthing & Hance 1991; Tomlin 1994)

2.96 (RP-HPLC-RT correlation, Saito et al. 1993)

3.03 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)

3.30 (recommended, Sangster 1993)

3.43 (Milne 1995)

3.30 (selected, Hansch et al. 1995)

3.03 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

1.00 (fish in static water, Leo et al. 1971; Kenaga & Goring 1980)

2.23 (motsugo, Kanazawa 1975)

2.34 (rainbow trout, Takimoto & Miyamoto 1976)

2.02 (mussel, McLeese et al. 1979)

1.96 (calculated-S, Kenaga 1980)

2.39 (*Pseudorasbora parva*, Kanazawa 1981)

2.34, 2.17 (mussel, calculated- K_{OW} & models, Zaroogian et al. 1985)

2.11 (mussel, Zaroogian et al. 1985)

2.74, 2.75 (*Oryzias latipes*, Takimoto et al. 1984)

2.48 (*Oryzias latipes*, Takimoto et al. 1987)

2.60 (willow shiner, Tsuda et al. 1989)

3.36 ± 0.04 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)

2.37, 2.72 (killifish, De Bruijn & Hermens 1991)

2.18, 2.31, 1.48 (minnow, motsugo, mullet, De Bruijn & Hermens 1991)

3.54 (*Poecilia reticulata*, De Bruijn & Hermens 1991)

2.30, 2.39 (rainbow trout, topmouth gudgeon, De Bruijn & Hermens 1991)

1.65, 1.68 (*Oryzias latipes*, Tsuda et al. 1995)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.83 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)

2.63 (average of 2 soils, Kanazawa 1989)

3.30 (20 – 25°C , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

2.54, 2.76 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 6.3$ d from the bottom of Palfrey Lake and $t_{1/2} = 7.2$ d from the surface of Palfrey Lake vs. a calculated $t_{1/2} = 20.6$ d; 0.9 d from Palfrey Brook vs. a calculated $t_{1/2} = 5.40$ d (Metcalf et al. 1980).

Photolysis: disappearance rate constant $k = 0.053 \text{ h}^{-1}$ with calculated first-order $t_{1/2} = 13 \text{ h}$ (Lacorte & Barcelo 1994).

Oxidation:

Hydrolysis: second-order alkaline hydrolysis rate constant $k = 4.2 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C (Maquire & Hale 1980; quoted, Wolfe 1980);

estimated half-lives at 22°C : $t_{1/2} \sim 108.8 \text{ d}$ at pH 4, $t_{1/2} \sim 84.3 \text{ d}$ at pH 7, and $t_{1/2} \sim 75 \text{ d}$ at pH 9 (Tomlin 1994).

Biodegradation: aerobic degradation $k = 2.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 13.0 \text{ d}$ for control system, $k = 0.4 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 73.0 \text{ d}$ for metabolism, $k = 5.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 8.50 \text{ d}$ for co-metabolism; anaerobic degradation $k = 1.7 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 17.0 \text{ d}$ for control system, $k = 3.9 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 9.6 \text{ d}$ for metabolism, $k = 38.0 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 1.0 \text{ d}$ for co-metabolism, by a mixture of microorganisms from activated sludge, soil and sediment in cyclone fermentors (Liu et al. 1981)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 88 \text{ d}^{-1}$ (rainbow trout, Takimoto & Miyamoto 1976; quoted, McLeese et al. 1976)

$k_2 = 0.4 \text{ d}^{-1}$ (rainbow trout, Takimoto & Miyamoto 1976; quoted, McLeese et al. 1976)

$k_2 = 0.070 \text{ h}^{-1}$ (willow shiner, Tsuda et al. 1989)

$k_1 = (3.89 \pm 1.39) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = (1.13 \pm 0.07) \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = 1.01 \text{ d}^{-1}$ (guppy, calculated- K_{OW} , De Bruijn & Hermens 1991)

$k_2 = (0.28 \pm 0.02) \times 10^{-3} \text{ (NADPH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

$k_2 = (0.15 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 15\text{--}168 \text{ h}$ in summer, Palfrey Lake, Canada at pH 6.7, 11°C under sunlight conditions (Metcalf et al. 1980);

$t_{1/2} = 36\text{--}48 \text{ h}$ at pH 7.0–7.5, $19\text{--}23^\circ\text{C}$ under sunlight conditions, $t_{1/2} = 518\text{--}1188 \text{ h}$ at pH 7.5, 23°C under dark conditions in Lac Bourgeois, Quebec (Greenhalgh et al. 1980);

$t_{1/2} = 5.5 \text{ d}$ and 1.0 d under aerobic and anaerobic co-metabolism conditions, $t_{1/2} = 73 \text{ d}$ under aerobic metabolism condition (Liu et al. 1981)

$t_{1/2} = 13 \text{ h}$ in winter, irrigation ditch from Ebre Delta, Spain under sunlight conditions, at pH 7.8, 11°C (Lacorte & Barcelo 1994);

$t_{1/2} = 202 \text{ d}$ at 6°C , $t_{1/2} = 62 \text{ d}$ at 22°C in darkness for Milli-Q water at pH 6.1; $t_{1/2} = 103 \text{ d}$ at 6°C , $t_{1/2} = 31 \text{ d}$ at 22°C in darkness, $t_{1/2} = 4 \text{ d}$ under sunlight conditions for river water at pH 7.3; $t_{1/2} = 143 \text{ d}$ at 6°C , $t_{1/2} = 27 \text{ d}$ at 22°C in darkness for filtered water at pH 7.3; $t_{1/2} = 224 \text{ d}$ at 6°C , $t_{1/2} = 34 \text{ d}$ at 22°C in darkness, $t_{1/2} = 3 \text{ d}$ under sunlight conditions in seawater (Arcachon Bay, France) at pH 8.1, $22\text{--}25^\circ\text{C}$ (Lartiges & Garri gues 1995);

$t_{1/2} = 11\text{--}19.3 \text{ h}$ at pH 7.8–8.2, $25\text{--}20^\circ\text{C}$ under sunlight conditions in rice crop field; $t_{1/2} = 70\text{--}74 \text{ h}$ at pH 8.2, $15\text{--}18^\circ\text{C}$ under dark conditions from Ebre Delta, Spain (Oubina et al. 1996).

Ground water:

Sediment:

Soil: selected field $t_{1/2} = 4 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);

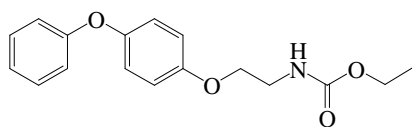
$t_{1/2} = 12\text{--}28 \text{ d}$ under upland conditions and $t_{1/2} = 4\text{--}20 \text{ d}$ under submerged conditions (Tomlin 1994).

Biota: excretion $t_{1/2} = 9.9 \text{ h}$ (willow shiner, Tsuda et al. 1989);

elimination rate constants $k = (0.28 \pm 0.02) \times 10^3 \text{ (NADPH)}$ and $(0.15 \pm 0.02) \times 10^3 \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993);

degradation $t_{1/2} = 4 \text{ d}$ in balsam fir and spruce foliage (Tomlin 1994).

18.1.1.40 Fenoxycarb



Common Name: Fenoxycarb

Synonym: Insegar, Logic, Pictyl, Torus, Varikil

Chemical Name: ethyl 2-(4-phenoxyphenoxy)ethylcarbamate; ethyl[2-(*p*-phenoxy)ethyl]- carbamate

Uses: insecticide to control lepidoptera, scale insects, and psyllids on fruit, cotton and ornamentals; and also cockroaches, fleas, mosquito larvae, and fire ants in public health situations.

CAS Registry No: 79127-80-3

Molecular Formula: C₁₇H₁₉NO₄

Molecular Weight: 301.338

Melting Point (°C):

53 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.23 (Tomlin 1994)

Molar Volume (cm³/mol):

344.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.531 (mp at 53°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

6.0 (20°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

5.7 (Worthing & Hance 1991)

6.0 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

1.7 × 10⁻⁶ (Hartley & Kidd 1987)

7.8 × 10⁻⁶ (20°C, Worthing & Hance 1991)

8.7 × 10⁻⁷ (Tomlin 1994)

1.7 × 10⁻⁶ (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol):

8.5 × 10⁻⁵ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow}:

4.30 (Worthing & Hance 1991; Milne 1995)

4.07 (Tomlin 1994)

4.30 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.35 (calculated-S as per Kenaga 1980, this work)

3.11 (calculated-K_{ow} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{oc}:

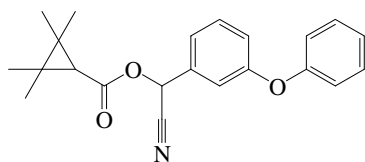
3.00 (20–25°C, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Half-Lives in the Environment:

Soil: t_{1/2} = 1.7–2.5 months in laboratory soil and water and t_{1/2} = few days to 31 d in field soil and water (Tomlin 1994);
field t_{1/2} = 1 d (20–25°C, selected, Hornsby et al. 1996).

18.1.1.41 Fenpropathrin



Common Name: Fenpropathrin

Synonym: Rody, Danitol, Meothrin, S-3206, Ortho Danitol, Herald, Meothrin

Chemical Name: (*R,S*)- α -cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate

CAS Registry No: 64257-84-7 (racemate); 39515-41-8 (unstated stereochemistry)

Uses: insecticide/acaricide (pyrethroid)

Molecular Formula: $C_{22}H_{23}NO_3$

Molecular Weight: 349.423

Melting Point ($^{\circ}C$):

47 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.15 (Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.608 (mp at $47^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.33 (Hartley & Kidd 1987)

0.0141 (Tomlin 1994)

0.33 (selected, Augustijn-Beckers et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00073 ($20^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

0.00130, 0.00133 (quoted, Augustijn-Beckers et al. 1994)

7.33×10^{-4} (selected, Augustijn-Beckers et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.0 ($20^{\circ}C$, Tomlin 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

6.75, 3.70 (quoted, estimated, Augustijn-Beckers et al. 1994)

3.70 (soil, estimated and selected, Augustijn-Beckers et al. 1994)

Environmental Fate Rate Constants, k , or Half-Lives:

Volatilization:

Photolysis: degraded principally by photolysis, $t_{1/2} = 2.7$ wk in river water (Hartley & Kidd 1987; Tomlin 1994).

Oxidation:

Hydrolysis: decomposed in alkaline solution (Hartley & Kidd 1987; Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: degraded principally by photolysis, $t_{1/2} = 2.7$ wk in river water (Hartley & Kidd 1987; Tomlin 1994).

Ground water:

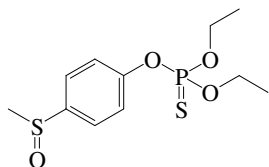
Sediment:

Soil: duration of activity in soil 1–5 d (Hartley & Kidd 1987; Tomlin 1994);

reported field $t_{1/2} = 8$ –144 d, recommended field $t_{1/2} = 5$ d (Augustijn-Beckers et al. 1994).

Biota:

18.1.1.42 Fensulfothion



Common Name: Fensulfothion

Synonym: Dassnit, Terracur

Chemical Name: *O,O*-diethyl *O*-4-methylsulphonylphenyl phosphorothioate

Uses: insecticide/nematicide

CAS Registry No: 115-90-2

Molecular Formula: $C_{11}H_{17}O_4PS_2$

Molecular Weight: 308.354

Melting Point ($^{\circ}C$):

yellow-brown oil (Spencer 1982; Hartley & Kidd 1987)

< 25 (Montgomery 1993)

Boiling Point ($^{\circ}C$):

138–141/0.01 mmHg (Hartley & Kidd 1987, Worthing & Walker 1987; Howard 1991)

Density (g/cm^3):

1.202 ($20^{\circ}C$, Spencer 1982, Hartley & Kidd 1987; Worthing & Walker 1987)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1600 (Spencer 1982)

2000 ($20^{\circ}C$, shake flask, Bowman & Sans 1979, 1983b)

1540 (Hartley & Kidd 1987; Worthing & Walker 1987)

1540 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

9.09×10^{-5} (Howard 1991)

6.67×10^{-3} (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

1.40×10^{-5} (calculated- P/C , Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.23 (shake flask-concn ratio-GC, Bowman & Sans 1983)

2.23 (Montgomery 1993)

2.23 (recommended, Sangster 1993)

2.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.46, 0.93 (calculated- K_{ow} , solubility, Howard 1991)

1.68 (killifish *Oryzias latipes*, after 48–72 h exposure, Tsuda et al. 1995)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.83, 2.11 (estimated, Howard 1991)
- 1.89 (calculated, Montgomery 1993)
- 2.09–2.57 (Augustijn-Beckers et al. 1994)
- 2.48 (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 2.52 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.45, 2.266, 2.11, 2.26, 2.85 (first generation EUROSOLS ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 3.05, 2.44, 2.15, 2.237, 2.85 (second generation EUROSOLS ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 3.053, 2.443, 2.150, 2.237, 2.848 (second generation EUROSOLS ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
- 2.52; 2.94, 2.62 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis: $t_{1/2} = 58\text{--}87$ d over pH range of 4.5–8.0 at 25°C in pure water (Howard 1991).

Biodegradation: field $t_{1/2} \sim 30$ d (estimated, Augustijn-Becker et al. 1994).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.17 \text{ h}^{-1}$ (killifish *Oryzias latipes*, Tsuda et al. 1995)

Half-Lives in the Environment:

Air: $t_{1/2} = 7.03$ h for reaction with OH radicals in the atmosphere (Howard 1991).

Surface water: $t_{1/2} = 58\text{--}87$ d in pure water at 25°C over the pH range of 4.5–8.0 (Howard 1991).

Ground water:

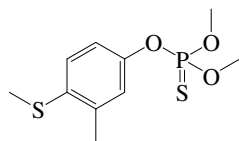
Sediment:

Soil: $t_{1/2} < 1$ wk to several weeks in soil (Howard 1991);

field $t_{1/2} = 3$ to 182 d and $t_{1/2} \sim 30$ d (estimated, Augustijn-Becker et al. 1994; Hornsby et al. 1996).

Biota:

18.1.1.43 Fenthion



Common Name: Fenthion

Synonym: Bay 29493, Baycid, Bayer 9007, Baytex, Baycid, DMTP, Ekalux, ENT 25540, Entex, Lebacid, Lebaycid, Mercaptophos, MPP, NCI-C08651, OMS 2, Queletox, Spottan, Talodex, Tiquvon

Chemical Name: *O,O*-dimethyl *O*-(3-methyl-4-(methylthio)phenyl) phosphorothioate; *O,O*-dimethyl *O*-4-methylthio-*m*-tolyl phosphorothioate

Uses: insecticide with contact, stomach and respiratory action and also used as acaricide and cholinesterase inhibitor.

CAS Registry No: 55-38-9

Molecular Formula: $C_{10}H_{15}O_3PS_2$

Molecular Weight: 278.328

Melting Point ($^{\circ}C$):

7.0 (Montgomery 1993)

7.5 (Tomlin 1994; Milne 1995)

Boiling Point ($^{\circ}C$):

87.0 (at 0.01 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.246 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

1.25 (Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm^3/mol):

264.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

89.31 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

55 (Günther et al. 1968; Martin & Worthing 1977; Budavari 1989)

54–56 (rm. temp., Spencer 1973, 1980)

56 ($22^{\circ}C$, Khan 1980)

55 ($22^{\circ}C$, Verschueren 1983)

7.51 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

9.3 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1985)

54–56 ($20^{\circ}C$, Hartley & Kidd 1987)

2.0 ($20^{\circ}C$, Worthing & Walker 1987; Worthing & Hance 1991; Milne 1995)

2.0, 4.2, 7.51, 9.3, 50 ($20^{\circ}C$, literature data variability, Heller et al. 1989)

4.2 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)

9.30, 11.3 ($20^{\circ}C$, $30^{\circ}C$, Montgomery 1993)

4.2 ($20^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

4.0×10^{-3} ($20^{\circ}C$, Eichler 1965)

4.0×10^{-3} ($20^{\circ}C$, Melnikov 1971)

4.0×10^{-3} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

4.0×10^{-3} ($20^{\circ}C$, Khan 1980; Budavari 1989; Worthing & Hance 1991; Montgomery 1993)

8.4×10^{-3} ($20^{\circ}C$, GC-RT correlation, Kim et al. 1984; Kim 1985)

4.0×10^{-3} , 10×10^{-3} (20°C, 30°C, Hartley & Kidd 1987)
 4.0×10^{-3} (20°C, selected, Suntio et al. 1988)
 2.5×10^{-3} , 4.0×10^{-2} , 0.43, 3.40, 21.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
 $\log(P_L/Pa) = 13.037 - 4665.2/(T/K)$; measured range 32.7–160°C (liquid, gas saturation-GC, Rordorf 1989)
 3.7×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 7.4×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.022 (20°C, calculated-P/C, Suntio et al. 1988)
 0.547 (Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.09 (shake flask-GC, Bowman & Sans 1983b)
 4.167 ± 0.009 (shake flask/slow-stirring method, De Bruijn & Hermens 1991)
 4.09, 4.84 (Montgomery 1993)
 3.56 (RP-HPLC correlation, Saito et al. 1993)
 4.09 (recommended, Sangster 1993)
 4.84 (Tomlin 1994)
 4.09 (selected, Hansch et al. 1995)
 4.17 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, $\log BCF$:

1.81 (calculated-S, Kenaga 1980)
 -4.50 (beef biotransfer factor $\log B_b$, correlated- K_{OW} , MacDougall 1972)
 -5.60 (milk biotransfer factor $\log B_m$, correlated- K_{OW} , Johnson & Bowman 1972)
 4.22 ± 0.08 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
 4.17 (*Poecilia reticulata*, De Bruijn & Hermens 1991)
 2.68 (whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992)
 1.34, 1.46, 1.43, 1.41 (whole body carp: 24 h, 72 h, 120 h, and 148 h; Tsuda et al. 1993)
 1.96 (killifish *Oryzias latipes*, after 12–72 h exposure, Tsuda et al. 1995)
 1.96, 2.02 (*Oryzias latipes*, Tsuda et al. 1995; quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

2.68 (calculated-S, Kenaga 1980)
 3.18 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 3.31 (soil, HPLC-screening test, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995a, b)
 0.89–1.58 (Montgomery 1993)
 3.18 (Tomlin 1994; Lohninger 1994)
 3.31; 3.37 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
 4.35, 3.55, 3.46, 3.146, 3.64 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
 3.10 (sandy loam soil, column equilibrium method-HPLC/UV, 20°C, Xu et al. 1999)
 3.716, 3.658, 3.450, 3.226, 3.292 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC-k' correlation, Gawlik et al. 2000)
 3.50, 3.00 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 223$ d at pH 4, $t_{1/2} = 200$ d at pH 7, and $t_{1/2} = 151$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: rate constants $k = -0.00745 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.00199 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.00129 \text{ h}^{-1}$ in nonsterile water by shake-tests at Range Point (Walker et al. 1988).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = (8.81 \pm 0.72) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = (0.60 \pm 0.02) \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = 0.42 \text{ d}^{-1}$ (guppy, calculated- K_{OW} , De Bruijn & Hermens 1991)

$k_2 = 0.07 \text{ h}^{-1}$ (whole body willow shiner, Tsuda et al. 1992)

$k_2 = 0.34 \text{ h}^{-1}$ (carp, Tsuda et al. 1992)

$k_2 = (0.64 \pm 0.09) \times 10^{-3} \text{ (NADPH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

$k_2 = (0.12 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993)

$k_2 = 0.14 \text{ h}^{-1}$ (killifish *Oryzias latipes*, Tsuda et al. 1995)

Half-Lives in the Environment:

Air:

Surface water: persistence of up to 4 wk in river water (Eichelberger & Lichtenberg 1971);

$t_{1/2} = 189 \text{ d}$ at 6°C , 71 d at 2°C in darkness for Mill-Q water at pH 6.1; $t_{1/2} = 149 \text{ d}$ at 6°C , $t_{1/2} = 42 \text{ d}$ at 22°C in darkness, $t_{1/2} = 2 \text{ d}$ under sunlight conditions for river water at pH 7.3; $t_{1/2} = 104 \text{ d}$ at 6°C , $t_{1/2} = 33 \text{ d}$ at 22°C in darkness for filtered river water, pH 7.3; $t_{1/2} = 227 \text{ d}$ at 6°C , $t_{1/2} = 26 \text{ d}$ at 22°C in darkness, $t_{1/2} = 5 \text{ d}$ under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment:

Soil: selected field $t_{1/2} = 34 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996);

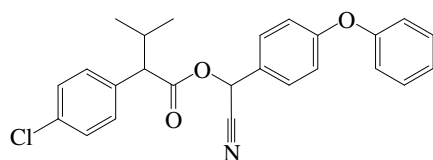
$t_{1/2} \sim 1 \text{ d}$ in soil and water (Tomlin 1994).

Biota: excretion rate constant $k = 0.07 \text{ h}^{-1}$ from whole body willow shiner (Tsuda et al. 1992);

elimination rate constants $k = (0.64 \pm 0.09) \times 10^{-3} \text{ (NADPH)}$ and $k = (0.12 \pm 0.02) \times 10^{-3} \text{ (GSH) min}^{-1} \cdot \text{mg protein}^{-1}$ (rainbow trout, De Bruijn et al. 1993);

excretion rate constant $k = 0.34 \text{ h}^{-1}$ with $t_{1/2} = 2.0 \text{ d}$ from carp (Tsuda et al. 1993).

18.1.1.44 Fenvalerate



Common Name: Fenvalerate

Synonym: Belmark, Ectrin, Pydrin, Pyrethroid, S 5602, Sanmarton, SD 43775, Sumicide, Somicidin, Sumifly, Sumipower, WL 43775

Chemical Name: (*RS*)- α -cyano-3-phenoxybenzyl (*RS*)-2-(4-chlorophenyl)-3-methylbutyrate; cyano-(3-phenoxyphenyl)-methyl 4-chloro- α -(1-methylethyl)benzeneacetate

Uses: non-systemic insecticide to control a wide variety of pests and also used as acaricide

CAS Registry No: 51630-58-1

Molecular Formula: $C_{25}H_{22}ClNO_3$

Molecular Weight: 419.901

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

decomposes on distillation (Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.26 (22 $^{\circ}C$, Spencer 1982)

1.17 (23 $^{\circ}C$, Hartley & Kidd 1987; Milne 1995)

1.175 (tech. grade at 25 $^{\circ}C$, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

479.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated):

0.085 (shake flask-GC, Coats & O'Donnell-Jafferey 1979)

0.085 (Verschuereen 1983; quoted, Pait et al. 1992)

0.024 (in seawater, Schimmel et al. 1983; Zaroogian et al. 1985; Clark et al. 1989)

<1.0 (20 $^{\circ}C$, Worthing 1979, 1987; Spencer 1982)

<1.0 (20 $^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

<0.02 (Davies & Lee 1987; quoted, Kawamoto & Urano 1989)

<1.0 (tech. grade at 20 $^{\circ}C$, Worthing & Walker 1991)

0.002 (20–25 $^{\circ}C$, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25 $^{\circ}C$ or as indicated):

4.90×10^{-7} (Barlow 1978)

3.07×10^{-5} (Worthing 1979)

1.33×10^{-5} (22 $^{\circ}C$, Spencer 1982)

3.70×10^{-5} (Hartley & Kidd 1987)

1.47×10^{-6} (Budavari 1989)

3.73×10^{-5} (Kawamoto & Urano 1989)

8.10×10^{-7} (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)

3.70×10^{-5} (tech. grade, Worthing & Hance 1991)

1.47×10^{-6} (20–25 $^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1.92×10^{-7} (20 $^{\circ}C$, Tomlin 1994)

1.78×10^{-6} (solid P^S , converted from P_L determined by GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.0152	($20\text{--}25^\circ\text{C}$, calculated-P/C, Montgomery 1993)
0.308	($20\text{--}25^\circ\text{C}$, calculated-P/C as per Wauchope et al. 1992, Majewski & Capel 1995)
0.0211	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C or as indicated:

4.42	(shake flask-GC, Coats & O'Donnell-Jafferey 1979)
6.20	(shake flask-GC, Schimmel et al. 1983)
5.2 ± 0.6	(HPLC-RT correlation, Muir et al. 1985)
6.65	(shake flask, Log P Database, Hansch & Leo 1987)
6.25	(HPLC-RT correlation, Kawamoto & Urano 1989)
4.09	(23°C , Worthing & Walker 1991)
6.25	(HPLC-RT correlation, Hu & Leng 1992)
4.09–6.25	(Montgomery 1993)
6.20	(recommended, Sangster 1993)
5.01	(23°C , Tomlin 1994)
6.20	(recommended, Hansch et al. 1995)
4.08	(23°C , Milne 1995)

Bioconcentration Factor, $\log \text{BCF}$:

3.67	(quoted, Schimmel et al. 1983)
1.67–1.84	(sand, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
2.01–2.24	(sand, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.30–1.53	(sand, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
1.62–1.87	(silt, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.36–2.06	(silt, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.26–1.97	(silt, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
1.36–1.51	(clay, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
2.09–2.19	(clay, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
0.95–1.70	(clay, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
4.48, 4.57	(oyster, calculated- K_{OW} & models, Zarogian et al. 1985)
4.48, 4.57	(sheepshead minnow, calculated- K_{OW} & models, Zarogian et al. 1985)
3.67	(oyster, Zarogian et al. 1985; quoted, Hawker & Connell 1986)
–3.09	(milk biotransfer factor $\log B_m$, correlated- K_{OW} , Wszolek et al. 1980; quoted, Travis & Arms 1988)
2.61, 2.96	(<i>Oncorhynchus mykiss</i> , Muir et al. 1994; quoted, Devillers et al. 1996)
2.70	(calculated, Pait et al. 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.58	(silt, reported as K_p on 78% DOC, Muir et al. 1985)
2.61	(clay, reported as K_p on 61% DOC, Muir et al. 1985)
1.30	(selected, USDA 1989; quoted, Neary et al. 1993)
3.72	(soil, $20\text{--}25^\circ\text{C}$, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.64	(calculated, Montgomery 1993)
3.72	(estimated-chemical structure, Lohninger 1994)
3.74	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Biodegradation: rate constant $k(\text{aerobic}) = 0.055 \text{ d}^{-1}$ with $t_{1/2} = 13 \text{ d}$ at 20°C by aerobic activated sludge, and $k(\text{anaerobic}) = 0.055 \text{ d}^{-1}$ with $t_{1/2} = 13 \text{ d}$ at 20°C by anaerobic microorganisms (batch contacting method, Kawamoto & Urano 1990).

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 14 \text{ d}$ in 100 mL of a pesticide-seawater solution under outdoor light, $t_{1/2} > 14 \text{ d}$ under outdoor dark condition and $t_{1/2} > 28 \text{ d}$ under indoor condition (Schimmel et al. 1983);

$t_{1/2} = 27\text{--}42$ d in an estuary (Schimmel et al. 1983; quoted, Montgomery 1993).

$t_{1/2} = 13$ d biodegradation by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990).

Ground water:

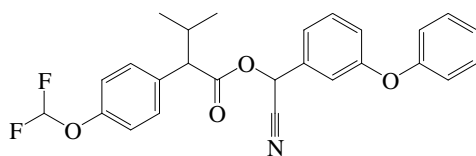
Sediment: $t_{1/2} = 34$ d in 10 g of sediment/100 mL of a pesticide-seawater solution in untreated condition and $t_{1/2} > 28$ d in sterile condition (Schimmel et al. 1983).

Soil: selected field $t_{1/2} = 35$ d (Wauchope et al. 1992; Hornsby et al. 1996).

soil $t_{1/2} = 50$ d (Pait et al. 1992).

Biota: average $t_{1/2} = 35$ d in the forest (USDA 1989; quoted, Neary et al. 1993).

18.1.1.45 Flucythrinate



Common Name: Flucythrinate

Synonym: AC 222705, Cybolt, Cythrin, Pay-Off

Chemical Name: (*RS*)- α -cyano-3-phenoxybenzyl(*S*)-2-(4-difluoromethoxyphenyl)-3-methylbutyrate; cyano(3-phenoxyphenyl)methyl 4-(difluoromethoxy)- α -(1-methylethyl)benzeneacetate

Uses: non-systemic insecticide with contact and stomach action to control a wide range of insect pests in cotton, fruit trees, strawberries, vines, fruits, olives, coffee, cocoa, hops, vegetables, soybeans, cereals, maize, alfalfa, sugar beet, sunflowers and ornamentals

CAS Registry No: 70124-77-5

Molecular Formula: $C_{26}H_{23}F_2NO_4$

Molecular Weight: 451.463

Melting Point ($^{\circ}C$):

<25 (dark amber liquid, Montgomery 1993)

Boiling Point ($^{\circ}C$):

108.0 (at 0.35 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.189 ($22^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

1.190 ($22^{\circ}C$, Worthing & Hance 1991)

Molar Volume (cm^3/mol):

499.9 (calculated-Le Bas method at normal boiling point)

379.4 ($22^{\circ}C$, calculated-density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.049 (in seawater, Schimmel et al. 1983)

0.50 ($21^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987, 1991; Tomlin 1994; Milne 1995)

0.06 (20 – $25^{\circ}C$, selected, Wauchope 1989; Hornsby et al. 1996)

0.50 ($21^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.2×10^{-6} (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

9.066 (Montgomery 1993)

2.69×10^{-6} , 2.2×10^{-6} (liquid P_L , GC-RT correlation; Donovan 1996)

1.2×10^{-6} (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

2.82×10^{-6} (solid P^S , converted from P_L determined by GC-RT correlation method, Tsuzuki 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

8187 (21 – $25^{\circ}C$, calculated-P/C, 8.08×10^{-2} atm· m^3/mol , Montgomery 1993)

0.0011 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.28 (shake flask-GC, Schimmel et al. 1983)

6.20 (Clark et al. 1989)

2.08	(Worthing & Hance 1991; Tomlin 1994; Milne 1995)
5.55	(shake flask, Huang & Leng 1993)
4.70	(Montgomery 1993)
6.20	(recommended, Sangster 1993)
6.20	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.96	(calculated-S as per Kenaga 1980, this work)
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Sorption Partition Coefficient, log K_{OC} :

3.81	(calculated, Montgomery 1993)
5.00	(20–25°C, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} \sim 21$ d for degradation on soil plates by simulated sunlight and $t_{1/2} = 4.0$ d in aqueous solutions (Tomlin 1994).

Oxidation:

Hydrolysis: $t_{1/2} = 40, 52,$ and 6.3 d at pH 3, 5, 9 all at 27°C (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 34$ d in an estuarine environment (Schimmel et al. 1983; quoted, Montgomery 1993).

Ground water:

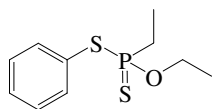
Sediment:

Soil: $t_{1/2} \sim 2$ months in soil (Tomlin 1994);

field $t_{1/2} = 21$ d (20–25°C, selected, Hornsby et al. 1996).

Biota:

18.1.1.46 Fonofos



Common Name: Fonofos

Synonym: Difonate, Dyfonate, ENT-25796, Fonophos, N 2788, N-2790, Stauffer NA 2790

Chemical Name: *O*-ethyl *S*-phenyl (*RS*)-ethylphosphorodithioate; (±)-*O*-ethyl *S*-phenyl ethylphosphorodithioate

Uses: soil insecticide to control rootworms, wireworms, crickets and similar crop pests in vegetables, sorghum, ornamentals, cereals, maize, vines, olives, sugar beet, sugar cane, potatoes, groundnuts, tobacco, turf, and fruit crops

CAS Registry No: 944-22-9 (unstated stereochemistry); 66767-39-3 (racemate); 62705-71-9 (*R*)-isomer; 62680-03-9 (*S*)-isomer

Molecular Formula: $C_{10}H_{15}OPS_2$

Molecular Weight: 246.329

Melting Point (°C): liquid

Boiling Point (°C):

130 (at 0.1 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm³ at 20°C):

1.160 (25°C, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

1.154 (Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm³/mol):

213.4 (calculated-density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F : 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

13 (22°C, Spencer 1973)

13 (Wauchope 1978)

15.7 (20°C, shake flask-GC, Bowman & Sans 1979, 1983b)

13 (Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

13 (20°C, Worthing & Walker)

16.9 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

13 (rm. temp., Montgomery 1993)

13 (22°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

0.0267 (Menn 1969; Fuhrmann & Lichtenstein 1980)

0.028 (Khan 1980; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

0.028 (Worthing & Walker 1987; Worthing & Hance 1991)

0.0453 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.5206 (calculated-P/C as per Worthing & Walker 1987, Schomburg et al. 1991)

0.5268 (20–25°C, calculated-P/C, Montgomery 1993)

0.530 (calculated-P/C as per Worthing & Walker 1987, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{ow} at 25°C or as indicated:

3.892 (shake flask-GC, Bowman & Sans 1983b)

3.94 (shake flask, Log P Database, Hansch & Leo 1987)

3.90 (20°C, Worthing & Hance 1991)

- 3.89, 3.90 (Montgomery 1993)
- 3.94 (recommended, Sangster 1993)
- 3.94 (Tomlin 1994)
- 3.90 (Milne 1995)
- 3.94 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 1.89 (mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 2.3–2.7 (selected, sediment/water, Schnoor & McAvoy 1981; Schnoor 1992)
- 1.83 (screening model calculations, Jury et al. 1987b)
- 1.18 (loam soil, Worthing & Hance 1991)
- 2.94 (soil, 20–25°C, selected, Wauchope et al. 1992)
- 3.03 (calculated, Montgomery 1993)
- 2.94 (estimated-chemical structure, Lohninger 1994)
- 2.94 (soil, 20–25°C, selected, Hornsby et al. 1996)
- 3.44; 3.0, 3.04 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 12$ d in water at pH 5 and 25°C (Worthing & Hance 1991; Tomlin 1994).

Oxidation:

Hydrolysis: alkaline chemical hydrolysis rate constant $k = 1 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} > 365$ d (selected, sediment/water, Schnoor & McAvoy 1981; quoted, Schnoor 1992);

hydrolysis $t_{1/2} = 74$ –127 d in water at 40°C and pH 7, $t_{1/2} = 101$ d at pH 4 (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil: persistence of less than one month in soil (Wauchope 1978);

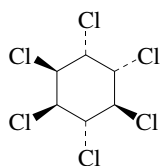
$t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} = 3.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 4.0$ wk in nonsterile organic soil (Miles et al. 1979);

$t_{1/2} = 60$ d from screening model calculations (Jury 1987b);

$t_{1/2} = 16.5$ –28 d at 24°C (Worthing & Hance 1991);

selected field $t_{1/2} = 40$ d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996).

Biota: biochemical $t_{1/2} = 60$ d from screening model calculations (Jury et al. 1987b).

18.1.1.47 α -HCH

Common Name: α -HCH

Synonym: α -BHC, α -Hexachlorocyclohexane

Chemical Name: α -1,2,3,4,5,6-hexachlorocyclohexane, (1 α , 2 α , 3 α , 4 α , 5 β , 6 β -1, 2, 3, 4, 5, 6-hexachloro-cyclohexane

CAS Registry No: 319-84-6

Molecular Formula: C₆H₆Cl₆

Molecular Weight: 290.830

Melting Point (°C):

158 (Lide 2003)

Boiling Point (°C): 288

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

243.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of fusion, ΔH_{fus} (kJ/mol):

30.96 (Ruelle & Kesselring 1997)

Entropy of fusion, ΔS_{fus} (J/mol K):

72.0 (Passivirta et al. 1999)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.0496 (mp at 158°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):

10 (20°C, Slade 1945, Günther et al. 1968; Ulmann 1972; Horvath 1982)

1.63 (shake flask-GC, Kanazawa et al. 1971)

2.03, 1.21 (28°C, shake flask-centrifuge, membrane filter-GC, max. 0.1 μm particle size, Kurihara et al. 1973)

1.77, 1.48 (28°C, shake flask-centrifuge, sonic and centrifuge-GC, max. 0.05 μm particle size, Kurihara et al. 1973)

1.21–2.03 (28°C, Kurihara et al. 1973)

2.0 (generator column-GC/ECD, Weil et al. 1974)

4.34 (shake flask-GC/ECD, Malaiyandi et al. 1982)

1.51 (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)

21.6 (supercooled liquid value, Majewski & Capel 1995)

0.666, 0.023 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

$\log [S_L/(\text{mol/L})] = 2.790 - 1621/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

85.22, 96.85 (supercooled liquid values: LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)

$\log S_L/(\text{mol m}^{-3}) = -398.5/(T/K) + 0.859$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.67* (20°C, static method, measured range 20–60°C, Slade 1945)

0.00333* (20°C, effusion manometer, measured range 15–30°C, Balson 1947)

0.27 (supercooled liquid value from Balson 1947; quoted, Hinckley et al. 1990)

0.0073 (20°C, Deutsche Forschungsgemeinschaft 1983; quoted, Ballschmiter & Wittlinger 1991; Fischer et al. 1991; Schreitmüller & Ballschmiter 1995)

0.0840 (20°C, supercooled liquid value, Bidleman et al. 1986)

0.313 (GC-RT correlation, Watanabe & Tatsukawa 1989)

0.227 (supercooled liquid P_L , GC-RT correlation, Hinckley et al. 1990)

$\log (P_L/\text{Pa}) = 10.49 - 3301/(T/K)$ (supercooled liquid, Hinckley et al. 1990)

$\log (P_L/\text{Pa}) = 11.34 - 3375/(T/K)$ (supercooled liquid, Hinckley et al. 1990)

0.003 (selected, Suntio et al. 1988, quoted, Calamari et al. 1991; Schreitmüller & Ballschmiter 1995)

0.0060 (quoted, Howard 1991)

0.00647 (quoted, supercooled liquid value, Majewski & Capel 1995)

0.159; 0.00464 (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/Pa) = 14.53 - 4954/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 10.77 - 3335/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

0.245, 0.245 (supercooled liquid P_L : LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)

$\log P_L/Pa = -3434/(T/K) + 10.91$ (supercooled liquid, linear regression of literature data, Xiao et al. 2004)

$\log P_L/Pa = -3497/(T/K) + 11.12$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ or at 25°C as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.47–0.792 (Callahan et al. 1979)

2.16 (gas stripping-GC, Atlas et al. 1982)

0.55 (calculated-P/C, Mabey et al. 1982)

0.87 (calculated-P/C, Suntio et al. 1988)

1.10 (calculated-P/C, Ballschmiter & Wittlinger 1991; Fischer et al. 1991)

1.07 (calculated-P/C, Howard 1991)

0.43 (calculated-P/C, Calamari et al. 1991)

0.677* (23°C, gas stripping-GC/ECD, distilled water, measured range 0.5–45°C, Kucklick et al. 1991)

$\log [H/(Pa \cdot m^3 \cdot mol^{-1})] = -2810/(T/K) + 9.31$, temp range 0.5–45°C (gas stripping-GC measurements, distilled water, Kucklick et al. 1991, McConnell et al. 1993)

0.104, 0.257, 0.710, 2.10, 5.99 (0.5, 10, 25, 23, 35, 45°C, gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)

$\log [H/(Pa \cdot m^3 \cdot mol^{-1})] = -2969/(T/K) + 9.88$, temp range 0.5–45°C (gas stripping-GC measurements, artificial seawater, Kucklick et al. 1991)

0.87 (20°C), 2.40, 1.10, 0.677, 0.710 (23°C) (quoted, Iwata et al. 1993)

0.215, 0.491, 0.373, 0.630, 0.630 (8.5°C in Green Bay, 18.9°C in Lake Michigan, 18.5°C in Lake Huron, 22.3°C in Lake Erie, 22.3°C in Lake Ontario, concn. ratio-GC, McConnell et al. 1993)

0.872 (calculated-P/C, this work)

1.239 (wetted wall column-GC, Altschuh et al. 1999)

$\log [H/(Pa \cdot m^3/mol)] = 8.98 - 1714/(T/K)$ (Passivirta et al. 1999)

0.43* (20°C, gas stripping-GC, measured range 10–40°C, Jantunen et al. 2000)

$\log [H/(Pa \cdot m^3/mol)] = 10.88 - 3298/(T/K)$; temp range 10–40°C (gas stripping-GC, Jantunen et al. 2000)

0.53 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 5.485 - 2682/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

0.38* (20°C, dynamic headspace-GC, DHS method, measured range 5–35°C, Sahsuvar et al. 2003)

0.42* (20°C, gas stripping-GC, BS method, measured range 5–35°C, Sahsuvar et al. 2003)

0.39* (20°C, mean value of DHS and BS methods, temp range 5–35°C, Sahsuvar et al. 2003)

$\log [H/(Pa \cdot m^3/mol)] = 10.13 - 3088/(T/K)$; temp range 5–35°C (Sahsuvar et al. 2003)

0.646, 0.741 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)

$\log [H/(Pa \cdot m^3/mol)] = -3171/(T/K) + 10.45$ (LDV linear regression of literature data, Xiao et al. 2004)

$\log [H/(Pa \cdot m^3/mol)] = -3099/(T/K) + 10.26$ (FAV final adjusted eq., Xiao et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.81 (shake flask-GC, Kurihara et al. 1973)

3.81 (HPLC-RT correlation, Sugiura et al. 1979)

3.90 (Veith et al. 1979)

3.776 ± 0.025 (shake flask/slow stirring method; De Bruijn et al. 1989)

3.80 (recommended, Sangster 1993)

3.80 (recommended, Hansch et al. 1995)

$3.79^* \pm 0.001$ (shake flask-slow stirring-GC, measured range 5–45°C, Paschke & Schüürmann 1998)

3.81; 4.57 (quoted lit.; calculated, Passivirta et al. 1999)

3.81, 3.94 (LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)

$\log K_{OW} = -374.5/(T/K) + 2.55$ (LDV linear regression of literature data, Xiao et al. 2004)

$\log K_{OW} = -266.2/(T/K) + 3.04$ (LDV linear regression of literature data, Xiao et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 6.90 (calculated- K_{OW}/K_{AW} , Wania & Mackay 1996)
- 7.26 (calculated, Finizio et al. 1997)
- 7.618*, 7.611 (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
- $\log K_{OA} = -3.23 + 3231/(T/K)$, temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
- 7.61, 7.464 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
- $\log K_{OA} = 3231/(T/K) - 3.23$ (LDV linear regression of literature data, Xiao et al. 2004)
- $\log K_{OA} = 3235/(T/K) - 3.90$ (FAV final adjusted eq., Xiao et al. 2004)

Bioconcentration Factor, $\log BCF$:

- 2.03 (mussels, Ernst 1977; quoted, Renberg & Sundström 1979; Hawker & Connell 1986)
- 3.08, 2.52, 2.78, 2.77 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
- 2.20, 2.82 (mussels, Geyer et al. 1982)
- 2.97–3.38 mean 3.20; 2.97–3.45 mean 3.38 (rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
- 3.20, 2.85 (rainbow trout: laboratory BCF, Lake Ontario field BCF, Oliver & Niimi 1985)
- 1.93 (paddy field fish, Soon & Hock 1987)
- 2.15 (calculated, Isnard & Lambert 1988)
- 6.01 (azalea leaves, Bacci et al. 1990)
- 3.04 (*Brachydanio rerio*, flow-through conditions, Butte et al. 1991)
- 2.33 (early juvenile of rainbow trout, Vigano et al. 1992)
- 5.72 (azalea leaves, calculated, Müller et al. 1994)
- 2.79; 2.606, 2.712 (fish, steady-state, quoted lit.; calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)
- 2.33; 2.44 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.81 (calculated-S, Lyman et al. 1982)
- 4.10, 3.5 (field sediment trap material, calculated- K_{OW} , Oliver & Charlton 1984)
- 3.25 (av. lit. value, Gerstl 1991)
- 3.32 (derived from exptl., Meylan et al. 1992)
- 3.53 (calculated-MCI χ , Meylan et al. 1992)
- 3.25 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 5.50 (soil, calculated-universal solvation model, Winget et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} \sim 6$ d from a model river of 1 m deep flowing 1 m/s with a wind speed of 3 m/s (Saleh et al. 1982);

$t_{1/2} \sim 500$ d from a model pond (estimated, Howard 1991).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.3$ d for reaction with OH radical in the gas phase (Atkinson 1987).

Hydrolysis: hydrolytic $t_{1/2} = 26$ yr at pH 8 and 5°C (Ngabe et al. 1993).

Biodegradation: overall degradation rate constant $k = 0.0648 \text{ h}^{-1}$ with $t_{1/2} = 10.7$ h for (+)- α -HCH and rate constant $k = 0.0298 \text{ h}^{-1}$ with $t_{1/2} = 23.3$ h for (–)- α -HCH were calculated from experiments S1–S3 of (35 ± 0.5) h for (+) enantiomer and 99 ± 3.5 h for (–) enantiomer in sewage sludge (Müller & Buser 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 3.82 \text{ h}^{-1}$; $k_2 = 0.036 \text{ h}^{-1}$ (mussels, Ernst 1977; quoted, Hawker & Connell 1986)

$k_1 = 0.52 \text{ d}^{-1}$, 0.56 d^{-1} , 0.91 d^{-1} , and 0.42 d^{-1} (golden orfe, carp, brown trout, and guppy at steady state, Sugiura et al. 1979)

$k_2 = 0.0009 \text{ h}^{-1}$ (azalea leaves, Peterson et al. 1991)

$k_1 = 27.6 \text{ h}^{-1}$; $k_2 = 0.13 \text{ h}^{-1}$ (early juvenile of rainbow trout, Vigano et al. 1992)

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.3$ d based on reaction with OH radical at 25°C (Atkinson 1987);

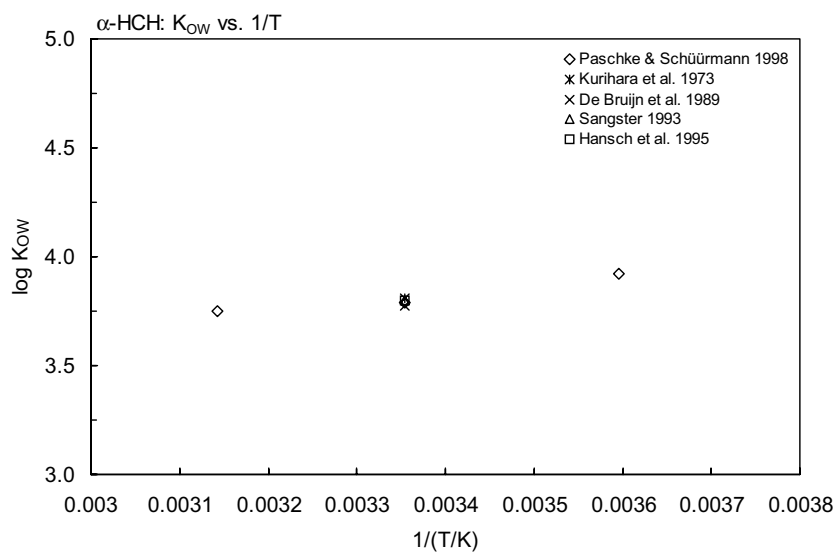


FIGURE 18.1.1.47.2 Logarithm of K_{OW} versus reciprocal temperature for α -HCH.

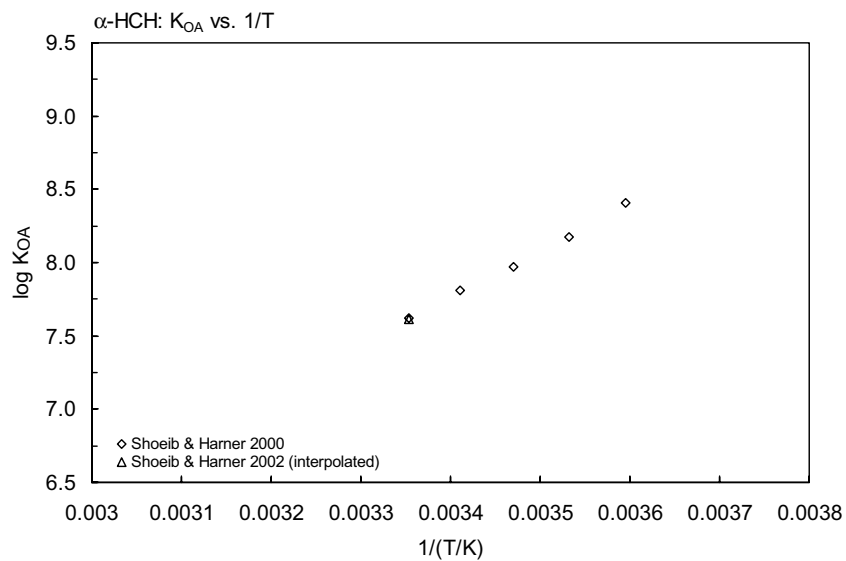


FIGURE 18.1.1.47.3 Logarithm of K_{OA} versus reciprocal temperature for α -HCH.

TABLE 18.1.1.47.2

Reported Henry's law constants of α -HCH at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)		
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)		
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)					
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)		
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)					
Kucklick et al. 1991		McConnell et al. 1993		Jantunen et al. 2000		Sahsuvar et al. 2003	
gas stripping-GC		concentration ratio		air stripping-GC		air stripping/dynamic HS	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
			Green Bay				dynamic headspace (DHS)
0.5	0.104	8.0	0.215	10	0.17	5	0.094
10	0.255		Lake Michigan	20	0.43	10	0.15
23	0.677	18.9	0.491	30	0.92	20	0.38
35	1.34		Lake Huron	35	1.52	30	0.79
45	3.27	18.5	0.373	40	2.21	35	1.32
			Lake Erie				
eq. 4a	H/(Pa m³/mol)	22.3	0.630	eq. 4a	H/(Pa m³/mol)		gas stripping-GC
A	9.31		Lake Ontario	A	10.88 ± 0.50	5	0.098
B	2810	22.3	0.630	B	3298 ± 149	10	0.13
seawater					20	0.42	
0.5	0.104					30	0.92
10	0.257					35	1.24
23	0.710						
35	2.10						combined - both methods
45	5.99					5	0.095
						10	0.15
eq.4a	H/(Pa m³/mol)					20	0.39
A	9.88					30	0.85
B	2969					35	1.30
						eq. 4a	H/(Pa m³/mol)
						A	10.13 ± 0.29
						B	3088 ± 84
							enthalpy of transfer air-water
							$\Delta H_{wA}/(\text{kJ mol}^{-1}) = 59.3$

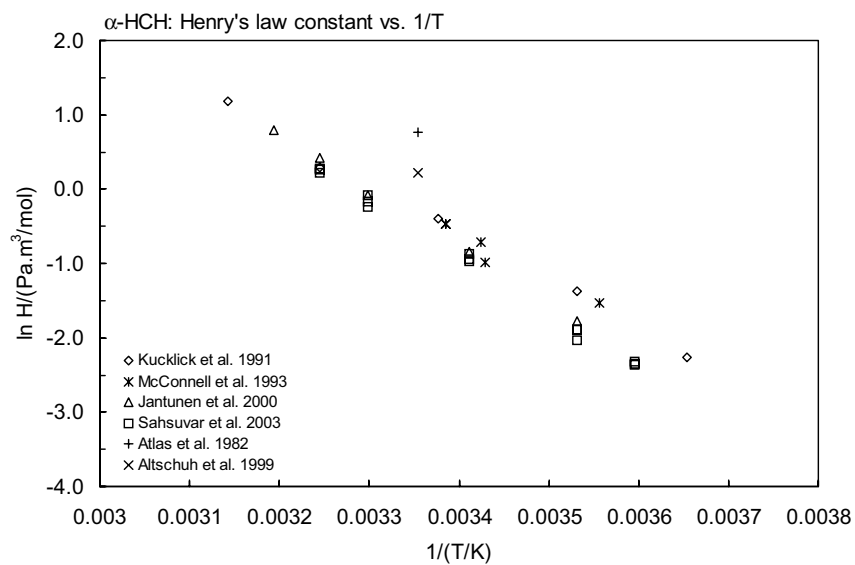
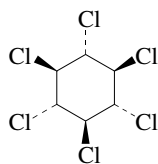


FIGURE 18.1.1.47.4 Logarithm of Henry's law constant versus reciprocal temperature for α -HCH.

18.1.1.48 β -HCH

Common Name: β -HCH

Synonym: β -BHC, β -Hexachlorocyclohexane, 1 α ,2 β ,3 α ,4 β ,5 α ,6 β -1,2,3,4,5,6-hexachloro-cyclohexane

Chemical Name: β -1,2,3,4,5,6-hexachlorocyclohexane

CAS Registry No: 319-85-7

Molecular Formula: C₆H₆Cl₆

Molecular Weight: 290.830

Melting Point (°C):

309 (Slade 1945; Ballschmiter & Wittlinger 1991)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

243.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of fusion, ΔH_{fus} (kJ/mol):

Entropy of fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.00164 (mp at 309°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations):

- 5.0 (20°C, Slade 1945; Gunther et al. 1968; Horvath 1982)
- 0.70 (20°C, shake flask-GC, Kanazawa et al. 1971)
- 0.20, 0.13 (28°C, shake flask-centrifuge, membrane filter-GC, max. 0.1 μ m particle size, Kurihara et al. 1973)
- 0.70 (20°C, Brooks 1974)
- 0.24 (generator column-GC/ECD, Weil et al. 1974)
- 0.13–0.70 (Callahan et al. 1979)
- 2.04 (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
- 7.0 (Worthing & Walker 1983)
- 69.5 (supercooled liquid value, Majewski & Capel 1995)
- 344, 418.8 (supercooled liquid: derivation of literature-derived value, final-adjusted value, Xiao et al. 2004)
- $\log [S_L/(\text{mol m}^{-3})] = -110.1/(T/K) - 0.211$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.67* (20°C, static method, measured range 20–60°C, Slade 1945)
- 3.73×10^{-5} * (20°C, effusion-manometer, measured range 0–110°C, Balson 1947)
- 4.90×10^{-5} (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
- 0.266 (GC-RT correlation, Watanabe & Tatsukawa 1989)
- 0.0272 (supercooled liquid value, Majewski & Capel 1995)
- 0.062, 0.0525 (supercooled liquid P_L LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)
- $\log (P_L/\text{Pa}) = -3563/(T/K) + 10.74$ (supercooled liquid, linear regression of literature data, Xiao et al. 2004)
- $\log (P_L/\text{Pa}) = -3563/(T/K) + 10.67$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.055 (20–25°C, Mabey et al. 1982)
- 0.120 (calculated-P/C, Suntio et al. 1988)
- 0.070 (calculated-P/C, Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
- 0.0446 (wetted-wall column-GC, Altschuh et al. 1999)

0.022* (dynamic headspace-GC, measured range 5–35°C, Sahsuvar et al. 2003)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 9.96 - 3400/(T/K)$; temp range 5–35°C (dynamic headspace-GC, Sahsuvar et al. 2003)
 0.037, 0.037 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -3454/(T/K) + 10.16$ (LDV linear regression of literature data, Xiao et al. 2004)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -3673/(T/K) + 10.89$ (FAV final adjusted eq., Xiao et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:

3.80 (shake flask-GC, Kurihara et al. 1973)
 4.15 (HPLC-RT correlation, Sugiura et al. 1979)
 3.842 ± 0.036 ; 3.78 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 3.81 (recommended, Sangster 1993)
 3.78 (recommended, Hansch et al. 1995)
 $3.88^* \pm 0.01$ (shake flask/slow stirring-GC, measured range 5–25°C, Paschke & Schüürmann 1998)
 3.84, 3.92 (LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)
 $\log K_{OW} = 847.5/(T/K) + 1.07$ (LDV linear regression of literature data, Xiao et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.965*, 8.875 (gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)
 $\log K_{OA} = -7.69 + 4937/(T/K)$, temp range 5–35°C, (gas saturation-GC, Shoeib & Harner 2002)
 8.87, 8.74 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
 $\log K_{OA} = 4937/(T/K) - 7.69$ (LDV linear regression of literature data, Xiao et al. 2004)
 $\log K_{OA} = 4391/(T/K) - 5.98$ (FAV final adjusted eq., Xiao et al. 2004)

Bioconcentration Factor, $\log BCF$:

2.99, 2.44, 2.82, 3.17 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
 3.08, 2.26, 2.62 (activated sludge, algae, golden ide, reported as $\log BF$, Freitag et al. 1985)
 2.66 (calculated, Isnard & Lambert 1988)
 3.16, 3.18 (*Brachydanio rerio*, flow-through conditions, Butte et al. 1991; quoted, Devillers et al. 1996)
 2.86; 2.606, 2.712 (fish, steady-state, quoted lit.; calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)
 2.50; 2.44 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, $\log K_{OC}$:

3.36 (av. lit. value, Gerstl 1991)
 3.98 (soil, calculated-S as per Kenaga 1980, this work)
 3.50 (derived from exptl., Meylan et al. 1992)
 3.53 (calculated-MCI χ , Meylan et al. 1992)
 3.36 (soil, calculated-MCI χ , Sabljic et al. 1995)
 5.50; 3.50 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: calculated $t_{1/2} = 178$ h in sewage sludge from experiments S1–S3 (Buser & Müller 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

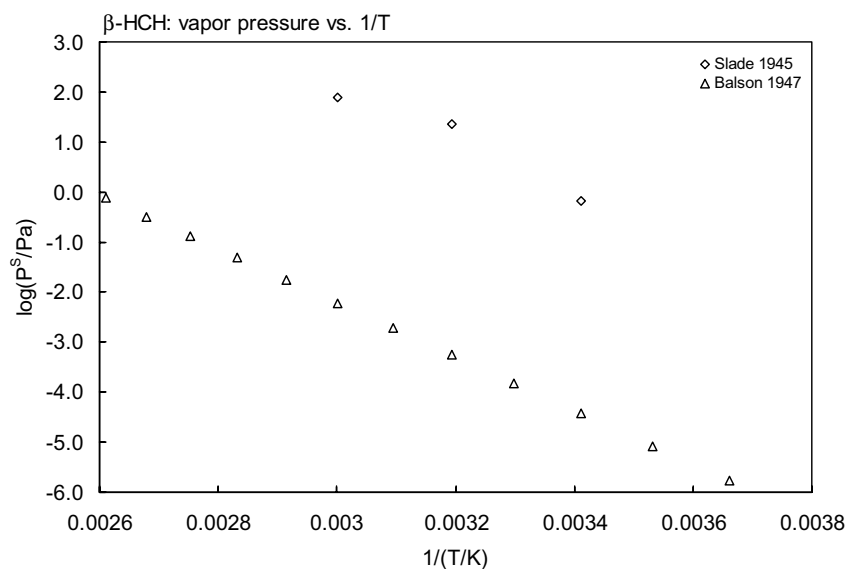
$k_1 = 0.46 \text{ d}^{-1}$, 0.33 d^{-1} , 0.53 d^{-1} , and 0.18 d^{-1} (golden orfe, carp, brown trout, and guppy at steady state, Sugiura et al. 1979)

Half-Lives in the Environment:

TABLE 18.1.1.48.1

Reported vapor pressures and Henry's law constants of β -HCH at various temperatures

Vapor pressure				Henry's law constant	
Slade 1945		Balson 1947		Sahsuvar et al. 2003	
static method		effusion manometer		dynamic headspace-GC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m ³ /mol)
20	0.667	0	1.733×10^{-6}	5	0.0054
40	22.7	10	8.399×10^{-6}	10	0.0092
60	77.3	20	3.733×10^{-5}	20	0.022
		30	1.533×10^{-4}	30	0.053
		40	5.60×10^{-4}	35	0.088
		50	1.907×10^{-3}		
		60	6.00×10^{-3}		
		70	0.01760	$\ln H = A - B/(t/K)$ H/(Pa m ³ /mol)	
		80	0.04933		
		90	0.1293	A	9.96 ± 0.23
		100	0.3200	B	3400 ± 68
		110	0.7653		
		$\log P = A - B/(T/K)$ P/mmHg		enthalpy of transfer air-water $\Delta H_{WA}/(\text{kJ mol}^{-1}) = 65.1$	
		A	11.790		
		B	5375		
		temp range: 95–117°C			

FIGURE 18.1.1.48.1 Logarithm of vapor pressure versus reciprocal temperature for β -HCH.

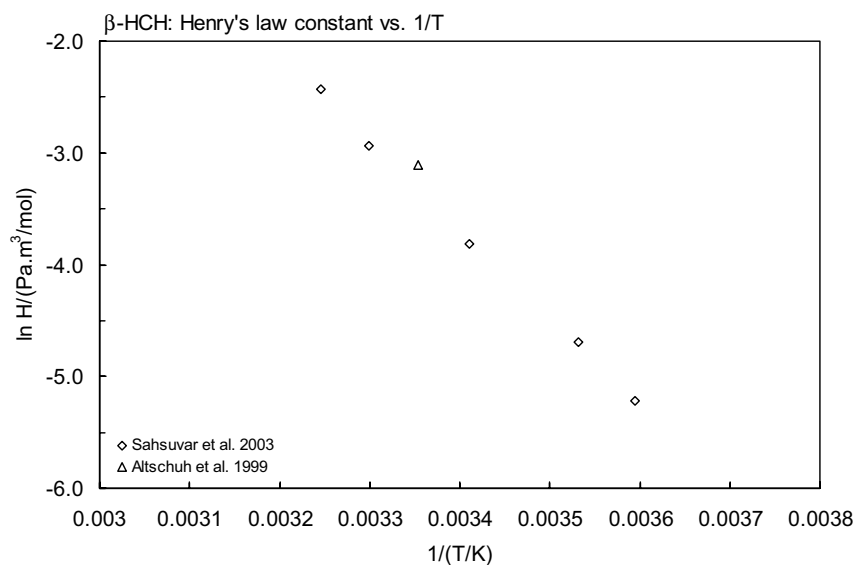


FIGURE 18.1.1.48.2 Logarithm of Henry's law constant versus reciprocal temperature for β-HCH.

TABLE 18.1.1.48.2
Reported octanol-water and octanol-air partition coefficients of β-HCH at various temperatures

log K _{OW}		log K _{OA}	
Paschke & Schüürmann 1998		Shoeib & Harner 2002	
shake flask-GC		generator column-GC/MS	
t/°C	log K _{OW}	t/°C	log K _{OA}
5	3.99	5	10.0686
25	3.88	15	9.4375
45	3.87	20	8.9875
		25	8.9651
		35	8.3682
		25	8.875
enthalpy of phase transfer: ΔH _{OW} /(kJ mol ⁻¹) = − 8.20		log K _{OA} = A + B/(T/K) A −7.692 B 4937	
entropy of phase transfer: ΔS _{OW} /(J K ⁻¹ mol ⁻¹) = 62.7			
		enthalpy of phase change ΔH _{OA} /(kJ mol ⁻¹) = 94.5	

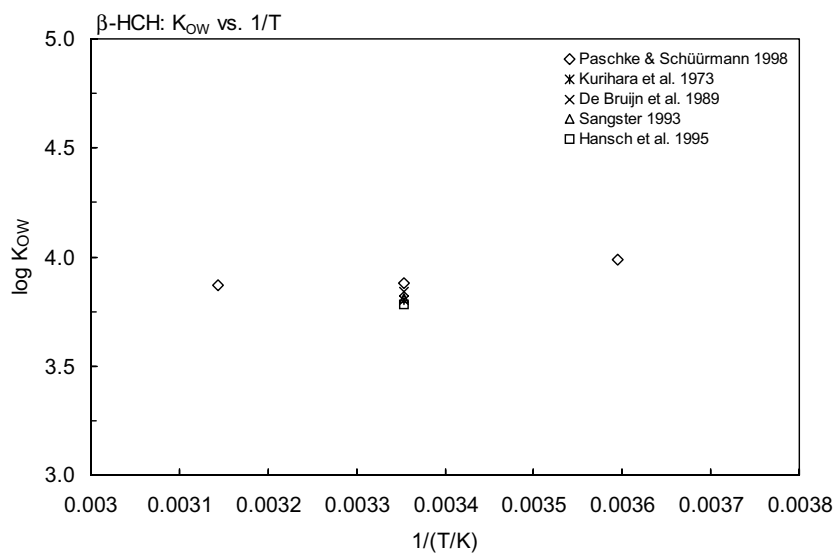


FIGURE 18.1.1.48.3 Logarithm of K_{OW} versus reciprocal temperature for β -HCH.

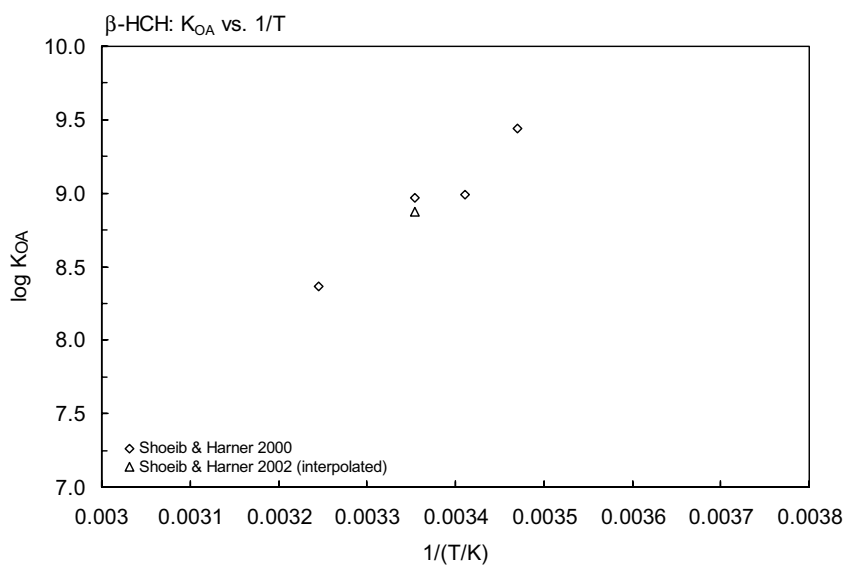
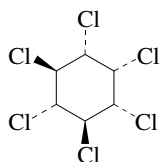


FIGURE 18.1.1.48.4 Logarithm of K_{OA} versus reciprocal temperature for β -HCH.

18.1.1.49 δ -HCH

Common Name: δ -HCH

Synonym: δ -BHC, δ -Hexachlorocyclohexane, $1\alpha,2\alpha,3\alpha,4\beta,5\alpha,6\beta$ -1,2,3,4,5,6-hexachloro-cyclohexane

Chemical Name: δ -1,2,3,4,5,6-hexachlorocyclohexane

CAS Registry No: 319-86-8

Molecular Formula: $C_6H_6Cl_6$

Molecular Weight: 290.830

Melting Point ($^{\circ}C$):

141.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

243.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.34 (DSC method, Plato 1972)

21.50 (Ruelle & Kesselring 1997)

Entropy of fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0719 (mp at $141.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

10 ($20^{\circ}C$, Slade 1945)

15.7, 10.7 ($28^{\circ}C$, shake flask-centrifuge, membrane filter-GC, max. $0.1 \mu m$ particle size, Kurihara et al. 1973)

11.6, 8.64 ($28^{\circ}C$, shake flask-centrifuge, sonic and centrifuge-GC, max. $0.05 \mu m$ particle size, Kurihara et al. 1973)

8.64–31.4 (shake flask-GC, Kurihara et al. 1973)

10 ($20^{\circ}C$, quoted, Günther et al. 1968)

21.3 ($20^{\circ}C$, shake flask-GC, Kanazawa et al. 1971)

31.4 (generator column-GC/ECD, Weil et al. 1974)

9.01 ($20^{\circ}C$, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2.67* ($20^{\circ}C$, static method, measured range 20 – $60^{\circ}C$, Slade 1945)

2.27×10^{-3} * ($20^{\circ}C$, effusion manometer, Balson 1947)

0.150 (GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0309 (supercooled liquid value, Majewski & Capel 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.018 (20 – $25^{\circ}C$, Mabey et al. 1982)

0.073 (calculated-P/C, Suntio et al. 1988)

0.0825 (calculated- P_L/C_L , Majewski & Capel 1995)

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

4.14 (shake flask-GC, Kurihara et al. 1973)

4.14 (recommended, Sangster 1993)

4.14 (recommended, Hansch et al. 1995)

4.17* ± 0.01 (shake flask-slow stirring-GC, measured range 5–45°C, Paschke & Schüürmann 1998)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

8.80*, 8.848 (gas saturation-GC/MS, calculated, measured range 5–35°C, Shoeib & Harner 2002)

log $K_{OA} = -7.45 + 4856/(T/K)$, temp range 5–35°C (gas saturation-GC, Shoeib & Harner 2002)

Bioconcentration Factor, log BCF:

1.95 (calculated-S as per Kenaga 1980, this work)

3.21, 3.25 (*Brachydanio rerio*, flow-through conditions, Butte et al. 1991; quoted, Devillers et al. 1996)

2.45 (rainbow trout, flow-through conditions, Vigano et al. 1992; quoted, Devillers et al. 1996)

2.34; 2.44 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

2.82 (soil, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Biodegradation: calculated $t_{1/2} = 126$ h in sewage sludge from experiments S1–S3 (Buser & Müller 1995).

Half-Lives in the Environment:

TABLE 18.1.1.49.1

Reported vapor pressures, octanol-water partition coefficients and octanol-water partition coefficients of δ -HCH at various temperatures

Vapor pressure				log K_{OW}		log K_{OA}	
Slade 1945		Balson 1947		Paschke & Schüürmann 1998		Shoeib & Harner 2002	
static method		effusion manometer		shake flask-GC		generator column-GC/MS	
t/°C	P/Pa	t/°C	P/Pa	t/°C	log K_{OW}	t/°C	log K_{OA}
20	2.67	0	1.213×10^{-4}	5	4.27	5	10.0436
40	12.0	10	5.466×10^{-4}	25	4.17	15	9.4587
60	45.33	20	2.266×10^{-3}	45	4.15	20	8.9251
		30	8.533×10^{-3}			25	8.7995
		40	0.02946		enthalpy of phase transfer:	35	8.4420
		50	0.09466		$\Delta H_{OW}/(\text{kJ mol}^{-1}) = -7.60$	25	8.848
		60	0.2780		entropy of phase transfer:		
		70	0.7866		$\Delta S_{OW}/(\text{J K}^{-1} \text{mol}^{-1}) = 69.9$		
			log P = A – B/(T/K)				log $K_{OA} = A + B/(T/K)$
		eq. 1	P/mmHg				A –7.447
		A	12.635				B 4856
		B	5100				
			temp range: 55–75°C				enthalpy of phase change
							$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 93.0$

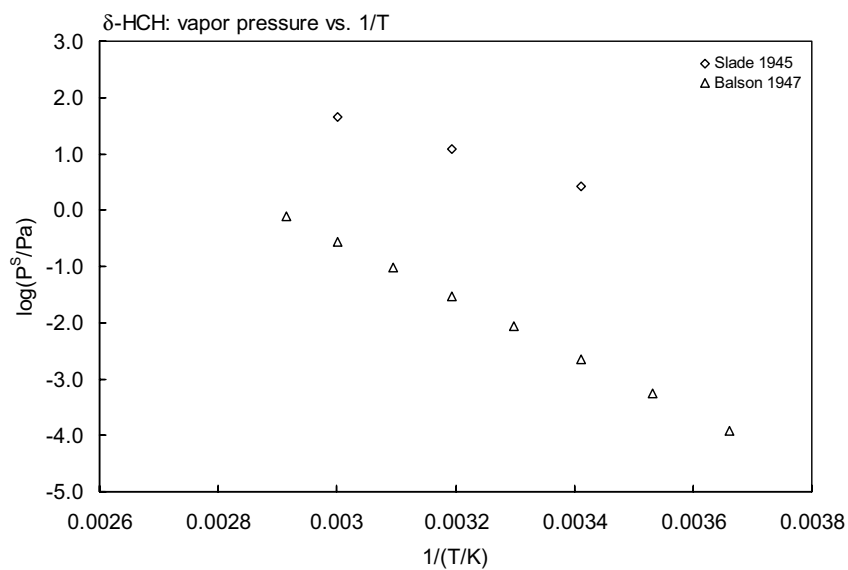


FIGURE 18.1.1.49.1 Logarithm of vapor pressure versus reciprocal temperature for δ-HCH.

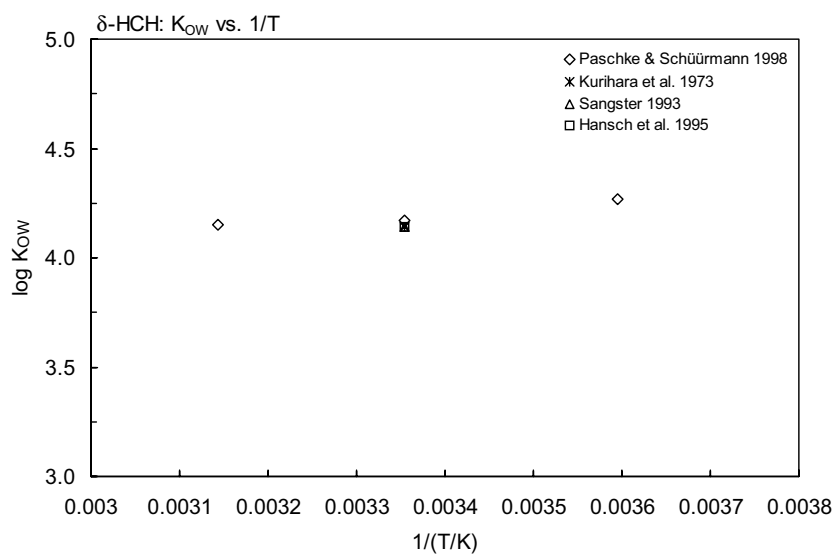


FIGURE 18.1.1.49.2 Logarithm of K_{OW} versus reciprocal temperature for δ-HCH.

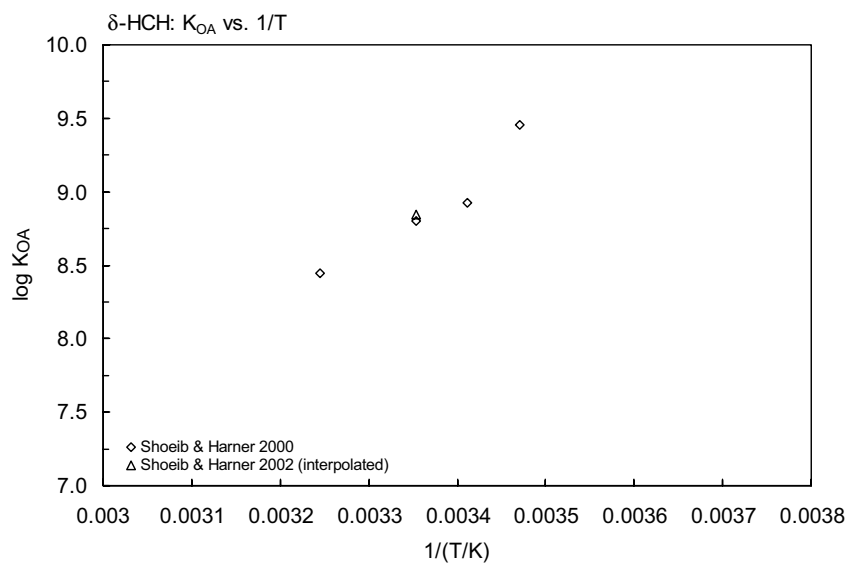
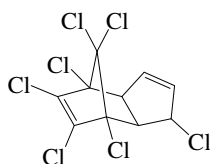


FIGURE 18.1.1.49.3 Logarithm of K_{OA} versus reciprocal temperature for δ -HCH.

18.1.1.50 Heptachlor



Common Name: Heptachlor

Synonym: Aahepta, Aathepta, Agroceres, Basaklor, 3-Chlorochlordene, Drinox, ENT 15152, Hepta, Heptachlorane, Heptagran, Heptagranox, Heptamak, Heptamul, Heptasol, Heptox, methanoindene, NA 2761, NCI-C00180, Rhodiachlor, Soleptax, Velsicol

Chemical Name: 1, 4, 5, 6, 7, 8, 8-heptachloro-3a, 4, 7, 7a-tetrahydro-4, 7-methanoindene; 3-4, 5, 6, 7, 8, 8a-heptachloro-dicyclopentadiene

Uses: non-systemic insecticide with contact, stomach, and some respiratory action to control termites, ants, and soil insects in cultivated and uncultivated soils; also used to control household insects

CAS Registry No: 76-44-8

Molecular Formula: $C_{10}H_5Cl_7$

Molecular Weight: 373.318

Melting Point ($^{\circ}C$):

95.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

135–145 (at 1–1.5 mmHg, Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.65–1.67 ($25^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

1.66 (Montgomery 1993)

Molar Volume (cm^3/mol):

308.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

73.06 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22 (Rordorf 1989)

22.97 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.203 (mp at $95.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.056 ($25-29^{\circ}C$, shake flask-GC, Park & Bruce 1968)

0.03, 0.125, 0.180* (particle size: 0.01, 0.05 & 5.0μ , shake flask-GC, measured range $15-45^{\circ}C$, Biggar & Riggs 1974)

0.03 (Martin & Worthing 1977; Kenaga 1980a, b; Kenaga & Goring 1980)

<1.0 (Wauchope 1978)

0.056 (Hartley & Graham-Bryce 1980; Worthing & Walker 1987; Hartley & Kidd 1987)

0.05 (Khan 1980)

0.30 (Herbicide Handbook 1983)

0.056 ($25-29^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

0.18 (Montgomery 1993)

0.056 ($20-25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

1.307, 1.307 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

$\log [C_L/(mol m^{-3})] = -770/(T/K) + 0.13$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Vapor Pressure (Pa at 25°C or as indicated or reported temperature dependence equations):

- 0.025 (Bowery 1964)
- 0.040 (Eichler 1965; Martin 1972; Quellette & King 1977)
- 0.021 (20°C, Hartley & Graham-Bryce 1980)
- 0.053 (Spencer 1982; Worthing 1983, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
- 0.0213 (20°C, selected exptl. value, Kim 1985)
- 0.021, 0.410, 5.10, 46, 320 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)
- $\log (P_s/\text{Pa}) = 14.977 - 4966.6/(T/K)$; measured range 36.4–95.6°C (solid, gas saturation-GC, Rordorf 1989)
- $\log (P_L/\text{Pa}) = 11.811 - 3816.5/(T/K)$; measured range 96.6–151°C (liquid, gas saturation-GC, Rordorf 1989)
- 0.031 (supercooled liquid P_L value, GC-RT correlation, Hinckley et al. 1990)
- $\log (P_L/\text{Pa}) = 11.88 - 3995/(T/K)$ (supercooled liquid, GC-RT correlation, Hinckley et al. 1990)
- 0.022 (20°C, selected, Taylor & Spencer 1990)
- 0.040 (20°C, Montgomery 1993)
- 0.0533 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 0.13, 0.13 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)
- $\log (P_L/\text{Pa}) = -3870/(T/K) + 12.11$ (supercooled liquid, linear regression of literature data, Shen & Wania 2005)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 150 (gas stripping-GC, Warner et al. 1987)
- 154 (WERL Treatability Database, Ryan et al. 1988)
- 112 (20°C, calculated-P/C, Suntio et al. 1988)
- 845.4 (calculated-P/C, Jury et al. 1990)
- 17.8 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)
- 233 (Montgomery 1993)
- 29.75 (wetted wall column-GC, Altschuh et al. 1999)
- 30, 38 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 5.44 (HPLC-RT correlation, Veith et al. 1979, 1980; Veith & Kosian 1983)
- 3.87 (quoted, Rao & Davidson 1980)
- 5.27 (HPLC-RT correlation, McDuffie 1981)
- 4.40–5.50 (Montgomery 1993)
- 5.27, 5.58 (quoted, Hansch et al. 1995)
- 6.02 (shake flask/slow stirring-GC, Simpson et al. 1995)
- 5.24 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 6.10, 5.94 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

- 7.705*, 7.643 (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
- $\log K_{OA} = -3.95 + 3455/(T/K)$, temp range 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
- 7.64, 7.76 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Bioconcentration Factor, $\log BCF$:

- 1.81 (beef biotransfer factor $\log B_b$, correlated- K_{OW} , Kenaga 1980)
- 1.48 (vegetation, correlated- K_{OW} , Lichtenstein 1960; Nash 1974)
- 2.49 (milk biotransfer factor $\log B_m$, correlated- K_{OW} , Saha 1969)
- 4.26 (oysters, wet wt. basis, Wilson 1963)
- 3.26 (bluegill, field tests, Andrews et al. 1966)
- 3.41 (soft clam, Butler 1971)
- 3.45–4.33 (estuarine fish for 96-h exposure, Schimmel et al. 1976)
- 3.76–3.92 (spot fish, whole body 24-d exposure, Schimmel et al. 1976)
- 3.67 (spot fish, edible tissue 24-d exposure, Schimmel et al. 1976)
- 3.58 (mosquito fish, Callahan et al. 1979)
- 3.56, 3.87 (spot fish for 72-h test, 96-h test. Callahan et al. 1979)

- 4.57, 4.32 (snails, algae, Callahan et al. 1979)
 3.98, 4.30 (fathead minnow, 32-d exposure, 276-d exposure, Veith et al. 1979, 1980)
 4.30 (sheepshead minnow, Veith et al. 1979)
 4.24, 3.33 (fish: flowing water, static water; Kenaga 1980; Kenaga & Goring 1980)
 3.65, 3.90 (estimated-S, K_{OW} , Bysshe 1982)
 3.11–3.56 (earthworm, Gish & Hughes 1982)
 3.98, 4.30 (fathead minnow, Veith & Kosian 1983)
 4.03 (clam fat, 60-d expt., Hartley & Johnson 1983)
 4.26 (oysters, Biddinger & Gloss 1984)
 3.90, 3.90, 3.90 (oyster, pinfish, sheepshead minnow, Zaroogian et al. 1985)
 4.30, 4.33 (measured for fathead minnow, sheepshead minnow, Zaroogian et al. 1985)
 3.93 (oyster, Zaroogian et al. 1985)
 3.98 (calculated, Isnard & Lambert 1988)
 4.11 (selected, Chessells et al. 1992)
 4.14; 4.406, 4.112 (fish, steady-state, quoted lit.; calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)
 4.23, 6.15 (oyster, uptake 6 months: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.30, 5.85 (fathead minnow, uptake 276-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.98; 3.67 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

- 4.48 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a)
 4.38 (screening model calculations, Jury et al. 1987b)
 4.34 (calculated- K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
 3.81 (Jury et al. 1990)
 5.21 (estimated-QSAR and SPARC, Kollig 1993)
 4.38 (Montgomery 1993)
 4.38 (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 4.76 (soil, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: measured rate constant $k = 3.0 \text{ d}^{-1}$ (Glotfelty et al. 1984; quoted, Glotfelty et al. 1989);
 calculated rate constant $k = 5.0 \text{ d}^{-1}$ (Glotfelty et al. 1989).

Photolysis:

Oxidation: $t_{1/2} = 5.2\text{--}51.7 \text{ h}$ in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order $t_{1/2} = 23.1 \text{ h}$, based on rate constant $k = 2.97 \times 10^{-2} \text{ h}^{-1}$ at pH 7.0 and 25°C (Demayo 1972; quoted, Callahan et al. 1979; Kollig et al. 1987; Howard et al. 1991);

rate constant $k = 61 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993)

$t_{1/2} = 5.4 \text{ d}$ at pH 2, $t_{1/2} = 0.96 \text{ d}$ at pH 7 in natural waters (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 360\text{--}1567 \text{ h}$, based on unacclimated aerobic soil grab sample test data (Castro & Yoshida 1971; quoted, Howard et al. 1991);

rate constant $k = 0.011 \text{ d}^{-1}$ by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);

estimated $t_{1/2} = 220 \text{ d}$ in soil (Jury et al. 1990);

aqueous anaerobic $t_{1/2} = 1440\text{--}6268 \text{ h}$, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 15 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 60 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 9.8\text{--}59.0 \text{ h}$, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $<1 \text{ d}$ (Kelly et al. 1994).

Surface water: persistence up to 2 wk in river water (Eichelberger & Lichtenberg 1971);

$t_{1/2} = 38$ d in surface waters in the Netherlands in case a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 23.1$ – 129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991)

Biodegradation $t_{1/2}$ (aerobic) = 15 d, $t_{1/2}$ (anaerobic) = 60 d, hydrolysis $t_{1/2} = 5.4$ d at pH 2, $t_{1/2} = 0.96$ d at pH 7 in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2} = 23.1$ – 129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} \sim 2$ – 5 yr persistence in soil (Nash & Woolson 1967);

estimated persistence of 2 yr in soil (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

Best estimated $t_{1/2} = 0.91$ yr, true value is between 0.86–0.97 yr when heptachlor was incorporated to 7.5 cm depth in an experimental field (Freeman et al. 1975)

persistence of >24 months (Wauchope 1978);

$t_{1/2} < 10$ d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988);

first-order $t_{1/2} = 63$ d from biodegradation rate constant $k = 0.011$ d⁻¹ by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);

field $t_{1/2} = 0.3$ d in moist fallow soil (Glottfelty 1981; quoted, Nash 1983);

microagroecosystem $t_{1/2} = 3$ d in moist fallow soil (Nash 1983);

measured dissipation rate $k = 0.28$ d⁻¹ (Nash 1983; quoted, Nash 1988);

estimated dissipation rate $k = 1.0$ and 0.20 d⁻¹ (Nash 1988);

reported $t_{1/2} = 9$ – 10 months in soil (Hartley & Kidd 1987; quoted, Montgomery 1993);

$t_{1/2} = 23.1$ – 129.4 h, based on hydrolysis half-lives (Kollig et al. 1987 and Chapman & Cole 1982; quoted, Howard et al. 1991);

estimated biodegradation $t_{1/2} = 220$ d in soil (Jury et al. 1990);

selected field $t_{1/2} = 250$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);

$t_{1/2} = 9$ – 10 months when used at agricultural rates (Tomlin 1994)

$t_{1/2} = 7$ – 14 yr in soil (Geyer et al. 2000)

Biota: biochemical $t_{1/2} = 2000$ d from screening model calculations (Jury et al. 1987b).

TABLE 18.1.1.50.1

Reported aqueous solubilities and octanol-air partition coefficients of heptachlor at various temperatures

Aqueous solubility				log K_{OA}	
Biggar & Riggs 1974				Shoeib & Harner 2002	
shake flask-GC				generator column-GC/MS	
t/°C	S/g·m ⁻³	S/g·m ⁻³	S/g·m ⁻³	t/°C	log K_{OA}
particle size	0.01μ	0.05μ	5.0μ		
15			0.100	5	8.5093
25	0.030	0.125	0.180	10	8.2625
35			0.315	15	7.9873
45			0.490	20	7.7934
				25	7.7046
				25	7.643
log $K_{OA} = A + B/(T/K)$					
				A	-3.951
				B	3455
enthalpy of phase change					
$\Delta H_{OA}/(kJ\ mol^{-1}) = 66.2$					

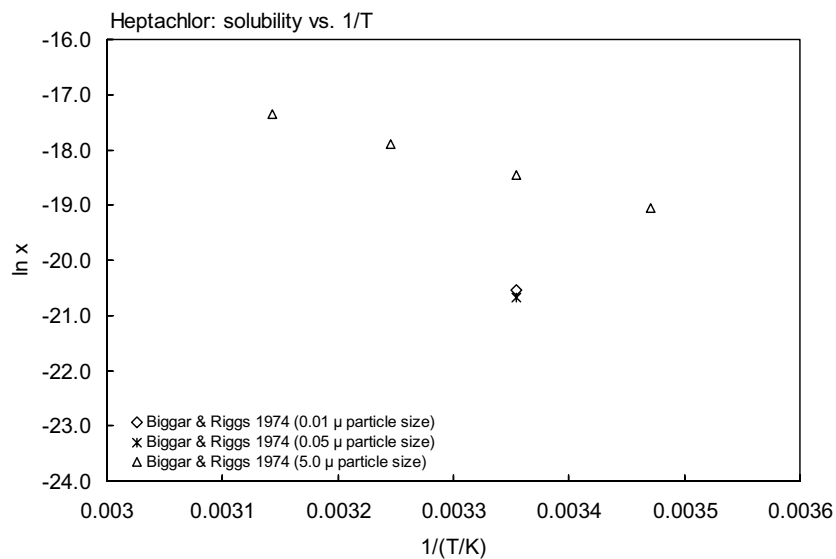


FIGURE 18.1.1.50.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for heptachlor.

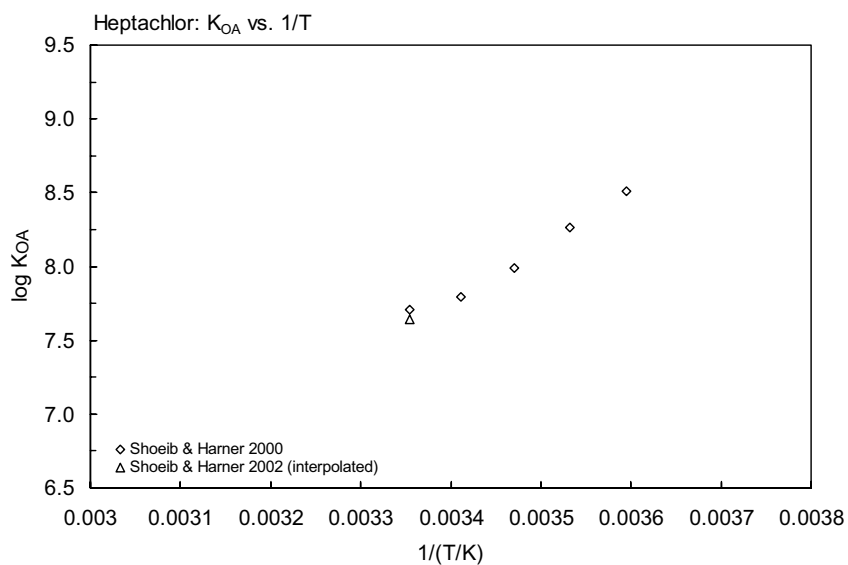
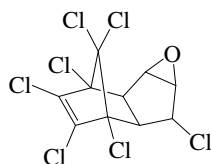


FIGURE 18.1.1.50.2 Logarithm of K_{OA} versus reciprocal temperature for heptachlor.

18.1.1.51 Heptachlor epoxide



Common Name: Heptachlor epoxide

Synonym: β -Heptachlorepoxyde, Epoxyheptachlor, HCE, Velsicol 53-CS-17

Chemical Name: 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-methanoindan; 2,3,4,5,7,8-hexa-hydro-2,5-methano-2*H*-indeno(1,2*b*)oxirene

Uses: a degradation product of heptachlor

CAS Registry No: 1024-57-3

Molecular Formula: $C_{10}H_5Cl_7O$

Molecular Weight: 389.317

Melting Point ($^{\circ}C$):

160 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

317.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.506 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} (J/mol K):

61.56 (Plato 1972)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0474 (mp at $160^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.035 (25–29 $^{\circ}C$, shake flask-GC, Park & Bruce 1968)

0.025, 0.120, 0.20* (shake flask-GC, particle size: 0.01, 0.05 and 5.0 μ , measured range 15–45 $^{\circ}C$, Biggar & Riggs 1974)

0.35 (generator column-GC/ECD, Weil et al. 1974)

0.20–0.35 (Mills et al. 1982; Mabey et al. 1982)

0.90 (Zaroogian et al. 1985)

0.275 (Montgomery 1993)

5.91 (supercooled liquid value, 20–25 $^{\circ}C$, Majewski & Capel 1995)

0.60, 0.0004 (predicted-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

7.0, 5.06 (supercooled liquid: LDV derivation of literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.045 (estimated, Mabey et al. 1982)

0.00256 (estimated, Howard 1991)

3.47×10^{-4} (20 $^{\circ}C$, Montgomery 1993)

0.0997 (supercooled liquid value, 20–25 $^{\circ}C$, Majewski & Capel 1995)

0.013, 0.022 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Shen & Wania 2005)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

395 (calculated-P/C, Mabey et al. 1982)

3.42 (gas-stripping, Warner et al. 1987)

3.25 (Montgomery 1993)

65.5 (20–25 $^{\circ}C$, Majewski & Capel 1995)

- 2.13 (wetted-wall column-GC, Altschuh et al. 1999)
 2.1, 1.7 (LDV literature-derived value, FAV final adjusted value, Shen & Wania 2005)

Octanol/Water Partition Coefficient, log K_{OW} :

- 4.43 (Briggs 1981)
 5.40 (HPLC-RT correlation, Veith et al. 1979)
 4.56 ± 0.05 (shake flask, Noegrohati & Hammers 1992)
 3.65 (Montgomery 1993)
 5.40, 5.42 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Octanol/Air Partition Coefficient, log K_{OA} :

- 8.62, 8.59 (LDV literature-derived value, FAV final-adjusted value, Shen & Wania 2005)

Bioconcentration Factor, log BCF:

- 3.30, 4.90, 3.78 (algae, snail, mosquito-microcosm expt., Lu & Metcalf 1975)
 3.23 (mussel, Ernst 1977)
 4.16 (fathead minnows, 32-d flow-through aquarium, Veith et al. 1979)
 2.03 (microorganism, calculated- K_{OW} , Mabey et al. 1982)
 3.37 (clam fat, 60-d expt., Hartley & Johnson 1983)
 2.93 (oyster, Zaroogian et al. 1985)
 3.87, 3.89 (sheepshead minnow, pinfish, mussel and oyster, Zaroogian et al. 1985)
 -1.45 (beef biotransfer factor log B_b , correlated- K_{OW} , Travis & Arms 1988)
 3.88 (calculated- K_{OW} , Howard 1991)
 >4.16, >5.14 (fathead minnow, uptake 32-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.16; 4.10 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 2.34 (sediment, calculated- K_{OW} , Mabey et al. 1982)
 2.00 (bentonite clay, Hill & McCarty 1967)
 4.0–4.3 (suspended solids in river, Frank 1981)
 3.89 (calculated-S, Howard 1991)
 4.32 (calculated, Montgomery 1993)
 3.98 (activated carbon-water, Blum et al. 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 60$ h from a model river (Howard 1991).

Photolysis:

Oxidation: oxidation rate Constants, $k < 3600 \text{ M}^{-1} \text{ h}^{-1}$ for reaction with singlet oxygen, and $k = 20 \text{ M}^{-1} \text{ h}^{-1}$ for reaction with peroxy radical (Mabey et al. 1982)

$t_{1/2} = 6\text{--}60$ h, based on estimated photooxidation half-life in air (Howard et al. 1991)

Hydrolysis: not expected to be important (Howard et al. 1991)

Biodegradation: $t_{1/2} \sim 25$ d under anaerobic conditions when incubated with thick digester sludge at 35°C (Howard 1991)

$t_{1/2}$ (aerobic) = 792–13248 h, based on aerobic soil grab sample data; $t_{1/2}$ (anaerobic) = 24–168 h, based on soil and freshwater mud grab sample data (Howard et al. 1991)

$t_{1/2}$ (aerobic) = 33 d, $t_{1/2}$ (anaerobic) = 1 d in natural waters (Capel & Larson 1995)

Biotransformation: rate constant for bacterial transformation in water $k = 3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}$ (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 1.5$ d for vapor-phase reaction with photochemically produced hydroxyl radical (Howard 1991)

$t_{1/2} = 6\text{--}60$ h, based on estimated photooxidation half-life in air (Howard et al. 1991)

Surface water: $t_{1/2} = 35$ d in lower Rhine River in case a first order reduction process may be assumed (Zoeteman 1980)

$t_{1/2} = 792\text{--}13248$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

biodegradation $t_{1/2}(\text{aerobic}) = 33$ d, $t_{1/2}(\text{anaerobic}) = 1$ d in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 24\text{--}26496$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 792\text{--}13248$ h, based on aerobic soil grab sample data (Howard et al. 1991)

$t_{1/2} \sim 3$ yr in soil (Geyer et al. 2000)

Biota:

TABLE 18.1.1.51.1

Reported aqueous solubilities of heptachlor epoxide at various temperatures

Biggar & Riggs 1974			
shake flask-GC			
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$S/\text{g}\cdot\text{m}^{-3}$	$S/\text{g}\cdot\text{m}^{-3}$
particle size	0.01 μ	0.05 μ	5.0 μ
15			0.110
25	0.025	0.120	0.200
35			0.350
45			0.600

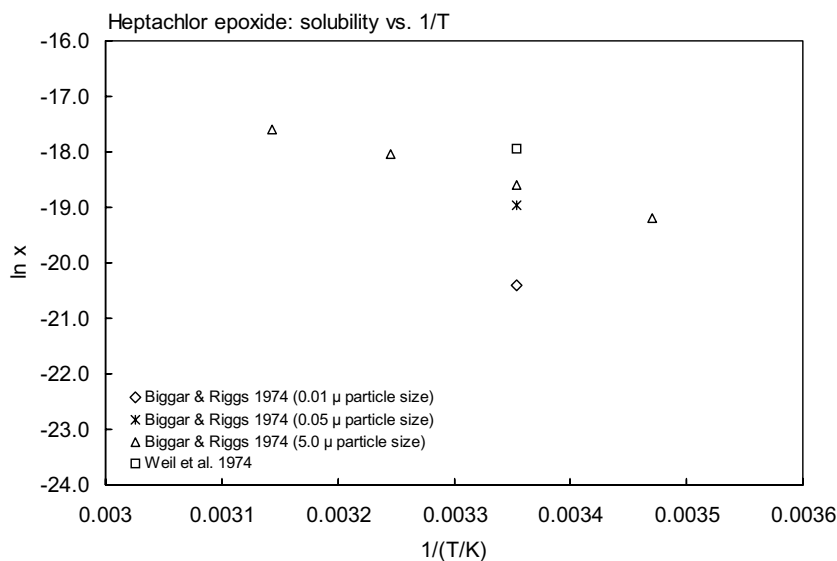
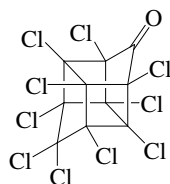


FIGURE 18.1.1.51.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for heptachlor epoxide.

18.1.1.52 Kepone



Common Name: Kepone

Synonym: Chlordecone, CIBA 8514

Chemical Name: 1,2,3,4,5,5,6,7,9,10,10-dodecachlorooctahydro-1,3,4-metheno-2-cyclobuta-[*c,d*]-pentalone

CAS Registry No: 143-50-0

Uses: Insecticide/Fungicide

Molecular Formula: $C_{10}Cl_{10}O$

Molecular Weight: 490.636

Melting Point ($^{\circ}C$):

350 (dec. Howard 1991; Montgomery 1993; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

369.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 6.5×10^{-4} (mp at $350^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.0 ($100^{\circ}C$, Günther et al. 1968)

2.7 (quoted Weil 1978 unpublished result, Kilzer et al. 1979)

3.0 ($20^{\circ}C$, Kenaga & Goring 1978, Kenaga 1980)

7.6 ($24^{\circ}C$, shake flask-nephelometry/fluor., Hollifield 1979; quoted, Howard 1991; Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

3.0×10^{-5} (Kilzer et al. 1979; quoted, Howard 1991; Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.00153 (calculated-P/C, Howard 1991)

0.00311 (calculated-P/C, Montgomery 1993)

0.00140 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.50 (Di Toro 1985)

5.41 (shake flask, $\log P$ database, Hansch & Leo 1987)

4.07 (calculated, Montgomery 1993)

5.41 (recommended, Sangster 1993)

5.44 (selected, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

4.04 (shrimp, 10–20 d exposure, Bahner et al. 1979)

3.92 (Kenaga & Goring 1980)

4.0, 2.65, 2.76 (sludge, algae, golden ide, Freitag et al. 1985)

3.84 (oyster, Zaroogian et al. 1985)

4.39, 4.46 (oyster, calculated- K_{ow} & models, Zaroogian et al. 1985)

- 4.39, 4.47 (sheephead minnow, calculated- K_{OW} & models, Zaroogian et al. 1985)
 3.85 (Spot *Leiostomus xanthurus*, 19-d uptake and 28-d clearance studies, Fisher et al. 1986)
 4.11 (grass shrimp *Palaemonetes pugio*, 16-d uptake and 21-d clearance studies, Fisher & Clark 1990)
 3.04–3.34 (fathead minnow, quoted, Howard 1991)
 3.19, 3.09, 2.84, 0.91 (*Cyprinodon variegatus*, *Leiostomus xanthurus*, *Palaemonetes pugio*, *Callinectes sapidus*, quoted, Howard 1991)
 3.36–3.99 (Atlantic menhaden, Howard 1991)
 4.34–4.78 (Atlantic silversides, Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.38–3.41 (calculated, Howard 1991)
 4.74 (calculated, Montgomery 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 3.8\text{--}46$ yr predicted for evaporation from a river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1991).

Photolysis: indefinite in air (Howard et al. 1991).

Oxidation:

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aerobic aqueous $t_{1/2} = 7488$ to 17,280 h (312 d to 2 yr), based on aerobic aquatic microcosm study, anaerobic $t_{1/2} = 29,952\text{--}69,120$ h (1248 d to 8 yr) based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Kinetic data of spot *Leiostomus xanthurus* in 19-d uptake and 28-d clearance studies (Fisher et al. 1986)

- $k_1 = 0.273\text{ d}^{-1}$; $k_2 = 0.037\text{ d}^{-1}$ with $t_{1/2} = 18.7$ d, uncontaminated water + 4% ration contaminated food,
 $k_1 = 217.3\text{ d}^{-1}$; $k_2 = 0.03\text{ d}^{-1}$ with $t_{1/2} = 23.5$ d, contaminated water + 4% ration uncontaminated food,
 $k_1 = 0.265\text{ d}^{-1}$; $k_2 = 0.037\text{ d}^{-1}$ with $t_{1/2} = 18.7$ d, uncontaminated water + 8% ration contaminated food,
 $k_1 = 185.5\text{ d}^{-1}$; $k_2 = 0.027\text{ d}^{-1}$ with $t_{1/2} = 25.5$ d, contaminated water + 8% ration uncontaminated food,
 $k_1 = 0.262\text{ d}^{-1}$; $k_2 = 0.032\text{ d}^{-1}$ with $t_{1/2} = 21.5$ d, contaminated food (4% ration) then water,
 $k_1 = 214\text{ d}^{-1}$; $k_2 = 0.023\text{ d}^{-1}$ with $t_{1/2} = 29.9$ d, contaminated water then food (a 4% ration)
 $k_1 = 0.292\text{ d}^{-1}$; $k_2 = 0.043\text{ d}^{-1}$ with $t_{1/2} = 16.2$ d, contaminated food (a 8% ration) then water,
 $k_1 = 154\text{ d}^{-1}$; $k_2 = 0.020\text{ d}^{-1}$ with $t_{1/2} = 35.4$ d, contaminated water then food (a 8% ration)

Kinetic data of grass shrimps in 16-d uptake and 21-d clearance studies (Fisher & Clark 1990)

- $k_1 = 0.475\text{ d}^{-1}$; $k_2 = 0.017\text{ d}^{-1}$ with $t_{1/2} = 28$ d, uncontaminated water + 4% ration contaminated food,
 $k_1 = 175\text{ d}^{-1}$; $k_2 = 0.014\text{ d}^{-1}$ with $t_{1/2} = 47.8$ d, contaminated water + 4% ration uncontaminated food,
 $k_1 = 0.499\text{ d}^{-1}$; $k_2 = 0.019\text{ d}^{-1}$ with $t_{1/2} = 36.3$ d, contaminated food (4% ration) then water,
 $k_1 = 182\text{ d}^{-1}$; $k_2 = 0.013\text{ d}^{-1}$ with $t_{1/2} = 51.5$ d, contaminated water then food (a 4% ration)
 $k_1 = 0.399\text{ d}^{-1}$; $k_2 = 0.021\text{ d}^{-1}$ with $t_{1/2} = 32.3$ d, contaminated food (a 8% ration) then water,
 $k_1 = 170\text{ d}^{-1}$; $k_2 = 0.011\text{ d}^{-1}$ with $t_{1/2} = 63.7$ d, contaminated water then food (a 4% ration)

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 438,000$ to 4.2×10^7 h or 50–200 yr (Howard et al. 1991).

Surface water: $t_{1/2} = 7488$ to 17,280 h or 312 d to 2 yr, based on aerobic aquatic microcosm study of soil and water grab samples (Howard et al. 1991).

Ground water: estimated $t_{1/2} = 14,976$ to 34,560 h (624 d to 4 yr) based on aqueous aerobic biodegradation (Howard et al. 1991).

Sediment:

Soil: estimated $t_{1/2} = 7488$ to 17,280 h (312 d to 2 yr) based on aerobic aquatic microcosm study (Howard et al. 1991).

Biota: clearance $t_{1/2} = 28$ d (shrimp, 10–20 d exposure, Bahner 1977)

Clearance $t_{1/2} = 16.2\text{--}35.4$ d for spot *Leiostomus xanthurus* (Fisher et al. 1986):

$t_{1/2}(4W) = 18.7$ d for kepone contaminated water + uncontaminated food at 4% ration

$t_{1/2}(4F) = 23.5$ d for uncontaminated water + kepone contaminated food at 4% ration

$t_{1/2}(8W) = 18.7$ d for kepone contaminated water + uncontaminated food at 8% ration,

$t_{1/2}(8F) = 25.5$ d for uncontaminated water + kepone contaminated food at 8% ration

$t_{1/2}(4FW\text{-}food) = 21.5$ d for dietary accumulation in combined exposure (food-water) at 4% ration

$t_{1/2}(4FW\text{-}water) = 29.9$ d for dietary accumulation in combined exposure (water-food) at 4% ration

$t_{1/2}(8FW\text{-}food) = 16.2$ d for dietary accumulation in combined exposure (food-water) at 8% ration

$t_{1/2}(8FW\text{-}water) = 35.4$ d for dietary accumulation in combined exposure (water-food) at 8% ration

Clearance $t_{1/2} = 32.3\text{--}63.7$ d for grass shrimps *Palaemonetes pugio* (Fisher & Clark 1990):

$t_{1/2}(4W) = 47.8$ d for kepone contaminated water + uncontaminated food at 4% ration

$t_{1/2}(4F) = 40.6$ d for uncontaminated water + kepone contaminated food at 4% ration

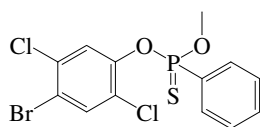
$t_{1/2}(4FW\text{-}food) = 36.3$ d for dietary accumulation in combined exposure (food-water) at 4% ration

$t_{1/2}(4FW\text{-}water) = 51.5$ d for dietary accumulation in combined exposure (water-food) at 4% ration

$t_{1/2}(8FW\text{-}food) = 32.3$ d for dietary accumulation in combined exposure (food-water) at 8% ration

$t_{1/2}(8FW\text{-}water) = 63.7$ d for dietary accumulation in combined exposure (water-food) at 8% ration

18.1.1.53 Leptophos



Common Name: Leptophos

Synonym: Abar, Phosvel, VCS-506

Chemical Name: *O*-(4-bromo-2,5-dichlorophenyl) *O*-methyl phenylphosphorothioate

Uses: insecticide

CAS Registry No: 21609-90-5

Molecular Formula: C₁₃H₁₀BrCl₂O₂PS

Molecular Weight: 412.066

Melting Point (°C):

71 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.53 (25°C, Merck Index 1989)

Molar Volume (cm³/mol):

317.8 (calculated-Le Bas method at normal boiling point)

269.3 (calculated-density)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.354 (mp at 71°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.03 (shake flask-UV, Carringer et al. 1975)

0.03 (20°C, GC, Freed 1976)

0.0047 (20°C, shake flask-GC, Chiou et al. 1977)

2.4 (Martin & Worthing 1977; Kenaga 1980; Kenaga & Goring 1980; Khan 1980)

0.07 (20°C, shake flask-GC, Bowman & Sans 1979)

0.0047 (20–25°C, shake flask-GC, Freed et al. 1979)

0.005 (20–25°C, shake flask-GC, Kanazawa 1981)

0.021 (20°C, shake flask-GC, Bowman & Sans 1983a, b)

0.03 (Budavari 1989)

Vapor Pressure (Pa at 25°C or as indicated):

3.07 × 10⁻⁶ (20°C, NIEHS 1975; quoted, Freed et al. 1977)

2.27 × 10⁻⁵ (30°C, NIEHS 1975; quoted, Freed et al. 1977)

3.07 × 10⁻⁶ (20–25°C, Freed et al. 1979)

3.00 × 10⁻⁶ (20°C, selected, Suntio et al. 1988)

0.0002 (Merck Index 1989)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.27 (20°C, calculated-P/C, Mackay & Shiu 1981)

0.25 (20°C, calculated-P/C, Suntio et al. 1988)

Octanol/Water Partition Coefficient, log K_{ow}:

6.30 (NIEHS 1975; quoted, Freed et al. 1977)

6.31 (20°C, shake flask-GC, Chiou et al. 1977)

6.31 (Hansch & Leo 1979)

4.32 (20°C, shake flask-GC, Kanazawa 1981)

- 5.88 (22°C, shake flask-GC, Bowman & Sans 1983b)
 6.31 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

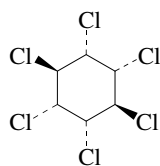
- 2.81 (*Daphnia magna*, wet wt. basis, Macek et al. 1979)
 2.88, 3.16 (fish: flowing water, static water; Kenaga 1980; Kenaga & Goring 1980)
 2.58, 2.86 (calculated-S, calculated- K_{OC} , Kenaga 1980)
 3.78 (*Pseudorasbora parva*, Kanazawa 1981)
 3.16 (mosquito fish, wet wt. basis, De Bruijn & Hermens 1991)
 3.78 (topmouth gudgeon, wet wt. basis, De Bruijn & Hermens 1991)
 2.88 (fish, reported as log BAF_w , LeBlanc 1995)

Sorption Partition Coefficient, log K_{OC} :

- 3.97 (soil, Carringer et al. 1975)
 3.43 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
 3.97, 4.45 (reported as log K_{OM} , estimated as log K_{OM} , Magee 1991)
 4.50 (soil, calculated-MCI χ , Sabljic et al. 1995)
 3.88, 4.74 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

18.1.1.54 Lindane (γ -HCH)

Common Name: Lindane (γ -HCH)

Synonym: Aalindan, Aficide, Agrisol G-20, Agrocide, Agronexit, Ambocide, Ameisenatod, Ameisenmittelmerck, Aparacin, Aparasin, Aphtiria, Aplidal, Arbitex, BBX, Ben-hex, Bentox 10, Benzenehexachloride, Benzex, Bexol, BHC, γ -BHC, Celanex, Chloran, Chloresene, Codechine, DBH, Detmol-extrakt, Detox 25, Devoran, Dolmix, ENT 7796, Entomoxan, Exagama, Forlin, Gallogama, Gamacid, Gamaphex, Gamene, Gamiso, Gamahexa, Gamalin, Gammexane, Gammopaz, Gexane, HCCH, Gyben, HCCH, HCH, γ -HCH, Heclotox, Hexa, Hexachlor, γ -Hexachlor, Hexachloran, γ -Hexachloran, Hexachlorane, γ -Hexachlorane, γ -Hexachlorobenzene, Hexamul, Hexapurdre, Hexatox, Hexaverm, Hexdow, Hexicide, Hexyclan, HGI, Hortex, Inexit, Isaton, Isotox, Jacutin, Kokotine, Kotol, Kwell, Lendine, Lentox, Lidenal, Lindafor, Lindagam, Lindagrain, Lindagranox, γ -Lindine, Lindapoudre, Lindatox, Lindosep, Lintox, Lorexane, Milbol 49, Mszycol, NA 2761, NCI-C00204, Neo-scabidol, Nexen FB, Nexit, Nexit-stark, Nexol-E, Nicochloran, Novigam, Omnitox, Ovadziak, Owadziak, Pedraczak, Pflanzol, Quellada, Silvanol, Soprocide, Spritz-rapidin, Spruehpflanzol, Streunex, Tap 85, TBH, Tri-6, Viton

Chemical Name: 1,2,3,4,5,6-hexachlorocyclohexane; γ -hexachlorocyclohexane; γ -1,2,3,4,5,6-hexachloro-cyclohexane; $1\alpha,2\alpha,3\beta,4\alpha,5\alpha,6\beta$ -1,2,3,4,5,6-hexachloro-cyclohexane

Uses: insecticide and pesticide with contact, stomach, and respiratory action to control a broad spectrum of phytophagous and soil inhibiting insects, public health pests, and animal ectoparasites.

CAS Registry No: 58-89-9

Molecular Formula: $C_6H_6Cl_6$

Molecular Weight: 290.830

Melting Point ($^{\circ}C$):

112.5 (Slade 1945; Howard 1991; Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

323.4 (Howard 1991; Montgomery 1993; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.87 (Montgomery 1993)

Molar Volume (cm^3/mol):

243.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

101.13 (Spencer & Cliath 1970)

76 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.4 (Rordorf 1989)

22.13 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

41.4 (Plato & Glasgow 1969)

58.0 (Rordorf 1989)

61.1 (Hinckley et al. 1990; Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.12 ($20^{\circ}C$, Suntio et al. 1988)

0.138 (Mackay et al. 1986)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

10 ($20^{\circ}C$, Slade 1945; Günther et al. 1968; Spencer 1973, 1982)

7.3* (shake flask-UV spectrophotometry, measured range $25-45^{\circ}C$, Richardson & Miller 1960)

0.50–6.60 (particle size of $0.04-5\mu$, shake flask-GC, room temp., Robeck et al. 1965)

5.7 (partition coefficient, Atkins & Eggleton 1971)

7.52 ± 0.041 (shake flask-centrifuge/GC, Masterton & Lee 1972)
 7.40, 5.75 (28°C, shake flask-centrifuge, membrane filter-GC, maximum 0.1 µm particle size, Kurihara et al. 1973)
 6.61, 6.24 (28°C, shake flask-centrifuge, sonic and centrifuge-GC, max. 0.05 µm particle size, Kurihara et al. 1973)
 12 (26.5°C, Bhavnagary & Jayaram 1974)
 0.15*, 0.60*, 6.80* (shake flask-GC, for different particle sizes: 0.01µ, 0.05µ, 5.0µ, measured range 15–45°C, Biggar & Riggs 1974)
 7.8 (generator column-GC/ECD, Weil et al. 1974)
 0.15 (Martin & Worthing 1977; Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
 2.0 (shake flask-nephelometry, Hollifield 1979)
 7.88 (20–25°C, shake flask-GC, Kanazawa 1981)
 6.50, 9.20 (15, 25°C, shake flask method, average values of 6–7 laboratories, OECD 1981)
 10 (20–25°C, shake flask-GC, Platford 1981)
 10.3 (shake flask-GC/ECD, Malaiyandi et al. 1982)
 9.50, 7.9–8.2 (shake flask-GC/ECD: Milli-Q water, environmental surface waters, Saleh et al. 1982)
 6.11 (20°C, Deutsche Forschungsgemeinschaft 1983; Ballschmiter & Wittlinger 1991; Fischer et al. 1991; 1993)
 7.87 (24°C, shake flask-GC, Chiou et al. 1986)
 7.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 $\log [S_L/(\text{mol/L})] = 2.220 - 1237/(T/K)$ (liquid, Passivirta et al. 1999)
 67.77, 71.84 (supercooled liquid S_L : derivation of literature-derived value, final-adjusted value, Xiao et al. 2004)
 $\log [S_L/(\text{mol m}^{-3})] = -749.8/(T/K) + 2.78$ (supercooled liquid, linear regression of literature data, Xiao et al. 2004)
 $\log [S_L/(\text{mol m}^{-3})] = -788.4/(T/K) + 2.04$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4.0, 18.7, 64 (20, 40, 60°C static method, Slade 1945)
 0.001253* (20°C, effusion manometer, measured range 0–90°C, Balson 1947)
 $\log (P/\text{mmHg}) = 15.515 - 6020/(T/K)$; temp range 50–90°C, (effusion manometer, Balson 1947)
 0.00435* (20°C, gas-saturation-GC, measured range 20–40°C, Spencer & Cliath 1970)
 $\log (P/\text{mmHg}) = 13.544 - 5288/(T/K)$, temp range 20–40°C (gas saturation-GC, Spencer & Cliath 1970)
 0.00413 (20°C, Partition coefficient, Atkins & Eggleton 1971)
 0.0213 (20°C, Demozay & Marechal 1972)
 0.00125 (20°C, Martin 1972, Melnikov 1971, Spencer 1973; Montgomery 1993)
 0.0028 (20°C, estimated from diffusion rate, Zimmerli & Marek 1974)
 0.0026 (20°C, estimated-relative loss rate, Dobbs & Grant 1980)
 0.00426 (20°C, volatilization rate, Burkhard & Guth 1981)
 $\log (P/\text{mmHg}) = 15.515 - 6020/(T/K)$ (Gückel et al. 1982)
 0.166 (GC-RT correlation, Watanabe & Tatsukawa 1989)
 0.0056 (20°C, Hartley & Kidd 1987; Worthing & Walker 1987, Worthing & Hance 1991; Tomlin 1994)
 0.107, 0.0654 (P_{GC} by GC-RT correlation, different stationary phases, Bidleman 1984)
 0.0552 (supercooled liquid P_L , converted from literature P_S with ΔS_{fus} Bidleman 1984)
 0.00321; 0.00368 (20°C, gas saturation-GC, gas saturation-mixed bed-GC, Kim 1985)
 0.00435 (20°C, GC-RT correlation, Kim 1985)
 6.70×10^{-3} * (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
 $\log (P_S/\text{Pa}) = 15.096 - 5148.9/(T/K)$; measured range 45–113°C (solid, gas saturation-GC, Rordorf 1989)
 $\log (P_L/\text{Pa}) = 12.05 - 3970.1/(T/K)$; measured range 115–171°C (liquid, gas saturation-GC, Rordorf 1989)
 0.0552, 0.0649 (supercooled P_L , converted from literature P_S with different ΔS_{fus} values, Hinckley et al. 1990)
 0.107, 0.0706 (P_{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)
 $\log (P_L/\text{Pa}) = 11.15 - 3680/(T/K)$ (GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990; quoted, Boehncke et al. 1996))
 7.426×10^{-4} (Howard 1991)
 0.0044 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0145, 0.0398, 0.1035 (supercooled liquid values at 10°C, 20°C, 30°C, calculated from Hinckley et al. 1990; Cotham & Bildeman 1992)

0.0094* (20°C, gas saturation-GC/ECD, measured range -30 to 30°C, Wania et al. 1994; quoted, Boehncke et al. 1996)

$\log (P_s/\text{Pa}) = 16.99 - 5566/(T/K)$, temp range -30 to +30°C (solid, gas saturation-GC, Wania et al. 1994)

0.00737* (Knudsen effusion method, measured range 19.63–53.07°C, Boehncke et al. 1996)

0.00383 (20°C, interpolated from vapor pressure eq. $\ln (P/\text{Pa}) = (34.53 \pm 0.21) - (11754 \pm 72)/(T/K)$, temp range 20–50°C, Boehncke et al. 1996)

0.0104* (torsion and Knudsen-effusion methods, measured range 310–384 K, Giustini et al. 1998)

$\log (P/\text{kPa}) = (11.23 \pm 0.50) - (4832 \pm 150)/(T/K)$; temp range 310–384 K (torsion and Knudsen-effusion methods, Giustini et al. 1998)

0.189, 0.131; 0.0167 (quoted supercooled liquid P_L : calculated, GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_L/\text{Pa}) = 13.80 - 4330/(T/K)$, (supercooled liquid, Passivirta et al. 1999)

0.0776, 0.0759 (supercooled liquid P_L : LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)

$\log (P_L/\text{Pa}) = -3890/(T/K) + 11.94$ (supercooled liquid, linear regression of literature data, Xiao et al. 2004)

$\log (P_L/\text{Pa}) = -3905/(T/K) + 11.98$ (supercooled liquid, final adjusted eq., Xiao et al. 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.005 (calculated-P/C, Mackay & Leinonen 1975)

0.22 (gas stripping, Atkins & Eggleton 1971)

0.32 (24°C, calculated-P/C, Chiou et al. 1980)

0.018–0.55 (calculated-P/C, Mabey et al. 1982)

0.124 (20°C, volatilization rate, Burkhard & Guth 1981)

0.27–0.32 (calculated-P/C, Mackay & Shiu 1981)

0.05 (calculated-P/C, Lyman et al. 1982; quoted, Suntio et al. 1988)

0.0486 (calculated-P/C, Thomas 1982)

0.322 (calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)

0.158 (calculated-P/C, Mackay et al. 1986)

0.202, 0.234 (23°C, wetted-wall column-GC/ECD, Fendinger & Glotfelty 1988)

1.49 (WERL Treatability Database, Ryan et al. 1988)

0.129 (20°C, calculated-P/C, Suntio et al. 1988)

0.322 (calculated-P/C, Taylor & Glotfelty 1988)

0.199, 0.209 (22–24°, fog chamber-concentration ratio-GC/ECD, Fendinger et al. 1989)

0.0486 (20°C, Lyman et al. 1990; quoted, Hemond & Fechner 1994)

0.10 (calculated-P/C, Ballshmiter & Wittlinger 1991; Fischer et al. 1991)

0.296 (calculated-P/C, Howard 1991)

0.353* (distilled water, gas stripping-GC/ECD, measured range 0.5–45°C, Kucklick et al. 1991)

$\log [H/(\text{Pa}\cdot\text{m}^3 \text{ mol}^{-1})] = -2382/(T/K) + 7.54$, temp range: 0.5–45°C (gas stripping-GC/ECD, Kucklick et al. 1991, McConnell et al. 1993)

0.0627, 0.137, 0.363, 0.996, 2.57 (0.5, 10, 23, 35, 45°C, gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)

$\log [H/(\text{Pa}\cdot\text{m}^3 \text{ mol}^{-1})] = -2703/(T/K) + 8.68$; temp range 0.5–45°C (gas stripping-GC/ECD, artificial seawater, Kucklick et al. 1991)

0.17 (calculated-P/C, Calamari et al. 1991)

0.10, 1.50 (calculated-P/C, Fischer et al. 1991)

25.9 (calculated-bond contribution method, Meylan & Howard 1991)

0.13 (20°C), 0.20, 0.339, 0.363 (23°C), 0.158 (Iwata et al. 1993)

0.121 at 8°C in Green Bay, 0.242 at 18.9°C in Lake Michigan, 0.236 at 18.5°C in Lake Huron, 0.301 at 22.3°C in Lake Erie and 0.301 at 22.3°C in Lake Ontario (concn ratio-GC, McConnell et al. 1993)

0.0246 (20°C, Montgomery 1993)

0.520 (wetted wall column-GC, Altschuh et al. 1999)

$\log [H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 11.58 - 3049/(T/K)$ (Passivirta et al. 1999)

0.18* (20°C, air stripping-GC, measured range 10–40°C, Jantunen et al. 2000)

$\log [H/(\text{Pa m}^3/\text{mol})] = 9.51 - 3005/(T/K)$; temp range 10–40°C (gas stripping, Jantunen et al. 2000)
 0.258 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{\text{AW}} = 3.715 - 2254/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 0.14* (20°C, dynamic headspace-GC, DHS method, measured range 5–35°C, Sahsuvar et al. 2003)
 0.15* (20°C, gas stripping-GC, BS method, measured range 5–35°C, Sahsuvar et al. 2003)
 0.14* (20°C, mean value of DHS and BS methods, temp range 5–35°C, Sahsuvar et al. 2003)
 $\log [H/(\text{Pa m}^3/\text{mol})] = 10.14 - 3208/(T/K)$; temp range 5–35°C (Sahsuvar et al. 2003)
 0.159, 0.193 (20, 23°C, dynamic equilibrium system-GC/MS, measured range 278–293 K, Feigenbrugel et al. 2004)
 0.269, 0.309 (LDV literature-derived value, FAV final adjusted value, Xiao et al. 2004)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -2940/(T/K) + 9.29$ (LDV linear regression of literature data, Xiao et al. 2004)
 $\log [H/(\text{Pa m}^3/\text{mol})] = -3117/(T/K) + 9.94$ (FAV final adjusted eq., Xiao et al. 2004)
 0.165* (seawater, dynamic equilibrium system-GC/MS, measured range 278–293 K, Xiao et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.72 (shake flask-GC, Kurihara et al. 1973)
 3.65 (HPLC-RT correlation, Sugiura et al. 1979)
 3.85 (HPLC-RT correlation, Veith et al. 1979)
 2.81 (Rao & Davidson 1980)
 3.66 (shake flask-GC, concn. ratio, Kanazawa 1981)
 3.62 (HPLC- k' correlation, McDuffie 1981)
 3.25 (shake flask-GC, Platford 1982)
 3.53 (shake flask-GC/FID, Hermens & Leeuwangh 1982)
 3.90 (Elgar 1983)
 3.61 (Hansch & Leo 1985)
 3.67 (HPLC-RT correlation, Eadsforth 1986)
 3.00 (HPLC-RT correlation, De Kock & Lord 1987)
 3.57 (shake flask-GC, Kishi & Hashimoto 1989)
 3.688 ± 0.021 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
 3.51 (shake flask-GC, Noegrohati & Hammers 1992)
 3.20–3.89 (Montgomery 1993)
 5.32 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
 3.55 (recommended, Sangster 1993)
 3.52 (RP-HPLC-RT correlation, Finizio et al. 1997)
 3.72* ± 0.01 (shake flask-slow stirring-GC, measured range 5–35°C, Paschke & Schüürmann 1998)
 3.80; 3.71 (quoted lit.; calculated, Passivirta et al. 1999)
 3.70, 3.83 (LDV literature-derived value, FAV final-adjusted value, Xiao et al. 2004)
 $\log K_{\text{OW}} = 282.2/(T/K) + 2.78$ (LDV linear regression of literature data, Xiao et al. 2004)
 $\log K_{\text{OW}} = 533.2/(T/K) + 2.04$ (LDV linear regression of literature data, Xiao et al. 2004)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

7.70 (calculated- $K_{\text{OW}}/K_{\text{AW}}$, Wania & Mackay 1996)
 8.08 (calculated, Finizio et al. 1997)
 7.847*, 7.849 (gas saturation-GC/MS, calculated, measured range 5–25°C, Shoeib & Harner 2002)
 $\log K_{\text{OA}} = -3.61 + 3415/(T/K)$, temp range: 5–25°C (gas saturation-GC, Shoeib & Harner 2002)
 7.84, 7.74 (LDV literature derived value, FAV final adjusted value, Xiao et al. 2004)
 $\log K_{\text{OA}} = 3415/(T/K) - 3.61$ (LDV linear regression of literature data, Xiao et al. 2004)
 $\log K_{\text{OA}} = 3521/(T/K) - 4.07$ (FAV final adjusted eq., Xiao et al. 2004)

Bioconcentration Factor, $\log \text{BCF}$:

-1.78 (beef biotransfer factor $\log B_b$, correlated- K_{OW} , Radeleff et al. 1952; Kenaga 1980;)
 -0.41 (vegetation, correlated- K_{OW} , Lichtenstein 1959; Voerman & Besemer 1975)
 -2.60 (milk biotransfer factor $\log B_m$, correlated- K_{OW} , Saha 1969)

- 2.15, 2.34 (Voerman & Tammes 1969)
 1.83, 3.24 (brine shrimp, silverside fish, Matsumura & Benezet 1973)
 1.98, 2.26 (brine shrimp in water, brine shrimp in sand, Matsumura & Benezet 1973)
 3.21 (northern brook silverside fish to lindane residues on sand, Matsumura & Benezet 1973)
 2.75, 2.66 (fish, snail, Metcalf et al. 1973)
 2.26 (fathead minnow, Canton et al. 1975)
 2.23, 2.65 (zooplankton, Hamelink & Waybrant 1976)
 2.00 (mussels, steady state, Ernst 1977)
 1.92, 2.34, 1.80, 2.69 (pink shrimp, pinfish, grass shrimp, sheepshead minnow, Schimmel et al. 1977; quoted, Howard 1991)
 2.88, 2.45, 2.65, 2.97 (golden orfe, carp, brown trout, guppy, Sugiura et al. 1979)
 2.68 (fathead minnow, Veith et al. 1979)
 2.26 (fathead minnow, 32-d exposure, Veith et al. 1979; Veith & Kosian 1983)
 2.51, 2.75 (fish: flowing water, static water; Kenaga 1980b; Kenaga & Goring 1980)
 3.26, 1.73 (calculated-S, K_{OC} , Kenaga 1980)
 -0.26 (average beef fat diet, Kenaga 1980b)
 2.67, 2.25 (fathead minnow, 30-d exposure, 32-d exposure, Veith et al. 1980)
 3.10 (topmouth gudgeon, Kanazawa 1981)
 2.19 (mussel, quoted average, Geyer et al. 1982)
 3.10 (topmouth gudgeon, Kanazawa 1983)
 3.42 (clam fat, 60-d exptl., Hartley & Johnson 1983)
 2.38, 2.46 (algae: exptl., calculated, Geyer et al. 1984)
 2.26 (fathead minnow, Davies & Dobbs 1984)
 2.38, 2.88, 2.91 (algae, fish, activated sludge, Klein et al. 1984)
 2.38, 2.57, 2.91 (algae, golden ide, activated sludge, Freitag et al. 1985)
 2.89–3.32 mean 3.08; 2.94–5.46 mean 3.30 (*p,p'*-DDE, rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study in 2 tanks with different water concn, Oliver & Niimi 1985)
 3.32, 3.20; 3.00 (rainbow trout: kinetic BCF, steady-state BCF; Lake Ontario field BCF, Oliver & Niimi 1985)
 2.50 (*Salmo gairdneri* Richardson fry, Ramamoorthy 1985)
 2.78, 2.73, 2.78; 2.61 (mussel, pinfish, sheepshead minnow; calculated- K_{OW} and models, Zaroogian et al. 1985)
 2.38, 2.67 (quoted values: mussel, sheepshead minnow, Zaroogian et al. 1985)
 2.76; 2.43 (salmon fry in humic water April 1982; Oct. 1983, at steady state, Carlberg et al. 1986)
 2.42, 2.84; 2.45–3.18 (salmon fry in lake water, quoted lit. values, Carlberg et al. 1986)
 2.33 (*Daphnia magna*, wet wt. basis, Korte & Freitag 1986)
 3.53 (azalea leaves, Bacci & Gaggi 1987)
 2.38 (paddy field fish, Soon & Hock 1987)
 4.30 (zooplankton, chum salmon, Kawano et al. 1988)
 3.53, 5.88 (dry leaf, wet leaf, Bacci et al. 1990)
 2.33 (*Daphnia magna*, Geyer et al. 1991)
 2.09, 2.70, 2.29, 2.34 (zebrafish: egg, embryo, yolk sac fry, juvenile, Gorge & Nagel 1990)
 1.96 (calculated, Banerjee & Baughman 1991)
 2.93, 2.96 (*Brachydanio rerio*, Butte et al. 1991)
 2.67 (selected, Chessells et al. 1992)
 1.58 (*Hydrilla*, Hinman & Klaine 1992)
 2.16–2.57 (rainbow trout in early life stages on wet wt. basis, Vigano et al. 1992; quoted, Devillers et al. 1996)
 3.77–3.85 (rainbow trout in early life stages on lipid basis, Vigano et al. 1992)
 2.65 ± 2.23; 1.63–3.63 (aquatic organisms, wet wt basis, average value; range, Geyer et al. 1997)
 4.04 (aquatic organisms, lipid basis, Geyer et al. 1997)
 2.65; 2.606, 2.676 (fish, steady-state, quoted lit.; calculated-MCI χ , calculated- K_{OW} , Lu et al. 1999)

Sorption Partition Coefficient, log K_{OC} :

- 2.96 (soil, Hamaker & Thompson 1972; Kenaga 1980a, b; Kenaga & Goring 1980)
 4.09 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
 3.40 (soil, Kenaga 1980)
 2.87 (average of 3 soils, HPLC-RT, McCall et al. 1980)

- 4.64 (calculated-S, Mill et al. 1980)
 3.03 (av. for 3 soils, Rao & Davidson 1982)
 2.88, 2.95, 2.74; 2.87 (Commerce soil, Tracy soil, Catlin soil; average soil, McCall et al. 1980)
 4.07, 2.90 (estimated-S, K_{OW} , Lyman 1982)
 3.11 (soil, screening model simulations, Jury et al. 1984, 1987a, b; Jury & Ghodrati)
 4.30, 3.50 (field data of river sediment, calculated- K_{OW} , Oliver & Charlton 1984)
 3.03 (Rao & Davidson 1982, Howard 1991)
 2.63–3.18 (reported as log K_{OM} , Mingelgrin & Gerstl 1983)
 3.04 (Caron et al. 1985)
 1.63 (log K_p with first-order adsorption rate 0.088 h^{-1} , Miller & Weber 1986)
 3.11, 2.82 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
 0.114 (screening model calculations, Jury et al. 1987b)
 4.02 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)
 3.47 (calculated- K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
 2.38 (average of 2 soils, Kanazawa 1989)
 2.84, 3.11, 3.08, 2.98, 2.88 (5 soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
 3.11 (soil, Mackay & Stiver 1991)
 3.04 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.38–3.52 (quoted lit. range, Montgomery 1993)
 3.00 (calculated-MCI χ , Sabljic et al. 1995)
 3.00; 4.57 (soil, quoted exptl.; estimated-general model, Gramatica et al. 2000)
 5.40; 3.30 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
 3.02, 3.00, 3.08 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
 3.49 (sediment: organic carbon $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2} = 191 \text{ d}$ was estimated from water (Mackay & Leinonen 1975, quoted, Howard 1991)
 estimated $t_{1/2} > 200 \text{ d}$ (Callahan et al. 1979);
 $t_{1/2}(\text{exptl.}) = 3.2 \text{ d}$ in nonstirred water and $t_{1/2}(\text{exptl.}) = 1.5 \text{ d}$ in stirred water from 4.5 cm deep distilled water at 24°C (Chiou et al. 1980; quoted, Howard 1991);
 estimated half-lives: 3.4 d in nonstirred water and 2.3 d in stirred water (Chiou et al. 1980);
 $t_{1/2} = 22 \text{ d}$, estimated from a model river of 1 m deep flowing 1 m/s with a wind speed of 3 m/s (Lyman et al. 1982; quoted, Howard 1991);
 initial $k = 4.4 \times 10^{-2} \text{ h}^{-1}$ and predicted $k = 1.4 \times 10^{-2} \text{ h}^{-1}$ from soil with $t_{1/2} = 49.5 \text{ h}$ (Thomas 1982);
 $t_{1/2}(\text{calc}) = 2760 \text{ h}$ from water (Thomas 1982);
 measured rate constant $k(\text{exptl.}) = 3.0 \text{ d}^{-1}$ (Glottfelty et al. 1984; quoted, Glottfelty et al. 1989);
 calculated rate constant $k = 0.01 \text{ d}^{-1}$ (Glottfelty et al. 1989);
 $t_{1/2} = 266 \text{ d}$ from lab. and field experiments (Jury et al. 1984; quoted, Spencer & Cliath 1990);
 half-lives in soil surfaces at $20 \pm 1^\circ\text{C}$: $t_{1/2} = 5.5$ to 15.9 d in peat soil and $t_{1/2} = 2.7$ to 6.7 d in sandy soil;
 half-lives in plant surfaces at $20 \pm 1^\circ\text{C}$: $t_{1/2} = 0.56 \text{ d}$ in bean, $t_{1/2} = 0.40 \text{ d}$ in turnips and $t_{1/2} = 0.31 \text{ d}$ in oats (Dörfler et al. 1991).
- Photolysis: $k_p(\text{aq.}) = 1.429 \times 10^{-2} \text{ d}^{-1}$ for photolysis in natural waters (Malaiyandi et al. 1982)
 $k_p(\text{aq.}) = 8.9 \times 10^{-4} \text{ h}^{-1}$ for Milli-Q water, $k_p = 4.1 \times 10^{-3} \text{ h}^{-1}$ for natural surface water samples from eutrophic pond, $k_p = 3.9 \times 10^{-4} \text{ h}^{-1}$ from eutrophic pond, $k_p = 4.5 \times 10^{-4} \text{ h}^{-1}$ from oligotrophic rock quarry and the half-lives were 779, 169, 1791, and 1540 h, respectively, under direct sunlight (Saleh et al. 1982; quoted, Howard 1991)
- Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 $k_{OH} = 6.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a $t_{1/2} \sim 2.3 \text{ d}$ (Atkinson 1987; quoted, Howard 1991)
 $k(\text{aq.}) = 4.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to DBCP) with hydroxyl radical in aqueous solutions at pH 2.9 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)
 $k(\text{aq.}) \leq 0.04 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.3 and 23°C , with a $t_{1/2} \geq 10 \text{ d}$ at pH 7 (Yao & Haag 1991).

calculated tropospheric lifetimes due to gas-phase reaction with OH radical was estimated to be about 7 d (Atkinson et al. 1992)

$k_{\text{OH}}(\text{aq.}) = (5.8 \pm 1.9) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ (Fenton with reference to DBCP); and $k = (5.2 \pm 0.9) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ (photo-Fenton with reference to DBCP) for the reaction with hydroxyl radicals in aqueous solutions at pH 2.9 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992)

Hydrolysis: $k(\text{neutral}) = 1.6 \times 10^{-4} \text{ h}^{-1}$ indicating that neutral hydrolysis is unimportant, rate constants of 7.5×10^{-3} , 8.99×10^{-4} , and $1.07 \times 10^{-3} \text{ h}^{-1}$ corresponded to half-lives of 92, 771 and 648 h in natural surface water samples from eutrophic pond, dystrophic reservoir and oligotrophic rock quarry, respectively (Saleh et al. 1982; quoted, Howard 1991)

$k(\text{neutral}) = (1.2 \pm 0.2) \times 10^{-4} \text{ h}^{-1}$ with a calculated $t_{1/2} = 206 \text{ d}$ at pH 7 (Ellington et al. 1987, 1988; quoted, Montgomery 1993)

$t_{1/2} = 42 \text{ yr}$ at pH 8 and 5°C (Ngabe et al. 1993)

$t_{1/2} = 191 \text{ d}$ at pH 7, and $t_{1/2} = 11 \text{ h}$ at pH 9 at 22°C (Tomlin 1994)

$t_{1/2} = 240 \text{ d}$ at pH 2, $t_{1/2} = 210 \text{ d}$ at pH 7 and $t_{1/2} = 0.015 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: $k = 0.0026 \text{ d}^{-1}$ by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);

$t_{1/2}$ = half-life of 266 d (soil, Jury et al. 1987);

$t_{1/2} = 3$ to 30, 30 to 300 d and $>300 \text{ d}$ for river, lake and ground water, respectively (Zoeteman et al. 1980; quoted, Howard 1991);

$t_{1/2} = 266 \text{ d}$ for 100-d leaching screening test in 0–10 cm depth of soil (Jury et al. 1984, 1987a, b; Jury & Ghodrati 1989)

$t_{1/2}(\text{aerobic}) = 31 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 5.9 \text{ d}$ in natural waters (Capel & Larson 1995)

$t_{1/2}(\text{calc}) = (20.4 \pm 0.1) \text{ h}$ in sewage sludge from experiments S1–S3 (Buser & Müller 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 3.13 \text{ h}^{-1}$; $k_2 = 0.0313 \text{ h}^{-1}$ (mussels, Ernst 1977)

$k_1 = 130 \text{ d}^{-1}$; $k_2 = 0.063 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_1 = 14, 179, 196 \text{ h}^{-1}$ (zebrafish: egg, yolk sac fry, juvenile, Gorge & Nagel 1990)

$k_2 = 0.06 \text{ h}^{-1}$ (*Chironomus riparius*-water only system, Lydy et al. 1992)

$k_2 = 0.0661 \text{ h}^{-1}$ (*Chironomus riparius*-screened system, Lydy et al. 1992)

$k_2 = 0.08 \text{ h}^{-1}$ (*Chironomus riparius*-3% organic carbon system, Lydy et al. 1992)

$k_2 = 0.0661 \text{ h}^{-1}$ (*Chironomus riparius*-15% organic carbon system, Lydy et al. 1992)

$k_1 = 9.0\text{--}26.4 \text{ h}^{-1}$; $k_2 = 0.04\text{--}0.18 \text{ h}^{-1}$ (rainbow trout in early life stages on wet wt. basis, Vigano et al. 1992)

$k_1 = 180\text{--}939 \text{ h}^{-1}$; $k_2 = 0.031\text{--}0.13 \text{ h}^{-1}$ (rainbow trout in early life stages on lipid basis, Vigano et al. 1992)

Half-Lives in the Environment:

Air: $t_{1/2} \sim 2.3 \text{ d}$ was estimated, based on rate constant $6.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{s}^{-1}$ for the vapor-phase reaction with hydroxyl radical in air (Howard 1991);

calculated tropospheric lifetimes due to gas-phase reaction with OH radical was estimated to be about 7 d (Atkinson et al. 1992);

atmospheric transformation lifetime was estimated to be $<1 \text{ d}$ (Kelly et al. 1994)

Lifetime of 13 d was estimated for atmospheric reaction with OH radical in the tropics (Schreitmüller and Ballschmiter 1995);

half-lives in the Great Lake's atmosphere. $t_{1/2} = 7.9 \pm 1.2 \text{ yr}$ at Eagle Harbor, $t_{1/2} = 4.3 \pm 0.5 \text{ yr}$ at Sleeping Bear Dunes and $t_{1/2} = 4.9 \pm 0.5 \text{ yr}$ at Sturgeon Point, when accounting the agricultural application effects, half-lives are, $t_{1/2} = 9.1 \pm 1.3 \text{ yr}$ at Eagle Harbor, $t_{1/2} = 4.6 \pm 0.4 \text{ yr}$ at Sleeping Bear Dunes and $t_{1/2} = 5.4 \pm 0.4 \text{ yr}$ at Sturgeon Point (Buehler et al. 2004)

Surface water: $t_{1/2} = 10\text{--}138 \text{ d}$ in various locations in the Netherlands in case a first order reduction process may be assumed; and $t_{1/2} = 3\text{--}30 \text{ d}$ in rivers and $t_{1/2} = 30\text{--}300 \text{ d}$ in lakes (Zoeteman et al. 1980);

hydrolysis $t_{1/2}(\text{exptl}) = 92 \text{ h}$, $t_{1/2}(\text{calc}) = 89 \text{ h}$ for Roselawn Cemetery Pond at pH 9.3; $t_{1/2}(\text{exptl}) = 771 \text{ h}$, $t_{1/2}(\text{calc}) = 578 \text{ h}$ for Cross Lake at pH 7.3; $t_{1/2}(\text{exptl}) = 648 \text{ h}$, $t_{1/2}(\text{calc}) = 231 \text{ h}$ for Indiana Quarry at pH 7.8; photolysis half-lives for direct sunlight during July and adjusted for mid-winter: $t_{1/2} = 779 \text{ h}$, 1560 h for Milli-Q water at pH 6.98, $t_{1/2} = 169 \text{ h}$, 339 h for Roselawn Pond at pH 9.3, $t_{1/2} = 1791 \text{ h}$, 3590 h for Cross Lake and $t_{1/2} = 1540 \text{ h}$, 3090 h for Indiana Quarry (Saleh et al. 1982);

$t_{1/2} > 10 \text{ d}$ for direction reaction with ozone in water at 23°C and pH 7 (Yao & Haag 1991);

hydrolysis $t_{1/2}$ = 191 d at pH 7, and $t_{1/2}$ = 11 h at pH 9 at 22°C (Tomlin 1994).

Biodegradation $t_{1/2}$ (aerobic) = 31 d, $t_{1/2}$ (anaerobic) = 5.9 d, hydrolysis $t_{1/2}$ = 240 d at pH 2, $t_{1/2}$ = 210 d at pH 7 and $t_{1/2}$ = 0.015 d at pH 12 in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2}$ –300 d (Zoeteman et al. 1980).

Sediment:

Soil: $t_{1/2}$ ~ 2 yr persistence in soil (Nash & Woolson 1967; quoted, Kaufman 1976);

persistence of 3 yr in soil (Edwards 1973; quoted, Morrill et al. 1982);

$t_{1/2}$ > 50 d and subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988)

First-order $t_{1/2}$ = 266 d in soil from biodegradation rate constant k = 0.0026 d⁻¹ by die-away test in soil (Rao & Davidson 1980; quoted, Scow 1982);

field $t_{1/2}$ = 0.3 d in moist fallow soil (Glottfelty 1981; quoted, Nash 1983);

microagroecosystem $t_{1/2}$ = 1–4 d in moist fallow soil (Nash 1983); measured dissipation rate of 0.16 d⁻¹ (Nash 1983; quoted, Nash 1988);

estimated dissipation rate of 0.20, 0.10 d⁻¹ (Nash 1988);

biodegradation $t_{1/2}$ = 266 d (soil, Jury et al. 1984, 1987);

first-order adsorption rate 0.088 h⁻¹ (Miller & Weber 1986; quoted, Brusseau & Rao 1989);

half-lives in soil surfaces at 20 ± 1°C: $t_{1/2}$ = 5.5 to 15.9 d in peat soil and $t_{1/2}$ = 2.7 to 6.7 d in sandy soil (Dörfler et al. 1991); reported $t_{1/2}$ = 266 d in soil (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);

reaction $t_{1/2}$ = 266 d (Mackay & Stiver 1991);

selected field $t_{1/2}$ = 400 d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996);

$t_{1/2}$ = 14 d for soil depth < 5 cm, $t_{1/2}$ = 90 d for 5–20 cm and $t_{1/2}$ = 180 d for >20 cm (Dowd et al. 1993)

$t_{1/2}$ = 14.5 and 16.0 yr for control and sludge-amended Luddington soils, respectively (Meijer et al. 2001)

Biota: $t_{1/2}$ = 22.1 h (mussels, Ernst 1977);

$t_{1/2}$ = 46 d (rainbow trout, Oliver & Niimi 1985);

biological half-lives for fishes: $t_{1/2}$ = 11 d for trout muscle, $t_{1/2}$ = 1 d for goldfish, $t_{1/2}$ < 1 d for sunfish and $t_{1/2}$ = 4 d for guppy (Niimi 1987);

$t_{1/2}$ = 678 h (azalea leaves, Bacci & Gaggi 1987);

biochemical $t_{1/2}$ = 266 d from screening model calculations (Jury et al. 1987b);

half-lives in plant surfaces at 20 ± 1°C: $t_{1/2}$ = 0.56 d in bean, $t_{1/2}$ = 0.40 d in turnips and $t_{1/2}$ = 0.31 d in oats (Dörfler et al. 1991);

elimination half-lives in the midge (*Chironomus riparius*) under varying sediment conditions: $t_{1/2}$ = 11 h for water only system, $t_{1/2}$ = 10 h for screened system, $t_{1/2}$ = 9 h for 3% organic carbon system and $t_{1/2}$ = 6 h for 15% organic carbon system (Lydy et al. 1992);

half-lives $t_{1/2}$ (in h) = 12.09 × L(% lipid) – 10.09, in different aquatic organisms (Geyer et al. 1997).

Average $t_{1/2}$ = 90 d (for pesticides used in conjunction with forest management, Neary et al. 1993).

TABLE 18.1.1.54.1

Reported aqueous solubilities of lindane at various temperatures

Richardson & Miller 1960		Biggar & Riggs 1974				OECD 1981	
shake flask-UV spectro.		shake flask-GC				shake flask method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	S/g·m ⁻³	S/g·m ⁻³	t/°C	S/g·m ⁻³
		particle size	0.01μ	0.05μ	5.0μ		
25	7.30	15	0.075	0.330	2.150	15	6.50
35	12.0	25	0.150	0.600	6.80	25	9.20
45	14.0	35	0.315	0.950	11.40		
		45	0.575	1.450	15.20		

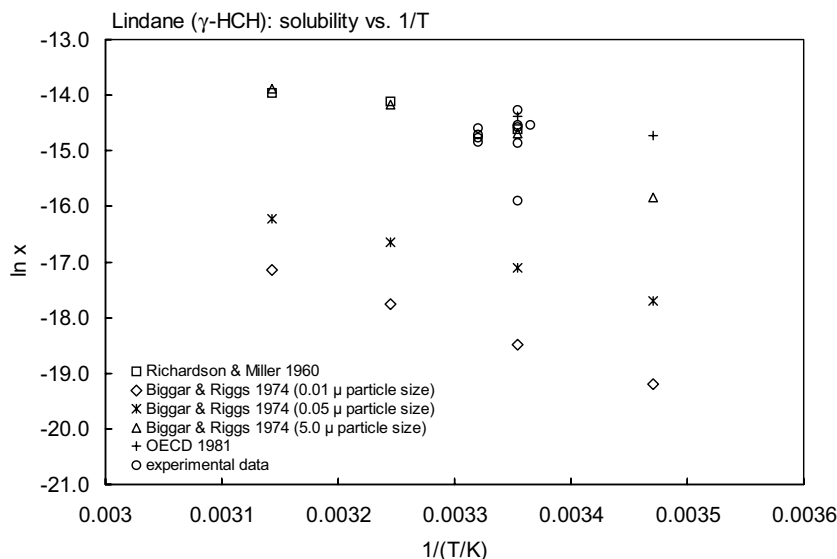


FIGURE 18.1.1.54.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for lindane (γ -HCH).

TABLE 18.1.1.54.2

Reported vapor pressures of lindane at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \log (T/K) & (4) \end{array} \quad \begin{array}{ll} \ln P = A - B/(T/K) & (1a) \\ P = A - B/(C + t/^{\circ}\text{C}) & (2a) \end{array}$$

1.

Balson 1947		Spencer & Cliath 1970		Wania et al. 1994		Boehncke et al. 1996	
effusion manometer		gas saturation-GC		gas saturation-GC		Knudsen effusion	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
0	3.87×10^{-5}	20	0.004346	-30	1.701×10^{-6}	19.63	0.00374
10	2.40×10^{-4}	30	0.0171	-20	7.353×10^{-6}	24.95	0.00737
20	1.253×10^{-3}	40	0.0608	-10	8.435×10^{-5}	28.42	0.0116
30	6.00×10^{-3}	30 wet	0.0167	0	4.489×10^{-4}	33.58	0.0225
40	0.0257	30 dry	0.0173	10	2.209×10^{-3}	37.82	0.0281
50	0.1027			20	9.395×10^{-3}	37.86	0.0386
60	0.3706	eq. 1	P/mmHg	30	4.192×10^{-2}	43.26	0.0718
70	1.233	A	13.544			48.06	0.123
80	3.853	B	5288			53.07	0.217
90	11.479			eq. 1	P/Pa	20	3.83×10^{-3}
		$\Delta H_v = 101.13 \text{ kJ/mol}$		A	16.99		
eq. 1	P/mmHg			B	5566	eq. 1a	P/Pa
A	15.515					A	34.53
B	6020					B	11754
temp range: 60–92 $^{\circ}\text{C}$				enthalpy of sublimation:		temp range: 293–323 K	
$\Delta H_v = 115.06 \text{ kJ/mol}$		Rordorf 1989		$\Delta H_{\text{sub}} = 106.6 \text{ kJ/mol}$		enthalpy of sublimation:	
		gas saturation-GC				$\Delta H_{\text{sub}} = 97.7 \text{ kJ/mol}$	
		25	0.067				
		50	0.15				
		75	2.0				

TABLE 18.1.1.54.2 (Continued)

Balson 1947		Spencer & Cliath 1970		Wania et al. 1994		Boehncke et al. 1996	
effusion manometer		gas saturation-GC		gas saturation-GC		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		100	20.0				
		125	150				
		eq. 1	P/Pa				
		A	15.096				
		B	5148.9				
		eq. 1	P/Pa				
		A	12.05				
		B	3970.1				
2.							
Giustini et al. 1998							
torsion		torsion		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
run 1–4		run 5–8		cell K.1		cell K.2	
50	0.162	73	1.9498	37.5	0.0562	70	1.5849
54	0.245	76	2.4547	39.5	0.0776	71.5	1.9055
59	0.407	79	3.3113	44.5	0.1023	72	1.7783
65	0.646	83	4.6774	45.0	0.1175	73.5	2.2387
69	1.148	88	7.2444	48.5	0.1622	74.5	2.3988
74	1.778	93	11.482	49.5	0.1995	75	3.0903
80	2.754	98	17.378	53.5	0.2951	80.5	4.0738
88	5.370	66	0.9550	55.0	0.3311	81	4.2658
97	11.220	69	1.5136	55.5	0.3631	84	7.0795
59	0.4074	76	2.3442	56.5	0.3981	87.5	7.0795
64	0.7244	79	3.0200	63.0	0.8318	89	9.3325
69	1.047	83	4.6774	63.5	0.8128	94	12.303
74	1.622	88	7.2444	65.5	0.9772	99.5	23.442
82	3.311	93	11.482	66.5	1.0471		
88	5.495	99	19.953				
92	8.710	68	1.2303	eq. 1	kPa	eq. 1	kPa
60	0.4074	72	1.7783	A	10.89	A	11.46
66	0.8128	77	2.7542	B	4706	B	4889
71	1.2303	82	4.3652	for temp 310.5–339.5 K		for temp 343–377 K	
76	1.8621	88	7.0795				
82	2.9512	94	13.490				
89	5.0119	101	24.547	Combining the above 4 equations, the final equation			
98	13.183	104	30.903	$\log (P/\text{kPa}) = 11.23 \pm 0.5 - (4832 \pm 150)/(T/\text{K})$			
66	0.8128	80	4.3652	for temperature range 310 to 384 K			
71	1.2303	83	5.6234	$\Delta H_{\text{sub}} = 92.5$ kJ/mol at 350 K			
76	2.0417	88	9.1201	at 25°C P = 0.0104 Pa			
81	2.8184	93	15.136				
87	4.6774	97	20.417				
92	7.7625	102	30.903				
96	11.482	106	48.978				
		111	66.069				

(Continued)

TABLE 18.1.1.54.2 (Continued)

Giustini et al. 1998							
torsion		torsion		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
eq. 1	kPa	eq. 1	kPa				
A	10.78	A	11.79				
B	4709	B	5025				
for temp 323–370 K		for temp 339–384 K					

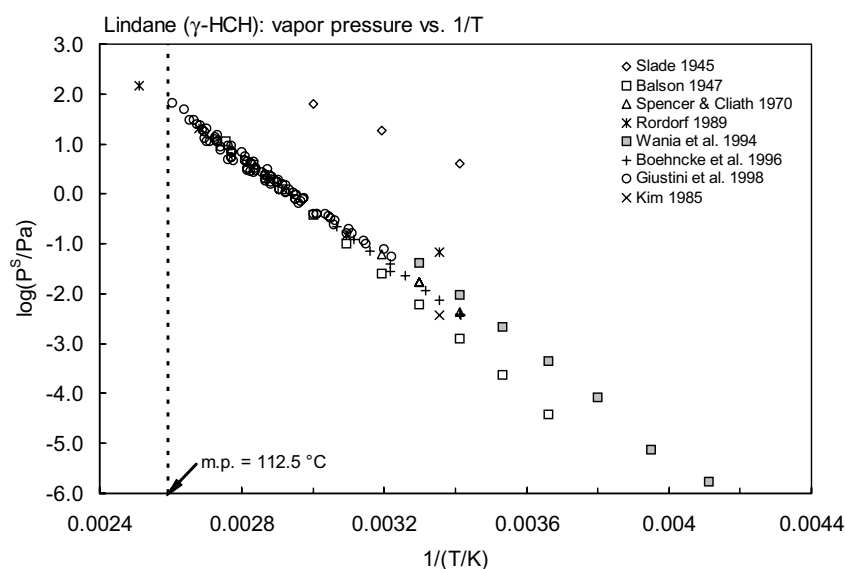
FIGURE 18.1.1.54.2 Logarithm of vapor pressure versus reciprocal temperature for lindane (γ -HCH).

TABLE 18.1.1.54.3

Reported Henry's law constants of lindane (-HCH) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln H = A - B/(T/K)$	(4)	$\log H = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

Kucklick et al. 1991		McConnell et al. 1993		Jantunen et al. 2000		Sahsuvar et al. 2003	
gas stripping-GC		concentration ratio		air stripping-GC		air stripping/dynamic HS	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
distilled water		Green Bay				dynamic headspace (DHS)	
0.5	0.0721	8.0	0.121	10	0.073	5	0.039
10	0.126		Lake Michigan	20	0.18	10	0.062
15	0.187	18.9	0.242	30	0.39	20	0.14
20	0.258		Lake Huron	35	0.58	30	0.33
23	0.339	18.5	0.236	40	0.80	35	0.60

TABLE 18.1.1.54.3 (Continued)

Kucklick et al. 1991		McConnell et al. 1993		Jantunen et al. 2000		Sahsuvar et al. 2003	
gas stripping-GC		concentration ratio		air stripping-GC		air stripping/dynamic HS	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
25	0.353		Lake Erie				
35	0.624	22.3	0.310	eq. 4a	H/(Pa m ³ /mol)		
45	1.170			A	9.51 ± 0.49	5	0.044
	22.3	0.301		B	3005 ± 145	10	0.054
eq.4a	H/(Pa m ³ /mol)					20	0.15
A	7.54 ± 0.54					30	0.34
B	2392 ± 160					35	0.55
seawater						combined - both methods	
0.5	0.0627					5	0.040
10	0.137					10	0.061
23	0.363					20	0.14
35	0.996					30	0.33
45	2.57					35	0.59
eq. 4a	H/(Pa m ³ /mol)					eq. 4a	H/(Pa m ³ /mol)
A	8.68 ± 0.96					A	10.14 ± 0.55
B	2703 ± 276					B	3208 ± 161
for temp range 0.5–23°C							

enthalpy of transfer, air-water
 $\Delta H_{WA}/(\text{kJ mol}^{-1}) = 61.4$

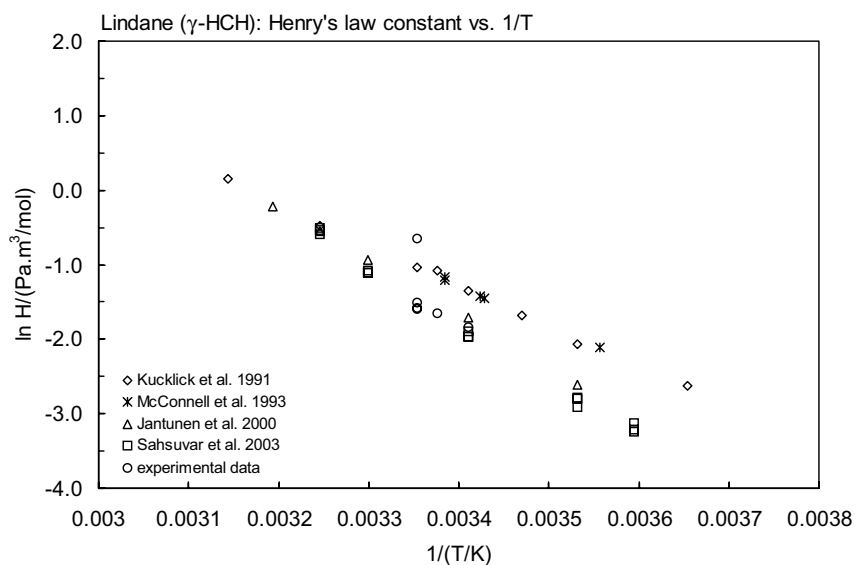
FIGURE 18.1.1.54.3 Logarithm of Henry's law constant versus reciprocal temperature for lindane (γ -HCH).

TABLE 18.1.1.54.4
Reported octanol-water and octanol-air partition coefficients
of lindane (γ -HCH) at various temperatures

$\log K_{OW}$		$\log K_{OA}$	
Paschke & Schüürmann 1998		Shoeib & Harner 2002	
shake flask-GC		generator column-GC/MS	
t/°C	$\log K_{OW}$	t/°C	$\log K_{OA}$
5	3.85	5	8.6845
25	3.72	10	8.4493
45	3.73	15	8.2181
		20	8.0643
		25	7.8473
		25	7.849
enthalpy of phase transfer:		$\log K_{OA} = A + B/(T/K)$	
$\Delta H_{OW}/(\text{kJ mol}^{-1}) = -10.40$		A	-3.611
entropy of phase transfer:		B	3415
$\Delta S_{OW}/(\text{J K}^{-1} \text{mol}^{-1}) = 52.2$		enthalpy of phase change	
		$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 65.4$	

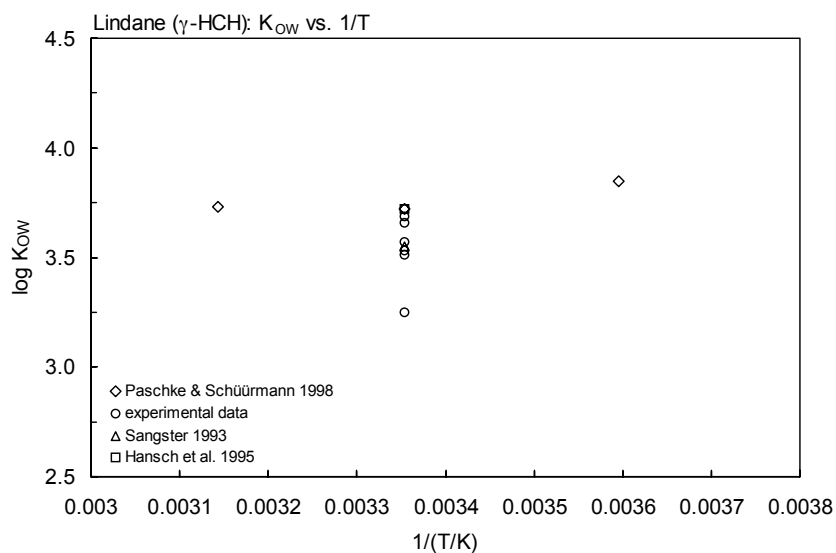


FIGURE 18.1.1.54.4 Logarithm of K_{OW} versus reciprocal temperature for lindane (γ -HCH).

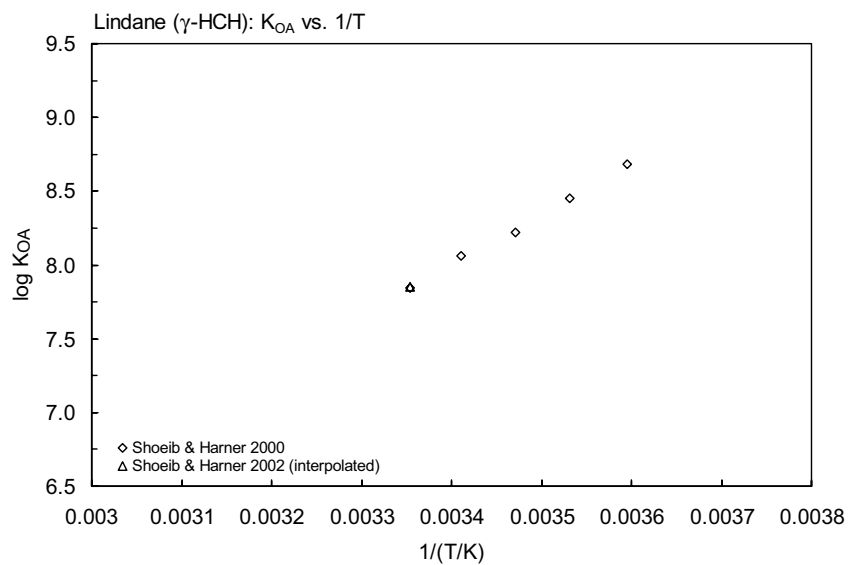
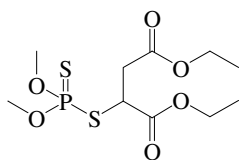


FIGURE 18.1.1.54.5 Logarithm of K_{OA} versus reciprocal temperature for lindane (γ -HCH).

18.1.1.55 Malathion



Common Name: Malathion

Synonym: American Cyanamid 4049, Calmathion, Carbethoxy malathion, Carbetovur, Carbetox, Carbofos, Carbophos, Celthion, Chemathion, Cimexan, Cythion, Detmol MA, EL 4049, Emmatos, Emmatos extra, ENT 17034, Ethiolacar, Etio, Fog 3, Formal, Forthion, Fosfothion, Fyfanon, Hithion, Karbofos, Kop-thion, Kypfos, Malacide, Malafor, Malakill, Malagran, Malamar, Malaphele, Malaphos, Malasol, Malaspray, Malatol, Malatox, Maldison, Malmed, Malphos, Maltox, Mercaptothion, MLT, Moscardia, NA 2783, NCI-C00215, Oleophosphothion, Orthomalathion, Phosphothion, Prioderm, Sadofos, Sadophos, SF 60, Siptox I, Sumitox, Tak, TM-4049, Vegfru malatox, Vetiol, Zithiol

Chemical Name: S-[1,2-bis(ethoxycarbonyl)ethyl] O,O-dimethyl phosphorodithioate

Uses: as insecticide to control sucking and chewing insects and spider mites on vegetables, fruits, ornamentals, field crops in greenhouses, gardens and forestry; also used as acaricide.

CAS Registry No: 121-75-5

Molecular Formula: C₁₀H₁₉O₆PS₂

Molecular Weight: 330.358

Melting Point (°C):

1.4 (Lide 2003)

Boiling Point (°C):

120 (at 0.2 mmHg, Melnikov 1971; Freed et al. 1977)

156–157 (at 0.7 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Density (g/cm³ at 20°C):

1.23 (25°C, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm³/mol):

319.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

145 (20°C, Macy 1948; Melnikov 1971; Spencer 1973)

145 (Spiller 1961; Willis & McDowell 1982)

145 (room temp., Spencer 1973; Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991; Hartley & Kidd 1987; Tomlin 1994)

150 (Hartley & Graham-Bryce 1980; Beste & Humburg 1983)

145 (22°C, Khan 1980)

143 (20°C, shake flask-GC, Bowman & Sans 1983a, b)

130 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

145, 164 (20°C, 30°C, Montgomery 1993)

Vapor Pressure (Pa at 2 5°C or as indicated):

1.67 × 10⁻⁴ (20°C, Wolfdietrich 1965; Melnikov 1971; Montgomery 1993)

7.33 × 10⁻⁴ (20°C, evaporation rate-gravimetric method, Gückel et al. 1973)

2.90 × 10⁻³ (Woolford 1975)

1.30 × 10⁻³ (20°C, Hartley & Graham-Bryce 1980)

5.30 × 10⁻³ (30°C, Khan 1980)

9.20 × 10⁻⁴ (20°C, GC, Seiber et al. 1981)

1.05 × 10⁻³ (gas saturation-GC, Kim et al. 1984; Kim 1985)

0.60 × 10⁻³ (20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984, Kim 1985)

- 0.67×10^{-3} (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
- 5.30×10^{-3} (30°C, Hartley & Kidd 1987; Tomlin 1994)
- 4.70×10^{-3} (GC-RT correlation, supercooled liquid value, Hinckley et al. 1990)
- 1.07×10^{-3} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 0.0063 (liquid P_L , GC-RT correlation; Donovan 1996)
- 1.07×10^{-3} (selected, Halfon et al. 1996)
- 0.00174 (gradient GC method; Tsuzuki 2000)
- 1.78×10^{-3} ; 1.35×10^{-3} ; 2.51×10^{-3} (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 0.038 (calculated-P/C, Mackay & Shiu 1981)
- 2.30×10^{-3} (20°C, calculated-P/C, Suntio et al. 1988)
- 3.22×10^{-3} (calculated-P/C, Taylor & Glotfelty 1988)
- 2.03×10^{-3} (calculated-P/C, Howard 1991)
- 4.96×10^{-4} (calculated-bond contribution method, Meylan & Howard 1991)
- 4.9×10^{-4} (23°C, quoted, Schomburg et al. 1991)
- 4.9×10^{-4} (Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.89 (20°C, shake flask-GC, Chiou et al. 1977)
- 2.89 (shake flask-GC, Freed et al. 1979; Yoshioka et al. 1986)
- 2.36 (Hansch & Leo 1979, 1985)
- 2.36 (Rao & Davidson 1980)
- 2.82 (shake flask-GC/FID, Hermens & Leeuwangh 1982)
- 2.94 (shake flask/slow-stirring method-GC, De Bruijn et al. 1991)
- 2.75 (Worthing & Hance 1991; Tomlin 1994)
- 2.36–2.89 (Montgomery 1993)
- 2.68 (RP-HPLC-RT correlation, Saito et al. 1993)
- 2.18 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
- 2.36 (recommended, Sangster 1993)
- 2.36 (selected, Hansch et al. 1995)
- 2.18 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 3.57 (RP-HPLC-RT correlation, Nakamura et al. 2001)
- 3.38 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log BCF$:

- 1.11 (carp, calculated. from k_1 of Bender 1969, McLeese et al. 1976)
- 4.74 (beef biotransfer factor $\log B_b$, correlated- K_{ow} , Pasarela et al. 1962)
- 0.867, 1.47 (lake trout, coho salmon, Howard 1991)
- 2.94, 2.98 (white shrimp, brown shrimp, Conte & Parker 1975)
- 1.57 (calculated-S, Kenaga 1980a; quoted, Howard 1991)
- 0.40 (*Triaenodes tardus*, Belluck & Felsot 1981)
- 1.54 (willow shiner, Tsuda et al. 1989)
- 0.85 (carp, wet wt. basis, De Bruijn & Hermens 1991)
- 2.00 (topmouth gudgeon, wet wt. basis, De Bruijn & Hermens 1991)
- 1.57 (Pait et al. 1992)

Sorption Partition Coefficient, $\log K_{oc}$:

- 2.45 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a)
- 3.26 (av. soils/sediments, Rao & Davidson 1980)
- 3.25 (Rao & Davidson 1980)
- 3.25 (Karickhoff 1981)
- 2.83, 3.29, 2.50 (estimated-S, calculated-S and mp, estimated- K_{ow} , Karickhoff 1981)
- 2.36 (Bomberger et al. 1983)

- 3.25 (screening model calculations, Jury et al. 1987b)
 0.903 (selected, USDA 1989; Neary et al. 1993)
 3.26 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 2.61 (Montgomery 1993)
 3.07 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 3.07; 2.76, 2.29 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
 3.08, 3.05 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)
 2.68–2.72 (sediments from San Diego Creek and Bonita Creek, shake flask-GC, Bondarenko & Gan 2004)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2} = 131$ d, based on volatilization rate from water with a wind speed of 0–2.5 m/s (Sanders & Seiber 1984; quoted, Howard 1991).
- Photolysis: $t_{1/2} = 15$ h for direct sunlight photolysis in aqueous media (Wolfe et al. 1976)
 $t_{1/2} = 900$ h in distilled water at pH 6 with wavelength $\lambda > 290$ nm; $t_{1/2} = 16$ h by sunlight in a natural water from Suwannee River (Wolfe et al. 1977)
 $t_{1/2} = 990$ –20000 h for both atmospheric and aqueous photolysis, based on experimental photolysis rate constant in aqueous solution at pH 6 exposure to >290 nm under summer sunlight at 40°N (Howard et al. 1991)
- Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 photooxidation $t_{1/2} = 1.0$ –9.8 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991)
 $k_{OH}(\text{calc}) = 64 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Winer & Atkinson 1990)
 calculated lifetime $\tau = 3$ h for reaction with OH radical in the troposphere (Atkinson et al. 1992)
- Hydrolysis: $t_{1/2} = 10.5$ d at pH 7.4 and 20°C (Freed et al. 1977, 1979; Montgomery 1993)
 $t_{1/2} = 120$ d at pH 6.1 and $t_{1/2} = 11$ d at pH 7.4 in water and soil at 20°C as per Ruzicka et al. 1967 using GC-RT correlation method for hydrolysis rates determination (Freed et al. 1979)
 $k(\text{acid}) = (4.8 \pm 0.2) \times 10^{-5}$ M⁻¹ s⁻¹ with $t_{1/2} > 4$ yr for acid degradation at pH 4 at 27°C; $k(\text{alkaline}) = (5.5 \pm 0.3) \text{ M}^{-1} \text{ s}^{-1}$ with a $t_{1/2} = 36$ h for alkaline degradation at pH 8 at 27°C, $t_{1/2} = 1$ h at 40°C and $t_{1/2} = 40$ h at 0°C and pH 8; all for 10^{-4} M in 1% acetonitrile and water at 27°C; $t_{1/2} = 20$ h for distilled water and $t_{1/2} = 22$ h for natural river water from Withlacoochee River, pH 8.2 (Wolfe et al. 1977)
 $k(\text{acid}) = 4.8 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$; $k(\text{neutral}) = 7.7 \times 10^{-9} \text{ s}^{-1}$ and $k(\text{alkaline}) = 5.5 \text{ M}^{-1} \text{ s}^{-1}$ all for 10^{-4} M in 1% acetonitrile and water at 27°C (Wolfe et al. 1977; quoted, Harris 1982)
 $t_{1/2} = 8.8$ yr, based on reported $k = 2.5 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at pH 7 and 0°C; $t_{1/2}(\text{base}) = 14$ h at pH 9 and 27°C (Howard et al. 1991)
 $t_{1/2} = 9$ d at pH 6 (Montgomery 1993)
 $t_{1/2} = 3200$ d at pH 7, $t_{1/2} = 0.0006$ d at pH 12 in natural waters (Capel & Larson 1995)
- Biodegradation: $k = 6.2 \times 10^{-8} \text{ mL cell}^{-1} \text{ d}^{-1}$ (Paris et al. 1975; quoted, Scow 1982)
 $k = 5.0 \times 10^{-8} \text{ mL cell}^{-1} \text{ d}^{-1}$ (Baughman & Lassiter 1978; quoted, Scow 1982)
 $k = 2.6$ – $16.1 \times 10^{-7} \text{ mL cell}^{-1} \text{ d}^{-1}$ (Paris et al. 1978; quoted, Scow 1982);
 $k = 1.4 \text{ d}^{-1}$ in soil (Rao & Davidson 1980; quoted, Scow 1982)
 $k = (4.5 \pm 0.74) \times 10^{-11} \text{ L cell}^{-1} \text{ h}^{-1}$ in North American waters (Paris et al. 1981)
 $t_{1/2}(\text{aq. aerobic}) = 100$ –1236 h, based on estimated aqueous aerobic biodegradation half-life; $t_{1/2}(\text{aq. anaerobic}) = 400$ –4944 h based on unacclimated aerobic biodegradation (Howard et al. 1991).
 $t_{1/2}(\text{aerobic}) = 4.2$ d, $t_{1/2}(\text{anaerobic}) = 17$ d in natural waters (Capel & Larson 1995)
- Biotransformation: transformation rate $k = 7.8 \times 10^{-3} \text{ mg (mg fungi)}^{-1} \text{ h}^{-1}$ by a fungi *Aspergillus orgzae* at 28°C in aqueous solution (Lewis et al. 1975)
 $k = 1.9 \times 10^{-1} \text{ mg (mg fungi)}^{-1} \text{ d}^{-1}$ in aquatic systems (Lewis et al. 1975; quoted, Scow 1982)
- Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
 $k_1 = 1.07 \text{ d}^{-1}$ (carp, Bender 1969; quoted, McLeese et al. 1976)
 $k_2 = 0.08 \text{ d}^{-1}$ (carp, calculated, from k_1 of Bender 1969, McLeese et al. 1976)
 $k_2 = 0.49 \text{ h}^{-1}$ (willow shiner, Tsuda et al. 1989)

Half-Lives in the Environment:

Air: $t_{1/2} = 1.0\text{--}9.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);
calculated lifetime of 3 h for the vapor-phase reaction with OH radical in the troposphere (Atkinson et al. 1992).

Surface water: persistence of up to 4 wk in river water (Eichelberger & Lichtenberg 1971);

$t_{1/2} = 100\text{--}1236$ h, based on unacclimated aerobic river die-away test data and estuarine water grab sample data (Howard et al. 1991);

$t_{1/2} = 1.65$ d in Indian River water, at 24 ppt salinity and pH 8.16 (Wang & Hoffman 1991);

$t_{1/2} = 212$ d at 6°C , $t_{1/2} = 42$ d at 22°C in darkness for Milli-Q water, pH 6.1; $t_{1/2} = 55$ d at 6°C , $t_{1/2} = 19$ d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 53$ d at 6°C , $t_{1/2} = 7$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 41$ d at 6°C , $t_{1/2} = 6$ d at 22°C in darkness, $t_{1/2} = 14$ d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995)

Biodegradation $t_{1/2}(\text{aerobic}) = 4.2$ d, $t_{1/2}(\text{anaerobic}) = 17$ d, hydrolysis $t_{1/2} = 3200$ d at pH 7 and $t_{1/2} = 0.0006$ d at pH 12 in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 200\text{--}2472$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} = 2$ d in sediment suspension (Cotham & Bidleman 1989)

first-order degradation $k = 0.902$ d^{-1} with $t_{1/2} = 0.8$ d under aerobic conditions, $k = 0.302$ d^{-1} with $t_{1/2} = 2.3$ d under anaerobic conditions in sediment from San Diego Creek, Orange County, CA; first-order degradation $k = 0.506$ d^{-1} with $t_{1/2} = 1.4$ d under aerobic conditions, $k = 0.431$ d^{-1} with $t_{1/2} = 1.6$ d under anaerobic conditions in sediment from Bonita Creek, Orange County, CA (Bondarendo & Gan 2004)

Soil: estimated persistence of one week (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987);

$t_{1/2} = 72\text{--}168$ h, based on unacclimated aerobic soil grab sample data (Walker & Stojanovic 1973; quoted, Howard et al. 1991);

biodegradation rate constant of 1.4 d^{-1} in soil (Rao & Davidson 1980; quoted, Scow 1982);

non-persistent in soil with $t_{1/2} < 20$ d (Willis & McDowell 1982);

$t_{1/2} = 1$ d in screening model simulations (Jury et al. 1987b);

Degradation $t_{1/2} = 8$ d in a coarse sandy soil, $t_{1/2} = 19$ d in sandy loam (Kjeldsen et al. 1990)

selected field $t_{1/2} = 1.0$ d (Wauchope et al. 1992; Dowd et al. 1993; Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2} = 11$ d (Pait et al. 1992);

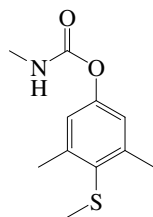
$t_{1/2} = 1$ d for soil depth < 5 cm, $t_{1/2} = 7$ d for soil depth $5\text{--}20$ cm and $t_{1/2} = 14$ d for soil depth > 20 cm (Dowd et al. 1993).

Biota: biochemical $t_{1/2} = 1$ d from screening model calculations (Jury et al. 1987b);

excretion $t_{1/2} = 1.4$ h (willow shiner, Tsuda et al. 1989);

average $t_{1/2} = 20$ d in the forest (USDA 1989; quoted, Neary et al. 1993).

18.1.1.56 Methiocarb



Common Name: Methiocarb

Synonym: Bayer 37344, Draza, Ensulol, Mercaptodimethur, Mesulol, Mesulol Phenol, metmercapturon

Chemical Name: 4-methylthio-3,5-xylyl methylcarbamate; 3,5-dimethyl-4-(methylthio)phenol methylcarbamate

Uses: Insecticide/Acaricide/Molluscicide/Repellent; to control slugs and snails in a wide range of agricultural situations; broad range control of lepidoptera, coleoptera, diptera, and homoptera and spider mites in pome fruit, stone fruit, citrus fruit, strawberries, hops, potatoes, beet, maize, oilseed rape, vegetables and ornamentals; also used as a bird repellent.

CAS Registry No: 2032-65-7

Molecular Formula: $C_{11}H_{15}NO_2S$

Molecular Weight: 225.308

Melting Point ($^{\circ}C$):

120 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.236 (Tomlin 1994)

Molar Volume (cm^3/mol):

261.4 (calculated-Le Bas method at normal boiling point)

182.3 (calculated-density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.117 (mp at $120^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

30 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987; Milne 1995)

27 ($20^{\circ}C$, Tomlin 1994)

24 ($20-25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.015 ($60^{\circ}C$, Hartley & Kidd 1987)

1.5×10^{-5} ($20^{\circ}C$, Tomlin 1994)

3.6×10^{-5} (Tomlin 1994)

0.016 ($20-25^{\circ}C$, selected, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.120 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.92 (shake flask as per Fujita et al. 1964; Briggs 1981)

2.92 (selected, Magee 1991)

3.34 (Tomlin 1994)

2.92 (recommended, Hansch et al. 1995)

2.82 (Pomona-database, Müller & Kördel 1996)

2.95 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

- 2.32 (20°C, sorption isotherm, converted from log K_{OM} of 2.08, Briggs 1981)
- 2.08, 2.33 (reported as log K_{OM} , converted from K_{OM} multiplied by 1.724, Magee 1991)
- 2.82 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
- 2.32 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 2.82; 2.26 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 2.48 (20–25°C, estimated, Hornsby et al. 1996)
- 3.12, 2.45, 2.38, 2.88, 2.80 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 2.25 (sandy loam soil, column equilibrium method-HPLC/UV, 20°C, Xu et al. 1999)
- 2.741, 2.641, 2.377, 2.493, 2.824 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
- 2.32; 2.23, 2.22 (soil, quoted exptl.; estimated-class specific model, estimated-general model, Gramatica et al. 2000)

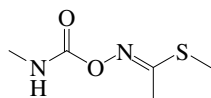
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Photolysis: photodegradation half-life of 6–16 d (Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2}$ = 30 d (20–25°C, estimated, Hornsby et al. 1996).

18.1.1.57 Methomyl



Common Name: Methomyl

Synonym: Du Pont 1179, ENT 27341, Lannate, Mesomile, Nu-bait II, Nudrin, SD 14999, WL 18236

Chemical Name: *S*-methyl-*N*-(methylcarbamoyloxy) thioacetimidate; methyl-*N*-(((methylamino)-carbonyl)oxy) ethan-imidothioate

Uses: insecticide/acaricide; control a wide range of insects and spider mites in fruit, vines, olives, hops, vegetables, ornamentals, field crops, cucurbits, flax, cotton, soya beans, etc.; also used for control of flies in animal and poultry houses and dairies.

CAS Registry No: 16752-77-5

Molecular Formula: C₅H₁₀N₂O₂S

Molecular Weight: 162.210

Melting Point (°C):

78–79 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

78 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.2946 (25°C, Spencer 1982; Worthing & Hance 1991; Tomlin 1994)

1.2946 (24°C, Milne 1995; Montgomery 1993)

Molar Volume (cm³/mol):

179.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.267 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.302 (mp at 78°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

58000 (Worthing 1979; Khan 1980; Worthing 1983, 1987, Worthing & Hance 1991)

10000 (Kenaga 1980a; Kenaga & Goring 1980)

> 1000 (20°C, shake flask-GC, Bowman & Sans 1983a)

57900 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

58000 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

3.47 × 10⁻³ (20°C, Hartley & Graham-Bryce 1980)

6.66 × 10⁻³ (Khan 1980; Spencer 1982)

0.162 (30°C, GC, Seiber et al. 1981)

6.67 × 10⁻³ (Worthing 1983)

3.47 × 10⁻³ (20°C, selected exptl. value, Kim 1985)

7.53 × 10⁻², 1.99 × 10⁻² (20°C, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)

6.65 × 10⁻³ (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

6.67 × 10⁻³ (20–25°C, selected, Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

1.82 × 10⁻⁵ (calculated, Lyman et al. 1982)

6.50 × 10⁻⁵ (20°C, calculated-P/C, Suntio et al. 1988)

6.48 × 10⁻⁵ (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, log K_{ow} :

0.30	(Dow Chemical data, Kenaga & Goring 1980)
1.08	(Rao & Davidson 1980)
0.131	(22°C, shake flask-GC, Bowman & Sans 1983b)
0.60	(shake flask-HPLC, Drabel & Bachmann 1983)
0.60	(Hansch & Leo 1985)
0.13, 1.08	(Montgomery 1993)
0.60	(recommended, Sangster 1993)
0.09	(Tomlin 1994)
0.60	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

0.477, 0.903	(calculated-S, calculated- K_{oc} , Kenaga 1980)
0.230, 0.110	(calculated- K_{ow} , calculated-S, Howard 1991)

Sorption Partition Coefficient, log K_{oc} :

2.20	(soil, Fung & Uren 1977)
1.45	(soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
1.71; 1.00	(calculated- K_{ow} ; calculated-S, Lyman et al. 1982)
2.20	(Worthing 1983)
1.08	(soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
1.86, 2.20	(Montgomery 1993)
1.86	(estimated-chemical structure, Lohninger 1994)
1.86	(Tomlin 1994)
1.30	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.86	(soil, 20–25°C, selected, Hornsby et al. 1996)
1.16, 1.62	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, Half-Lives, $t_{1/2}$

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} \sim .14$ months, based on vapor-phase reaction with hydroxyl radical in air (GEMS 1986; quoted, Howard 1991).

Hydrolysis: experimental $t_{1/2} = 262$ d from rate constant $k = 8.9 \times 10^{-5} \text{ h}^{-1}$ has been determined in pure water at pH 7 and 25°C (Ellington et al. 1987, 1988; quoted, Howard 1991; Montgomery 1993).

Biodegradation: rate constants $k = -0.000215 \text{ h}^{-1}$ in nonsterile sediment, $k = -0.000747 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.000175 \text{ h}^{-1}$ in nonsterile water and $k = -0.000383 \text{ h}^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} \sim 1.14$ months, based on rate constant $k = 2.919 \times 10^{-13} \text{ cm}^3/\text{molecules}$ for the vapor-phase reaction with $8 \times 10^5/\text{cm}^3$ hydroxyl radical in air (GEMS 1986; quoted, Howard 1991).

Surface water: experimental $t_{1/2} = 262$ d has been determined in pure water at 25°C (Ellington et al. 1988; quoted, Howard 1991).

Ground water: $t_{1/2} < 0.2$ d in ground water samples (Smelt et al. 1983; quoted, Tomlin 1994).

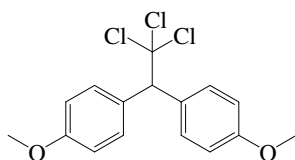
Sediment:

Soil: field $t_{1/2} = 30$ d (20–25°C, selected, Hornsby et al. 1996).

Biota: $t_{1/2} \sim 3\text{--}5$ d in plants following leaf application (Harvey & Reiser 1973; quoted, Tomlin 1994);

$t_{1/2} = 0.4\text{--}8.5$ d on cotton plants, $t_{1/2} = 0.8\text{--}1.2$ d on mint plants and $t_{1/2} \sim 2.5$ d on Bermuda grass (Willis & McDowell 1987; quoted, Howard 1991).

18.1.1.58 Methoxychlor



Common Name: Methoxychlor

Synonym: Chemform, Dimethoxy-DDT, DMDT, DMTD, ENT 1716, Maralate, Marlate, Methoricide, Methoxo, Metox, Moxie NCI-C00497

Chemical Name: 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)ethane; 1,1'-(2,2,2-trichloroethylidene)bis[4-methoxybenzene]

Uses: insecticide to control mosquito larvae, house flies, and other insect pests in field crops, fruits, and vegetables; also to control ectoparasites on cattle, sheep, and goats.

CAS Registry No: 72-43-5

Molecular Formula: $C_{16}H_{15}Cl_3O_2$

Molecular Weight: 345.648

Melting Point ($^{\circ}C$):

87 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.41 ($25^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

354.3 (calculated-Le Bas method at normal boiling point)

245.1 (calculated-density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.614 (DSC method, Plato & Glasgow 1969)

23.88 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.246 (mp at $87^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

0.10* (shake flask-UV, measured range $25-45^{\circ}C$, Richardson & Miller 1960)

0.62 (Karpoor et al. 1970)

0.003, 0.01, 0.045* (particle size of 0.01, 0.05 and 5.0μ ; shake flask-GC, measured range $15-45^{\circ}C$, Biggar & Riggs 1974)

0.10 (generator column-GC/ECD, Weil et al. 1974)

0.12 (shake flask-GC/ECD, Zepp et al. 1976, Karickhoff et al. 1979; Karickhoff 1981)

0.1-0.25 (Wauchope 1978)

0.10 (Weber et al. 1980)

0.10 (Worthing 1983, 1987, Worthing & Hance 1991; Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

0.10 ($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.04 ($24^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

$< 1.33 \times 10^{-4}$ ($20-25^{\circ}C$, Weber et al. 1980)

1.910×10^{-4} (estimated, Howard 1991)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

1.60 (estimated, Hine & Mookerjee 1975; quoted, Howard 1991)

0.999 (calculated-P/C, this work)

0.0206 (wetted wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{ow} :

- 4.68 (HPLC-RT correlation, Veith & Morris 1978)
- 5.08 (shake flask-UV, Karickhoff et al. 1979; Karickhoff 1981)
- 4.30 (HPLC-RT correlation, Veith et al. 1979, 1980)
- 4.20 (Mackay et al. 1980)
- 4.83 (Belluck & Felsot 1981)
- 4.51 (HPLC- k' correlation, McDuffie 1981)
- 4.83 (shake flask-UV, Nishimura & Fujita 1983)
- 4.68–5.08 (Hansch & Leo 1985)
- 4.91, 4.26 (shake flask, RP-TLC-RT correlation, Renberg et al. 1985)
- 3.31, 5.08 (Montgomery 1993)
- 4.95 (recommended, Sangster 1993)
- 5.08 (recommended, Hansch et al. 1995)
- 4.58 (RP-HPLC-RT correlation, Finizio et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

- 1.70 (bioaccumulation factor logBF, adipose tissue in female Albino rats, Harris et al. 1974)
- 4.68, 3.08, 3.72, 3.92 (*Bacillus subtilis*, *Flavobacterium harrisonii*, *Aspergillus sp.*, *Chlorella pyrenoidosa*, Paris et al. 1975; Paris & Lewis 1976)
- 4.40 (bacterial sorption, Paris & Lewis 1976)
- 2.14 (sheepshead minnow, Parrish et al. 1977)
- 3.92, 3.72 (algae, fungi, Wolfe et al. 1977)
- 3.92 (fathead minnows, 32 d exposure, Veith et al. 1979, 1980)
- 3.70–3.93, 2.54–3.05 (snail, Stonefly, Anderson & Defoe 1980)
- 2.27, 3.19 (fish: flowing water, static water; Kenaga 1980b; Kenaga & Goring 1980)
- 4.21, 3.91 (calculated-S, K_{OC} , Kenaga 1980)
- 1.15 (*Triaenodes tardus*, Belluck & Felsot 1981)
- 4.20, 3.04, 3.91 (estimated-S, K_{ow} , K_{OC} , Bysshe 1982)
- 3.92 (fathead minnows, Veith & Kosian 1983)
- 4.08 (mussel, Renberg et al. 1985)
- 3.18 (soft clams, Hawker & Connell 1986)
- 3.92 (calculated, Isnard & Lambert 1988)
- 5.40 (calculated field bioaccumulation, Thomann 1989)
- 5.29 (rainbow trout lipid base, estimated, Noegrohati & Hammers 1992)
- 3.98; 4.05 (*Oncorhynchus mykiss*, wet wt. basis: quoted exptl.; calculated-QSAR model based on quantum chemical parameters, Wei et al. 2001)

Sorption Partition Coefficient, log K_{OC} :

- 2.79 (water-sediment, Wolfe et al. 1977)
- 4.90 (av. for isotherms on sediments, Karickhoff et al. 1979)
- 3.99–4.61, 4.90–5.00, 4.86–4.96 (sand, fine silt, clay Karickhoff et al. 1979)
- 4.90 (soil, quoted, Kenaga 1980a, b; Kenaga & Goring 1980; Bysshe 1982)
- 5.03 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 6.04 (calculated-S, Mill et al. 1980)
- 4.90 (av. soils/sediments, Rao & Davidson 1980)
- 4.67, 4.69, 5.54 (estimated-S, K_{ow} , S and mp, Karickhoff 1981)
- 4.26 (soil, screening model calculations, Jury et al. 1987b)
- 4.99 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)
- 4.63 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 4.90 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 4.90 (estimated-QSAR and SPARC, Kollig 1993)
- 4.90, 4.95 (Montgomery 1993)
- 4.90 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 4.5$ d from water was estimated based on Henry's law constant for a model river 1 m deep with a current of 1 m/s and a wind speed of 3 m/s (Howard 1991).

Photolysis: midsummer direct photolysis $t_{1/2} = 690$ h in water, $t_{1/2} = 4100$ h in hydrocarbon media; midday $t_{1/2} = 1100$ h average over all seasons in water at latitude 40°N , daily average direct photolysis $t_{1/2} = 4.5$ months (12-h days) in water in the Central U.S. (Zepp et al. 1976)

photodecomposition $t_{1/2} > 300$ h in distilled water, $t_{1/2} = 2.2$ h in Suwannee River water, $t_{1/2} = 5.4$ h in Tombigbee River water, $t_{1/2} = 2.9$ h in Alabama River water with methoxychlor at 40 ppb under sunlight (Zepp et al. 1976)
 $t_{1/2} = 300\text{--}2070$ h in both air and natural water, based on measured photolysis rates in distilled water under midday sunlight and adjusted for approximate winter sunlight intensity (Howard et al. 1991).

Oxidation:

photooxidation $t_{1/2} = 2.2\text{--}5.4$ h in natural water, based on measured photooxidation in river water exposed to midday May sunlight (Zepp et al. 1976; quoted, Howard et al. 1991);

photooxidation $t_{1/2} \sim 1.12\text{--}11.2$ h in air, based on rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k(\text{aq.}) = (270 \pm 80) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $24 \pm 1^\circ\text{C}$, with $t_{1/2} = 21$ min at pH 7 (Yao & Haag 1991).

$k_{\text{OH}}(\text{aq.}) = 2 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radicals in aqueous solutions at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992).

Hydrolysis: $k(\text{alkaline}) = 3.8 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 2100$ d at 27°C , $k(\text{neutral}) = 2.2 \times 10^{-8} \text{ s}^{-1}$ at pH 3–7 corresponds to a $t_{1/2} = 367$ d at pH 9 and 27°C (Wolf et al. 1977)

Overall rate constant $k = 5.5 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} = 147$ d; $k = 3.0 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} = 270$ d at 25°C and pH 7 (Mabey & Mill 1978)

$k(\text{alkaline}) = 3.8 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$, $k(\text{neutral}) = 2.2 \times 10^{-8} \text{ s}^{-1}$, $1 \times 10^{-8} \text{ M}$ in water at 27°C (Harris 1982)

$t_{1/2} = 1.05$ yr, based on neutral and base catalyzed hydrolysis rate constants Howard et al. 1991)

$k = 0.60 \text{ yr}^{-1}$ at pH 7 and 25°C (Kollig 1993)

$t_{1/2} = 370$ d at pH 2, $t_{1/2} = 370$ d at pH 7 and $t_{1/2} = 270$ d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 4320\text{--}8760$ h (6 months to 1 yr), based on very slow biodegradation observed in an aerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 1200\text{--}4320$ h (50 d to 6 months), based on anaerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991)

$k = -0.00236 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.000639 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and $k = -0.000139 \text{ h}^{-1}$ in nonsterile water and $k = -0.00000327 \text{ h}^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988)

$t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 50$ d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 14.4\text{--}37.5 \text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 11.4\text{--}82.0 \text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 35.8\text{--}54.9 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)

$k_1 = 35.8\text{--}54.9 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

$k_2 = 45.4\text{--}38.6 \text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.030 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air: $t_{1/2} \sim 1.12\text{--}11.2$ h, based on rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: midsummer direct photolysis $t_{1/2} = 690$ h in water; midday $t_{1/2} = 1100$ h average over all seasons in water at latitude 40°N , daily average direct photolysis $t_{1/2} = 4.5$ months (12-h days) in water in the Central U.S. (Zepp et al. 1976)

$t_{1/2} = 2.2\text{--}5.4$ h, based on measured photooxidation in river water exposed to midday May sunlight (Zepp et al. 1976; quoted, Howard et al. 1991);

measured $k = (270 \pm 80) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.7–6.4 and $24 \pm 1^\circ\text{C}$, with a $t_{1/2} = 2.1$ min at pH 7 (Yao & Haag 1991)

biodegradation $t_{1/2}(\text{aerobic}) = 180$ d, $t_{1/2}(\text{anaerobic}) = 50$ d, hydrolysis $t_{1/2} = 370$ d at pH 2, $t_{1/2} = 370$ d at pH 7 and $t_{1/2} = 270$ d at pH 12 in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2} = 1200\text{--}8760$ h, based on aerobic and anaerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 1.5$ wk at pH 4.7 and 6.5 and $t_{1/2} = 1.0$ wk at pH 7.8 (Carlo et al. 1952; quoted, Kaufman 1976);

$t_{1/2} = 4320\text{--}8760$ h, based on very slow biodegradation observed in an aerobic soil die-away test study data (Fogel et al. 1982; quoted, Howard et al. 1991);

$t_{1/2} = 42$ d in screening model calculations (Jury et al. 1987b);

selected field $t_{1/2} = 120$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: elimination $t_{1/2} = 9.6$ h in pond sediment-water, $t_{1/2} = 23.2$ h in sand-water system (*Chironomus tentans* larvae, Muir et al. 1983);

$t_{1/2} = 0.4\text{--}8.5$ d on cotton plants, $t_{1/2} = 0.8\text{--}1.2$ d on mint plants and $t_{1/2} \sim 2.5$ d on Bermuda grass (Willis & McDowell 1987; quoted, Howard 1991).

TABLE 18.1.1.58.1

Reported aqueous solubilities of methoxychlor at various temperatures

Richardson & Miller 1960		Biggar & Riggs 1974			
shake flask-UV spec.		shake flask-GC			
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$	$\text{S/g}\cdot\text{m}^{-3}$
		particle size	0.01 μ	0.05 μ	5.0 μ
25	0.10	15	-	-	0.020
35	0.20	25	0.003	0.010	0.045
45	0.40	35	-	-	0.095
		45	-	-	0.185

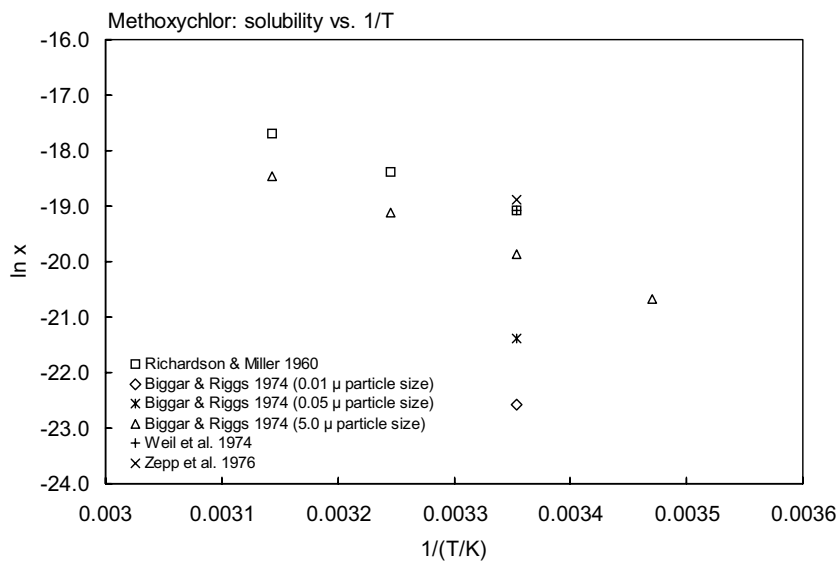
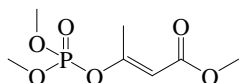


FIGURE 18.1.1.58.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for methoxychlor.

18.1.1.59 Mevinphos



Common Name: Mevinphos

Synonym: Apavinfos, CMDP, Compound 2046, Duraphos, ENT 22374, Fosdrin, Gesfid, Gestid, Meniphos, Menite, NA 2783, OS 2046, PD 5, Phosdrin, Phosfene

Chemical Name: 2-carbomethoxy-1-methylvinyl dimethyl phosphate; 1-methoxycarbonyl-1-propen-2-yl dimethyl phosphate; methyl-3-(dimethoxyphosphinoyloxy)but-2-enoate 2-carbomethoxy-1-methylvinyl dimethyl phosphate

Uses: contact insecticide and acaricide to control chewing insects and spider mites in fruits, vegetables, and ornamentals.

CAS Registry No: 7786-34-7 [formerly 298-01-1 for (E) isomer & 338-45-4 for (Z) isomer] for cis-isomer and 338-45-4 for *trans*-isomer]

Molecular Formula: C₇H₁₃O₆P

Molecular Weight: 224.1 48

Melting Point (°C):

–56.1 (Montgomery 1993; Lide 2003)

21 ((E) isomer, Lide 2003)

6.9 ((Z) isomer, Lide 2003)

Boiling Point (°C)

99–103 (at 0.03 mmHg, Martin 1971; Freed et al. 1977; Milne 1995)

76.0 (at 0.2 mmHg, Melnikov 1971; Freed et al. 1979)

110 (at 1.6 mmHg, Hartley & Kidd 1987)

106–107.5 (at 1 mmHg, Montgomery 1993)

Density (g/cm³ at 20°C):

1.24 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

1.25 (Montgomery 1993)

1.235, 1.245 ((E) isomer, (Z) isomer, Tomlin 1995)

Molar Volume (cm³/mol):

180.7 (calculated from density)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

miscible (Spencer 1973; Worthing 1979; Freed et al. 1979)

> 2000 (shake flask-GC, Bowman & Sans 1983a)

miscible (Hartley & Kidd 1987; Tomlin 1994)

miscible (Worthing & Walker 1987)

600000 (20–25°C, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

0.293 (20°C, Eichler 1965)

0.293 (20–25°C, Melnikov 1971)

0.757 (20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)

0.017 (20°C, Hartley & Kidd 1987; Tomlin 1994)

0.0173 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.293 (20°C, Montgomery 1993)

Henry's Law Constant (Pa·m³/mol):

6.35 × 10^{–6} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

0.845	(Melnikov 1971)
0.954	(Freed et al. 1977)
0.550	(selected, Dao et al. 1983)
1.20	(shake flask, Log P Database. Hansch & Leo 1987)
0.200	(selected, Boehncke et al. 1990)
0.130	(Tomlin 1994)
1.20	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc} :

1.64	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.64	(estimated-chemical structure, Lohninger 1994)
2.30	(soil, calculated-MCI χ , Sabljic et al. 1995)
2.12, 1.56	(soil, <i>cis</i> -mevinphos, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.28, 1.67	(soil, <i>trans</i> -mevinphos, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} = 1.8$ h for *cis*- and $t_{1/2} = 3.0$ h for *trans*-isomer at pH 11.6 (Casida et al. 1956; quoted, Montgomery 1993);
 $t_{1/2} = 30$ –35 d (Melnikov 1971; quoted, Freed et al. 1977);
 $t_{1/2} = 120$ d at pH 6, $t_{1/2} = 35$ d at pH 7, $t_{1/2} = 3$ d at pH 9, and $t_{1/2} = 1.4$ h at pH 11 (Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water:

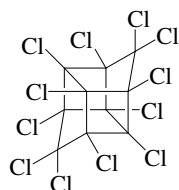
Ground water:

Sediment:

Soil: selected field $t_{1/2} = 3$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: estimated $t_{1/2} = 19 \pm 2$ and 24 ± 7 h in lettuce in the summer and $t_{1/2} = 20 \pm 11$ h in the fall, $t_{1/2} = 50$ h in cauliflower in the summer and $t_{1/2} = 18 \pm 1$ h in the fall, $t_{1/2} = 25 \pm 2$ h in celery in the summer and $t_{1/2} = 16$ h in the fall (Spencer et al. 1992)

18.1.1.60 Mirex



Common Name: Mirex

Synonym: Bichlorendo, Declorane, ENT 25719, Ferriamicide, Paramex, Perclordecone

Chemical Name: 1,1a,2,2,3,3a,4,5,5,5a,5b,6-dodecachloro-octahydro-1,3,4-methano-1H-cyclobuta(cd) pentalene; dodecachloro-pentacyclodecane

Uses: Insecticide.

CAS Registry No: 2385-85-5

Molecular Formula: $C_{10}Cl_{12}$

Molecular Weight: 545.542

Melting Point ($^{\circ}C$):

485 (dec., Smith et al. 1978; Spencer 1982; Kühne et al. 1995; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Molar Volume (cm^3/mol):

403.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio, at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 3.1×10^{-5} (mp at $485^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.001 (from D. Dollar of Miss. State Chem. Lab. unpublished results, Alley 1973)

0.085 (shake flask-LSC, Metcalf et al. 1973)

0.60 (Neely 1978; quoted, Kenaga 1980; Kenaga & Goring 1980)

7.0×10^{-5} ($22^{\circ}C$, shake flask-GC, Smith et al. 1978)

0.02 ($24^{\circ}C$, Verschueren 1983)

7.0×10^{-5} (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or indicated and reported temperature dependence equations):

8.0×10^{-4} ($50^{\circ}C$, Smith, et al. 1978)

1.3×10^{-4} ($20^{\circ}C$, Smith et al. 1978)

1.0×10^{-4} ($20^{\circ}C$, selected, Suntio et al. 1988)

9.0×10^{-7} ($10^{\circ}C$, estimated, McLachlan et al. 1990)

2.5×10^{-4} , 2.9×10^{-4} , 2.8×10^{-4} (GC-RT correlation, supercooled liquid, Hinckley et al. 1990)

5.2×10^{-5} ($12^{\circ}C$, extrapolated supercooled liquid value, Hinckley et al. 1990)

1.1×10^{-4} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ and reported temperature dependence equations):

1013 ($20^{\circ}C$, calculated, Smith et al. 1978)

53.2 ($22^{\circ}C$, gas stripping-GC/ECD, Yin & Hassett 1986)

$\log [H/(atm \cdot m^3/mol)] = 12.709 - 4711/(T/K)$, temp range: 8 – $24^{\circ}C$ (gas stripping-GC, Yin & Hassett 1986)

840 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

44.1 ($20^{\circ}C$, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 13.899 - 4585/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.50 (Hansch & Leo 1979)

6.89 (HPLC-RT correlation, Veith et al. 1979; Veith & Kosian 1983)

- 5.28 (shake flask, Log P Database, Hansch & Leo 1987)
 5.28 (recommended, Sangster 1993)
 5.28 (recommended, Hansch et al. 1995)
 7.13–7.24 (shake flask/slow stirring-GC/ECD, both phases, Fisk et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 2.34, 3.07 (*Gambusia*, *Physa*, Metcalf et al. 1973)
 2.78 (*Oedogonium* sp., Metcalf et al. 1973)
 2.18 (bioaccumulation factor $\log BF$, adipose tissue in female Albino rats, Ivie et al. 1974)
 -2.02 (milk biotransfer factor $\log B_m$, correlated- K_{OW} , Dorough & Ivie 1974)
 2.34 (fish in static water, Metcalf 1974)
 -1.25 (beef biotransfer factor $\log B_b$, correlated- K_{OW} , Bond et al. 1975)
 -1.14 (vegetation, correlated- K_{OW} , De La Cruz & Rajanna 1975)
 3.86; 3.51; 3.61; 3.70 (*Chlorococcum* sp.; *Chlamydomonas* sp.; *Dunaliella tertiolecta*; *Thalassidsira pseudomana*, Hollister et al. 1975)
 5.60 (bacterial sorption, Smith et al. 1978)
 4.26 (fathead minnows, 32-d exposure, Veith et al. 1979, 1980)
 2.91 (calculated-S, Kenaga 1980)
 4.71 (fathead minnow to ^{14}C mirex, Huckins et al. 1982)
 4.34 (fish, correlated, Mackay 1982)
 4.26 (fathead minnow, Veith & Kosian 1983)
 4.09, 3.41 (algae, fish, Verschueren 1983)
 6.50 (fish, selected, Paterson & Mackay 1985)
 1.78–2.87 highest value 2.87 but not equilibrated (rainbow trout, 15°C, steady-state BCF on 7- to 96-d laboratory study, Oliver & Niimi 1985)
 > 4.08; 2.87 (rainbow trout, kinetic $BCF-k_1/k_2$; steady-state BCF in laboratory studies, Oliver & Niimi 1985)
 6.08; 7.18 (rainbow trout, calculated- K_{OW} , Lake Ontario field data, Oliver & Niimi 1985)
 2.87 (fish, Oliver & Niimi 1985; Oliver 1987)
 4.34 (worms, Oliver 1987)
 6.17 (oligochaetes, Connell et al. 1988)
 6.41 (smelt, Oliver & Niimi 1988)
 4.31 (*Poecilia reticulata*, Gobas et al. 1989; quoted, Devillers et al. 1996)
 6.42, 7.16 (guppy, correlated, Gobas et al. 1989)
 6.40 (Markwell et al. 1989)
 4.72, 7.07 (dry leaf, wet leaf, Bacci et al. 1990)
 7.07 (wet leaf, Bacci et al. 1990)
 5.97, 7.16 (guppy 6.5% lipid: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.79–4.26, 3.95–4.40 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

Bioaccumulation Factor $\log BAF$:

- 8.27 (calculated field bioaccumulation, Thomann 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

- 5.56 (natural sediment, Smith et al. 1978)
 7.38 (av. soils/sediments, Smith et al. 1978)
 3.76 (soil, quoted exptl., Kenaga 1980)
 3.08 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
 6.00, 5.67 (derived from exptl., calculated-MCI χ , Meylan et al. 1992)
 6.42 \pm 0.39 (suspended particulate matter of the St. Lawrence River, Comba et al. 1993)
 6.00 (20–25°C, soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
 6.00 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Rate Constants, k , and Environmental Half-Lives, $t_{1/2}$:

Volatilization: $k = 5.37 \times 10^{-2} \text{ h}^{-1}$ (Hill et al. 1976) with $t_{1/2} = 500 \text{ h}$ from river, $t_{1/2} = 700 \text{ h}$ from pond, $t_{1/2} = 1980 \text{ h}$ from eutrophic lake, and 1 $t_{1/2} = 980 \text{ h}$ from oligotrophic lake (Smith et al. 1978).

Photolysis: rate constants $k < 5.0 \times 10^{-8} \text{ s}^{-1}$ (laboratory data, Smith et al. 1978);

$k = 4.2 \times 10^{-3} \text{ d}^{-1}$ (field data, Smith et al. 1978);

$t_{1/2} = 3.9 \times 10^3 \text{ h}$ (aquatic half-life, Haque et al. 1980);

$k = 0.123 \text{ d}^{-1}$ (sunlight, distilled water containing 2.0 mg DOC/L humic acid, Mudambi & Hassett 1988);

$k = 0.033 \text{ d}^{-1}$ (sunlight, distilled water, summer, Mudambi & Hassett 1988);

$k = 0.102 \text{ d}^{-1}$ (sunlight, Lake Ontario water, Mudambi & Hassett 1988);

$k = 0.019 \text{ d}^{-1}$ (sunlight, distilled water, fall, Mudambi & Hassett 1988).

Oxidation: laboratory data $k < 30 \text{ M}^{-1} \text{ s}^{-1}$ (Smith et al. 1978); $t_{1/2} \gg 0.7 \text{ yr}$ (Smith et al. 1978; quoted, Cheung 1984).

Hydrolysis: laboratory data rate constant $k = 1 \times 10^{-10} \text{ s}^{-1}$ (Smith et al. 1978); $k = 2 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 250 \text{ yr}$ (Cheung 1984);

degradation rate constant $k = 1.93 \times 10^{-4} \text{ h}^{-1}$ (Mackay et al. 1985; quoted, Mackay & Paterson 1991).

Biodegradation: slow process (Cheung 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 > 8.50 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_2 < 0.0007 \text{ d}^{-1}$ (rainbow trout, Oliver & Niimi 1985)

$k_2 = 0.017 \text{ d}^{-1}$ with $t_{1/2} = 42 \text{ d}$ and $k_2 = 0.009 \text{ d}^{-1}$ with $t_{1/2} = 78 \text{ d}$ for food concn of 21 ng/g and 145 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for juvenile rainbow trout (Fisk et al. 1998)

Half-Lives in the Environments:

Air:

Surface water: overall $t_{1/2} = 0.83 \text{ h}$ in river or stream, $t_{1/2} = 420 \text{ h}$ in pond, and $t_{1/2} = 1480 \text{ h}$ by sorption in both eutrophic lake and oligotrophic lake; with photolysis $t_{1/2} > 8000 \text{ h}$ and oxidation $t_{1/2} > 1000 \text{ h}$ in pond, river, eutrophic lake and oligotrophic lake (Smith et al. 1978);

degradation rate constant $k = 1.93 \times 10^{-4} \text{ h}^{-1}$ (Mackay et al. 1985; quoted, Mackay & Paterson 1991);

$t_{1/2} = 7 \text{ d}$ in sunlit, air-equilibrated humic acid solution, or natural water (Mudambi & Hassett 1988; Burns et al. 1996).

Ground water:

Soil: estimated field $t_{1/2} = 3000 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

$t_{1/2} = 8.2 \text{ yr}$, extremely persistent in soil (Geyer et al. 2000)

Biota: $t_{1/2} > 1000 \text{ d}$ (Skea et al. 1981; Oliver & Niimi 1985);

$t_{1/2} > 28 \text{ d}$ in fathead minnow to ^{14}C mirex (Huckins et al. 1982);

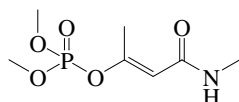
$t_{1/2} > 500 \text{ d}$ (4°C , rainbow trout, Niimi & Palazzo 1985);

$t_{1/2} = 114 \text{ d}$ as observed and $t_{1/2} = 495 \text{ d}$ as adjusted (12°C , rainbow trout, Niimi & Palazzo 1985);

$t_{1/2} = 103 \text{ d}$ as observed and $t_{1/2} > 1000 \text{ d}$ as adjusted (18°C , rainbow trout, Niimi & Palazzo 1985).

Depuration $t_{1/2} = 42\text{--}78 \text{ d}$ in 30-d uptake and 160-d depuration studies (juvenile rainbow trout, Fisk et al. 1998)

18.1.1.61 Monocrotophos



Common Name: Monocrotophos

Synonym: Apadrin, Azodrin, Bilobran, Crotos, ENT 27129, Monocron, Nuvacron

Chemical Name: dimethyl (E)-1-methyl-2-(2-methylcarbamoyl)vinyl phosphate

Uses: systemic insecticide and acaricide to control pests in cotton, sugar cane, coffee, tobacco, olives, rice hops, sorghum, maize, deciduous fruits, citrus fruits, potatoes, sugar beet, tomatoes, soya beans, and ornamentals.

CAS Registry No: 6923-22-4

Molecular Formula: $C_7H_{14}NO_5P$

Molecular Weight: 223.164

Melting Point ($^{\circ}C$):

55 (Lide 2003)

Boiling Point ($^{\circ}C$):

125 (at 0.0005 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.33 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Milne 1995)

1.22 (Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.508 (mp at $55^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

miscible (Spencer 1973; Budavari 1989)

miscible (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

1000000 (Worthing & Walker 1987, Worthing & Hance 1991; Milne 1995)

1000000 (20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

9.33×10^{-3} ($20^{\circ}C$, Eichler 1965)

9.33×10^{-3} ($20^{\circ}C$, Wolfdietrich 1965; Melnikov 1971; Budavari 1989)

9.33×10^{-4} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

5.09×10^{-3} ($20^{\circ}C$, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)

2.30×10^{-3} ($20^{\circ}C$, GC-RT correlation with mp correction, Kim 1985)

9.00×10^{-3} (Hartley & Kidd 1987)

2.90×10^{-4} ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

9.33×10^{-3} (20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

9.00×10^{-3} ($20^{\circ}C$, Montgomery 1993)

0.0295; 0.0039, 0.019 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

2.08×10^{-6} (20– $25^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

-1.97 (calculated, Montgomery 1993)

-0.22 (calculated, Tomlin 1994)

-0.20 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$

Sorption Partition Coefficient, $\log K_{OC}$:

0.0 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

2.29, 1.65 (soil, *trans*-isomer, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

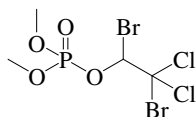
Hydrolysis: calculated $t_{1/2} = 96$ d at pH 5, $t_{1/2} = 66$ d at pH 7 and $t_{1/2} = 17$ d at pH 9 and 20°C (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Soil: selected field $t_{1/2} = 30$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 1$ –5 d in laboratory soil (Tomlin 1994).

18.1.1.62 Naled



Common Name: Naled

Synonym: Arthodibrom, Dibrom, Bromex, Bromchlophos

Chemical Name: 1,2-dibromo-2,2-dichloroethyl dimethyl phosphate

CAS Registry No: 300-76-5

Uses: insecticide

Molecular Formula: $C_4H_7Br_2Cl_2O_4P$

Molecular Weight: 380.784

Melting Point ($^{\circ}C$):

27 (Lide 2003)

Boiling Point ($^{\circ}C$):

110/0.5 mmHg (Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987; Montgomery 1993; Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.96 ($20^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

1.97 ($20^{\circ}C$, Worthing 1987)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.23 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.956 (mp at $27^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

practically insoluble in water (Hartley & Kidd 1987; Worthing & Walker 1987)

0.3, 2000 (quoted, Wauchope et al. 1992)

2000 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

10 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.266 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987; Tomlin 1994)

6.0×10^{-2} , 0.67, 5.20, 31.0, 150 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 12.307 - 4034.2/(T/K)$; measured range 50.5 – $120^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

0.267, 0.00267 (Wauchope et al. 1992)

0.0267 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.267 ($20^{\circ}C$, Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.38 (shake flask-GC/UV, Hussain et al. 1974)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

133, 2.26; 2.26 (soil, quoted values; selected, Wauchope et al. 1992; Hornsby et al. 1996)

2.14, 3.38 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: degraded by sunlight (Tomlin 1994).

Oxidation:

Hydrolysis: completely hydrolyzed in water within 2 d (Windholz 1983; quoted, Montgomery 1993);

rapidly hydrolyzed in water > 90% in 48 h at room temp. (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: completely hydrolyzed within 2 d (Windholz 1983; quoted, Montgomery 1993);

rapidly hydrolyzed in water > 90% in 48 h at room temp. (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994).

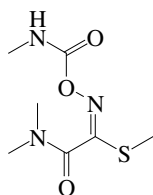
Ground water:

Sediment:

Soil: field $t_{1/2} = 1$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

18.1.1.63 Oxamyl



Common Name: Oxamyl

Synonym: D 1410, Dioxamyl, Dupont 1410, Nematicide 1410, Thioxamyl, Vydate

Chemical Name: *N,N*-dimethylcarbamoyloxyimino-2-(methylthio)acetamide; ethanimidothioic acid, 2-(dimethylamino)-*N*-[[[(methylamino)carbonyl]oxy]-2-oxo-methyl ester

Uses: insecticide/acaricide/nematicide

CAS Registry No: 23135-22-0

Molecular Formula: $C_7H_{13}N_3O_3S$

Molecular Weight: 219.261

Melting Point ($^{\circ}C$):

109 (Lide 2003)

Boiling Point ($^{\circ}C$):

dec (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.97 (Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

212.4 (calculated-Le Bas method at normal boiling point)

226.1 (calculated-density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.150 (mp at $109^{\circ}C$)

0.15 ($20^{\circ}C$, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

281000 (Martin & Worthing 1977)

280000 (Khan 1980, Spencer 1982; Montgomery 1993; Tomlin 1994; Milne 1995)

282500 (Briggs 1981, Gerstl & Helling 1987)

282000 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0306 (Khan 1980; Spencer 1982)

0.0306 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0311 (Montgomery 1993)

0.0310 (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.00026 (calculated-P/C, Suntio et al. 1988)

0.260 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

-0.432 (Briggs 1973)

-0.47 (20 – $25^{\circ}C$, shake flask- ^{14}C -labeled compound-LSC, Briggs 1981)

-0.432 (shake flask-centrifuge-liquid scintillation counting method, Gerstl 1984; Gerstl & Helling 1987)

-0.40	(Montgomery 1993)
-0.44	(pH 5, Tomlin 1994)
-0.47	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

0.707	(soil, sorption isotherm, converted from reported log K_{OM} of 0.47, Briggs 1981)
1.66, 1.07, 1.20, 1.32, 1.84	(5 Israeli soils, organic matter: 0.11% pH 8.5; 0.68% pH 7.9; 0.95% pH 7.8; 1.23% pH 7.2; and 2.03% pH 7.7, reported as K_{OM} , batch equilibrium-adsorption isotherms, Gerstl 1984)
0.176–1.16, -0.886–0.38	(reported as K_{OM} , estimated-S, estimated- K_{OW} , Gerstl 1984)
0.778	(soil, screening model calculations, Jury et al. 1987b)
2.47	(calculated-MCI χ , Gerstl & Helling 1987)
0.70	(soil, Carsel 1989)
1.40	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
-0.70 to 1.40	(Montgomery 1993)
1.00	(soil, calculated-MCI χ , Sabljic et al. 1995)
1.06, 1.68	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
1.43, 1.36	(soils: organic carbon OC \geq 0.1%, OC \geq 0.5%, average, Delle Site 2001)
1.08	(sediment: organic carbon OC \geq 0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 55.4$ h (absorbance wavelength 223 nm) (Montgomery 1993).

Oxidation:

$k(aq.) = (620 \pm 150) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2–7 and $24 \pm 1^\circ\text{C}$, with a $t_{1/2} = 54$ s at pH 7 (Yao & Haag 1991).

Hydrolysis: hydrolysis $t_{1/2} > 31$ d at pH 5, 8 d at pH 7 and $t_{1/2} = 3$ h at pH 9 (Tomlin 1994).

Biodegradation: decomposition rate constants range from $k = 0.182 \text{ d}^{-1}$ to 0.021 d^{-1} corresponding to $v = 4$ to 33 d in Bet Dagan soil depending on moisture, and decomposition rate constant ranges from $k = 0.23$ to 0.11 d^{-1} corresponding to $t_{1/2} = 3.1$ to 6.5 d in five Israeli soils (Gerstl 1984);
 $t_{1/2} = 6$ d in screening model calculations (Jury et al. 1987b); .

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: measured rate constant $k = (620 \pm 150) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.0–7.0 and $24 \pm 1^\circ\text{C}$, with $t_{1/2} = 54$ s at pH 7 (Yao & Haag 1991).

Ground water:

Sediment:

Soil: $t_{1/2} = 9$ –15 d (Harvey & Han 1978);

$t_{1/2} = 12$ –68 d for soils from Holland depending on the moisture content (Smelt et al. 1979);

$t_{1/2} = 15$ d in several soils at 15°C (Bromilow et al. 1980);

decomposition in soil was as a function of moisture content, and followed first-order kinetics with reported soil $t_{1/2} = 4$ –13 d at 25°C and, $t_{1/2} = 32.7$ d at 15°C , $t_{1/2} = 3.8$ d at 35° in Bet Dagan soil; rate constants between $k = 0.11$ – 0.23 d^{-1} and with $t_{1/2} \sim 4$ d in 5 Israeli soils (Gerstl 1984);

$t_{1/2} = 6$ d in screening model calculations (Jury et al. 1987b);

$t_{1/2} = 7$ d (Worthing & Hance 1991);

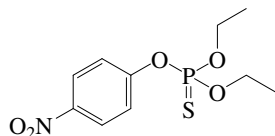
$t_{1/2} = 8$ –50 d (Ou & Rao 1986) and

$t_{1/2} = 10.2$ –13.1, 6.2, 7.1 and 17.8 d in Pitstone, Devizes, Sutton, Veany soils, respectively (Montgomery 1993);

field $t_{1/2} = 4$ d (selected, Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

18.1.1.64 Parathion



Common Name: Parathion

Synonym: AAT, AATP, AC 3422, Alkron, Alleron, American Cyanamid 3422, Aphamite, Aralo, B 404, Bay E-605, Bladan, Corothion, Corthion, Corthione, Danthion, DDP, Diethyl parathion, DNDP, DPP, E 605, Ecatox, Ekatox, ENT 15108, Ethlon, Ethyl parathion, Etilon, Folidol, Fosfermo, Fosferno, Fosfex, Fosfive, Fosova, Fostern, Fostox, Gearphos, Genithion, Kolphos, Kypthion, Lethalaire G54, Lirothion, Murfos, NA 2783, NCI-C00226, Niran, Nitrostigmine, Orthophos, Pac, Panthion, Paradust, Paraflow, Paramar, Paraphos, Paraspray, Parathene, Parathion-ethyl, Parawet, Penphos, Pestox plus, Pethion, Phoskil, Phosphemol, Phosphenol, Phosphostigmine, RB, Rhodiasol, Rhodiatox, Rhodiatrox, Selephos, SNP, Soprathion, Stathion, Strathion, Sulphos, Super rodiatox, T-47, Thiofos, Tiophos, Tox 47, Vapophos, Vitrex

Chemical Name: *O,O*-diethyl *O*-4-(nitrophenyl) phosphorothioate; diethyl 4-nitrophenyl phosphorothioate; phosphorothioic acid *O,O*-diethyl *O*-(4-nitrophenyl) ester

Uses: insecticide and acaricide to control chewing and sucking insects and mites in fruits, vegetables, ornamentals and field crops.

CAS Registry No: 56-38-2

Molecular Formula: $C_{10}H_{14}NO_5PS$

Molecular Weight: 291.261

Melting Point ($^{\circ}C$):

6.1 (Melnikov 1971; Freed et al. 1977; Montgomery 1993; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

115 (at 0.05 mmHg, Melnikov 1971; Freed et al. 1977)

375 (Montgomery 1993; Milne 1995)

105 (at 80 Pa, Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.265 ($25^{\circ}C$, Spencer 1982; Hartley & Kidd 1987; Milne 1995)

1.26 ($25^{\circ}C$, Merck Index 1989; Montgomery 1993)

1.2694 ($25^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

Molar Volume (cm^3/mol):

251.9 (calculated-Le Bas method at normal boiling point)

230.3 (calculated from density)

Dissociation Constant, pK_a :

7.14 (Kortum et al. 1961; Wolfe 1980)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

89.92 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.87 (DSC method, Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

24 (Macy 1948; Günther et al. 1968; Melnikov 1971; Spencer 1973)

18–31 (rm temp., > 95% purity with max. particle size 0.07–5.0 μ , shake flask-GC, Robeck et al. 1965)

11.9 ($20^{\circ}C$, NIEHS 1975; quoted, Freed et al. 1977)

11.9 ($20^{\circ}C$, O'Brien 1975)

24 (Martin & Worthing 1977; Worthing & Walker 1987; Hartley & Kidd 1987)

24 (Wauchope 1978; Khan 1980; Lyman 1982; Willis & McDowell 1982)

12.4 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983b)

6.54 (shake flask-GC, Felsot & Dahm 1979)

20	(Windholz 1983, Budavari 1989)
14.0	(shake flask-GC or LSC, Gerstl & Mingelgrin 1984)
11	(20°C, Worthing & Hance 1991; Tomlin 1994; Milne 1995)
12.9, 15.2	(20°C, 30°C, Montgomery 1993)
12	(20°C selected, Siebers & Mattusch 1996)
24	(20° C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5.04×10^{-3} *	12.3×10^{-3} (20, 30°C, calculated by Spencer et al. 1979-gas saturation, temp range 20–45°C, Bright et al. 1950)
$\log (P/\text{mmHg}) = 7.761 - 3395/(T/K)$	temp range 25.2–65.5°C (gas saturation, Bright et al. 1950)
2.56×10^{-3}	(20°C, effusion, measured range 25.2–65.5°C, Williams 1951)
$\log (P/\text{mmHg}) = 10.30 - 4400/(T/K)$	temp range 25.2–65.5°C (effusion, Williams 1951)
0.76×10^{-3}	(20°C, Wolfdietrich 1965)
5.07×10^{-3}	(20°C, Spencer 1973)
5.85×10^{-4}	(20°C, evaporation rate-gravimetric method Gückel et al. 1973, 1974)
0.76×10^{-3}	(20°C, Gückel et al. 1973, 1974)
1.29×10^{-3} *	(25°C, gas saturation method, measured range 25–45°C, Spencer et al. 1979)
$\log (P/\text{mmHg}) = 12.66 - 5274/(T/K)$	temp range 24.9–45°C (gas saturation Spencer et al. 1979)
6.41×10^{-4} *	(20°C, evaporation rate, measured range 20–60°C, Gückel et al. 1982)
1.29×10^{-3}	(Spencer 1983)
1.30×10^{-3} *	(25.3°C, gas saturation-GC, measured range 25.3–45°C, Kim et al. 1984; Kim 1985)
$\log (P/\text{mmHg}) = 10.5655 - 4645.07/(T/K)$	temp range 25.3–45°C (gas saturation, Kim 1985)
0.69×10^{-3}	(20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984; Kim 1985)
8.13×10^{-4}	(20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
5.0×10^{-3}	(20°C, Hartley & Kidd 1987)
1.80×10^{-3} *	(gas saturation-GC, measured range 25–125°C Rordorf 1989)
$\log (P_L/\text{Pa}) = 13.006 - 4697.2/(T/K)$	measured range 32.3–160°C (gas saturation-GC, Rordorf 1989)
6.7×10^{-3}	(P_L , GC-RT correlation, Hinckley et al. 1990)
8.90×10^{-4}	(20°C, Worthing & Hance 1991; Tomlin 1994)
0.0533	(20°C, Montgomery 1993)
6.67×10^{-4}	(20°C, selected, Hornsby et al. 1996)
1.30×10^{-3}	(20°C, selected, Siebers & Mattusch 1996)
0.00316; 0.0066, 0.0013, 0.00059, 0.0025	(gradient GC method; quoted lit. values, Tsuzuki 2000)
3.23×10^{-3} ; 1.12×10^{-3} , 0.00145	(gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

0.120	(20°C, calculated-P/C, Mackay & Shiu 1981)
0.074	(20°C, volatilization rate, Burkhard & Guth 1981)
0.096	(24°C, calculated-P/C, Chiou et al. 1980)
0.015	(calculated-P/C, Jury et al. 1984, 1987a; Jury & Ghodrati 1989)
0.012	(20°C, calculated-P/C, Suntio et al. 1988)
0.015	(calculated-P/C, Taylor & Glotfelty 1988)
0.0087	(23°C, Fendinger & Glotfelty 1990)
0.057	(calculated-P/C, Howard 1991)
0.030	(calculated-bond contribution method, Meylan Howard 1991)
0.0087	(calculated-P/C, Montgomery 1993)
0.020	(selected, Siebers & Mattusch 1996)

Octanol/Water Partition Coefficient, log K_{OW} :

3.81	(shake flask-GC, Chiou et al. 1977; Freed et al. 1977)
3.40	(shake flask-LSC, Felsot & Dahm 1979)
3.81	(shake flask-GC, Freed et al. 1979)

- 3.80 (Hansch & Leo 1979)
- 3.93 (shake flask-UV, Lord et al. 1980)
- 3.93 (shake flask-GC, Briggs 1981)
- 3.76 (shake flask-GC, Bowman & Sans 1983b)
- 3.83 (Hansch & Leo 1985)
- 2.15–3.93 (Montgomery 1993)
- 3.83 (recommended, Sangster 1993)
- 3.83 (Tomlin 1994)
- 3.83 (recommended, Hansch et al. 1995)
- 3.45 (RP-HPLC-RT correlation, Finizio et al. 1997)
- 4.32 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 2.53 (fish in static water, Metcalf & Sanborn 1975)
- 1.81 (tadpoles, Hall & Kolbe 1980)
- 2.00, 2.54 (calculated-S, K_{OC} , Kenaga 1980)
- 3.14 (earthworms, Lord et al. 1980)
- 4.00 (log BCF_{lipid}, Briggs 1981)
- 2.68 (calculated- K_{OW} , Hansch & Leo 1985)
- 2.48 (Am. oysters after 84 d.; Howard 1991)
- 1.48, 2.34 (av., fathead minnow after 70 d, 820, 138 d, Howard 1991)
- 2.34 (av., fathead minnow after 82–138 d, Howard 1991)
- 1.91, 2.27, 2.40, 1.43 (av., bluegill after 12 h, 29 h, 46 h, 504 d, Howard 1991)
- 1.95, 2.39, 2.50 (average, brook trout muscle after 8 h, 6 d, 180 d, Howard 1991)
- 1.90 (Isnard & Lambert 1988)
- 2.53 (Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

- 3.68 (soil, Swoboda & Thomas 1968; quoted, Kenaga 1980; Kenaga & Goring 1980)
- 4.02 (average, 4 soils, Hamaker & Thompson 1972)
- 3.30 (average, soils, Chiou et al. 1979)
- 2.88 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 2.90 (calculated-S, Mill et al. 1980)
- 4.03 (average soils/sediments, Rao & Davidson 1980)
- 3.02 (soil, sorption isotherm, converted from the reported log K_{OM} of 2.78, Briggs 1981)
- 3.25, 3.95, 3.42 (estimated-S, calculated-S and mp, calculated- K_{OW} , Karickhoff 1981)
- 2.26–3.96 (reported as log K_{OM} , Mingelgrin & Gerstl 1983)
- 2.83 (average, 8 Israeli soils, Gerstl & Mingelgrin 1984)
- 3.19 (average, 4 Israeli sediments, Gerstl & Mingelgrin 1984)
- 3.52, 2.58 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
- 3.04 (screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
- 3.68, 3.33 (reported, estimated as log K_{OM} , Magee 1991)
- 3.15 (estimated-QSAR and SPARC, Kollig 1993)
- 2.50–4.20 (Montgomery 1993)
- 3.70 (20°C, selected, Hornsby et al. 1996)
- 3.20 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.20; 3.57, 3.14 (soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 3.05, 3.09, 2.94 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)
- 3.17, 3.09 (average values for sediments with $OC \geq 0.5\%$, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: exptl. $t_{1/2} = 14$ d in nonstirred aqueous solutions and $t_{1/2} = 9.3$ d in stirred aqueous solutions, and estimated $t_{1/2} \sim 13$ d in nonstirred aqueous solutions and $t_{1/2} \sim 8.7$ d in stirred aqueous solutions (Chiou et al. 1980).

Photolysis: photoreacted 390 times more rapidly when sorbed by algae than in distilled water (Zepp & Schlotzhauer 1983)

direct photolysis has a $t_{1/2} < 1$ d to 10 d in surface waters, the presence of photosensitizers, free radicals, hydrogen peroxide, or algae which are found in eutrophic waters may accelerate degradation considerably (GEMS 1986; quoted, Howard 1991)

photodegradation $t_{1/2} = 88$ h (Hazardous Substances Data Bank 1989; quoted, Montgomery 1993)

$t_{1/2} = 55$ d without addition of humic substances; $t_{1/2} = 18$ d and $t_{1/2} = 9$ d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda \geq 290$ nm (Mansour & Feicht 1994).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{calc}) = 92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Winer & Atkinson 1990).

Hydrolysis:

$k(\text{second-order alkaline}) = 1.2 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C (Ketelaar 1950; quoted, Wolfe 1980)

$t_{1/2} = 130$ d at pH 7.4 and 20°C (NIEHS 1975; quoted, Freed et al. 1977, 1979; Montgomery 1993)

$t_{1/2} = 5240$ h, 180 h, 30 h, 4.47 h at room temp, 50, 70, 90°C , respectively, in estuarine water with salinity of 25.7‰ at pH 7.8; and $t_{1/2}$ ranging from 15.7–40.5 h in seawater or distilled water containing NaCl, NaOH or salt at 30 g/L at pH ranging from 1–8.0 at 70°C (Weber 1976)

$t_{1/2} = 24$ wk at pH 6, $t_{1/2} = 19$ wk at pH 7.4 and 20°C (Freed et al. 1979; quoted, Howard 1991; Montgomery 1993)

$t_{1/2} = 43$ wk at pH 5, $t_{1/2} = 24$ wk at pH 6, and $t_{1/2} = 15$ wk at pH 8 and 20°C (Chapman & Cole 1982; quoted, Howard 1991; Montgomery 1993)

$k(\text{alkaline}) = 2.3 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$, $k(\text{neutral}) = 4.5 \times 10^{-8} \text{ s}^{-1}$ in aqueous buffer at 20°C (Harris 1982)

$k = 2.4 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993); $t_{1/2} = 3.5$ wk at pH 6 (Montgomery 1993)

$t_{1/2} = 272$ d at pH 4, $t_{1/2} = 260$ d at pH 7, and $t_{1/2} = 130$ d at pH 9 at 22°C (Tomlin 1994).

Biodegradation: generally occurs with a half-life of several weeks but in well acclimated water, complete degradation may occur in two weeks (Eichelberger & Lichtenberg 1971; Sharom et al. 1980; quoted, Howard 1991)

$t_{1/2} > 4250$ d from biodegradation rate constant in aquatic systems from river water samples (Williams 1977; quoted, Scow 1982);

$k = 0.029 \text{ d}^{-1}$ in soil by die-away tests from soil incubation studies (Rao & Davidson 1980; quoted, Scow 1982)

$t_{1/2} = 18$ d for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1987a, b; Jury & Ghodrati 1989)

$k < 0.00016 \text{ d}^{-1}$ of aerobic degradation observed in incubations of river water samples (Lyman et al. 1990; quoted, Hemond & Fechner 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: persistence of up to 8 wk in river water (Eichelberger & Lichtenberg 1971)

$t_{1/2} = 3670$ h at pH 5 and $t_{1/2} = 523$ h at pH 9 in water at 20°C (Gomaa & Faust 1972)

estimated $t_{1/2} > 4250$ d from biodegradation rate constant in aquatic systems from river water samples (Williams 1977; quoted, Scow 1982);

$t_{1/2} = 5240$ h, 180 h, 30 h, 4.47 h at room temp, 50, 70, 90°C , respectively, in estuarine water with salinity of 25.7‰ at pH 7.8; and $t_{1/2}$ ranging from 15.7–40.5 h in seawater or distilled water containing NaCl, NaOH or salt at 30 g/L at pH ranging from 1–8.0 at 70°C (Weber 1976)

$t_{1/2} = 7.84$ d in the Indian River water at 24 ppt salinity; pH 8.16 (Wang & Hoffman 1991);

photolysis $t_{1/2} = 55$ d without addition of humic substances; $t_{1/2} = 18$ d and 9 d with concn of humic acid 20 mg/L and 50 mg/L, respectively, under light intensity $\lambda > 290$ nm (Mansour & Feicht 1994);

$t_{1/2} = 120$ d at 6°C , $t_{1/2} = 84$ d at 22°C in darkness for Milli-Q water at pH 6.1; $t_{1/2} = 120$ d at 6°C , $t_{1/2} = 86$ d at 22°C in darkness, 8 d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 122$ d at 6°C , $t_{1/2} = 33$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 542$ d at 6°C , $t_{1/2} = 44$ d at 22°C in darkness, $t_{1/2} = 18$ d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995).

Ground water:

Sediment:

Soil: persistence of one week (Edwards 1973; quoted, Morrill et al. 1982);

persistence of less than one month (Wauchope 1978);

$t_{1/2} > 24$ wk in sterile sandy loam and $t_{1/2} < 1.0$ wk in nonsterile sandy loam; $t_{1/2} > 24$ wk in sterile organic soil and $t_{1/2} = 1.5$ wk in nonsterile organic soil (Miles et al. 1979);

estimated first-order $t_{1/2} = 23.9$ d from biodegradation rate constant $k = 0.029$ d⁻¹ in soil by die-away tests from soil incubation studies (Rao & Davidson 1980; quoted, Scow 1982);

moderately persistent in soil with $t_{1/2} = 20$ –100 d (Willis & McDowell 1982);

reported $t_{1/2} = 18$ d calculated using screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989; quoted, Montgomery 1993);

av. degradation rate constant $k = 0.030$ d⁻¹ in silty clay with $t_{1/2} = 23$ d and av. degradation rate constant $k = 0.0315$ d⁻¹ in sandy clay with $t_{1/2} = 22$ d (Sattar 1990);

$t_{1/2} = 14$ d (selected, Halfon et al. 1996);

field $t_{1/2} = 14$ d (20–25°C, selected, Hornsby et al. 1996);

soil $t_{1/2} = 6$ d (Pait et al. 1992)

Biota: biochemical $t_{1/2} = 15$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

TABLE 18.1.1.64.1

Reported vapor pressures of parathion at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Bright et al. 1950		Williams 1951		Spencer et al. 1979		Gückel et al. 1982	
gas saturation		dynamic/microdistillation		gas saturation-GC		evaporation rate	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
	calc- eq. 1*				observed		
20	5.04×10^{-3}	20	2.61×10^{-3}	25	1.29×10^{-3}	20	6.41×10^{-4}
25	7.96×10^{-3}	25.4	4.68×10^{-3}	35	4.32×10^{-3}	40	7.29×10^{-3}
30	1.23×10^{-2}	54.5	0.088	45	0.01680	60	6.10×10^{-2}
35	1.86×10^{-2}	70.7	0.373				
40	2.79×10^{-2}	100	2.866		calculated from eq. 1		
45	0.04135	140	58.66	20	6.27×10^{-4}		
		160	142.7	25	1.26×10^{-3}		
eq. 1	P/mmHg		#extrapolated	30	2.45×10^{-3}		
A	7.161			35	4.71×10^{-3}		
B	3395	eq. 1	P/mmHg	40	8.83×10^{-3}		
		A	10.30	45	0.0162		
*calc by Spencer et al. 1979		B	4400				
				eq. 1	P/mmHg		
				A	12.66		
				B	5274		

TABLE 18.1.1.64.1 (Continued)

2.

Kim et al. 1984, Kim 1985		Rordorf 1989	
gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
25.3	0.00131	25	0.0018
34.9	0.00409	50	0.030
45.0	0.0120	75	0.330
20.0	0.0693	100	2.60
25.0	0.00131	125	16.0
eq. 1	P/mmHg	eq. 1	P/Pa
A	10.5654	A	13.006
B	4645.07	B	4697.2

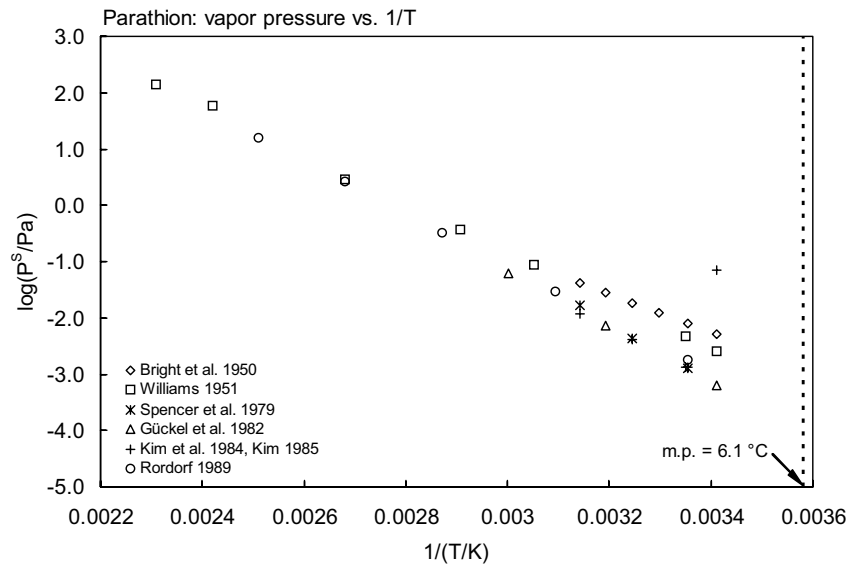
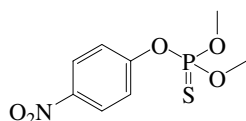


FIGURE 18.1.1.64.1 Logarithm of vapor pressure versus reciprocal temperature for parathion.

18.1.1.65 Parathion-methyl



Common Name: Parathion-methyl

Synonym: Bladan M, Folidol-M, Metacide, Nitrox 80

Chemical Name: *O,O*-dimethyl *O*-4-(nitrophenyl) phosphorothioate; dimethyl 4-nitrophenyl phosphorothioate

Uses: insecticide to control chewing and sucking insects, and mites in a wide range of crops, including fruits, vines, vegetables, ornamentals, cotton, and also used as acaricide.

CAS Registry No: 298-00-0

Molecular Formula: $C_8H_{10}NO_5PS$

Molecular Weight: 263.208

Melting Point ($^{\circ}C$):

38 (Lide 2003)

Boiling Point ($^{\circ}C$):

109 (at 0.05 mmHg, Freed et al. 1977)

119 (at 0.1 mmHg, Hartley & Kidd 1987)

154 (at 1.0 mmHg, Hartley & Kidd 1987; Tomlin 1994)

143 (Howard 1991)

Density (g/cm^3 at $20^{\circ}C$):

1.358 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Molar Volume (cm^3/mol):

207.5 (calculated-Le Bas method at normal boiling point)

194.0 (calculated from density)

Dissociation Constant, pK_a :

7.15 (Kortum et al. 1961; Wolfe 1980)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

24.06 (Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.746 (mp at $38^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

55 (Melnikov 1971)

60 (Leonard et al. 1976; Khan 1980)

57 (Martin & Worthing 1977)

50 (Smith et al. 1978; Wauchope 1978)

37.7 ($19.5^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983b)

55 ($20^{\circ}C$, Freed et al. 1979)

55–60 (Worthing 1979, 1983; Hartley & Kidd 1987)

60 (Khan 1980)

53 (Weber et al. 1980)

55 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

60 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00133 ($20^{\circ}C$, Wolfdietrich 1965; von Rümker & Horay 1972)

0.00129 ($20^{\circ}C$, Gückel et al. 1973)

0.0023 (Grover et al. 1976)

0.00229* ($24.9^{\circ}C$, gas saturation-GC, measured range 24.9 – $45.1^{\circ}C$, Spencer et al. 1979)

$\log(P/mmHg) = 14.37 - 3700/(T/K)$; temp range 24.9 – $34.9^{\circ}C$ (gas saturation, Spencer et al. 1979)

$\log(P/mmHg) = 10.61 - 4543/(T/K)$; above mp 35.2 – $35.4^{\circ}C$ (gas saturation, Spencer et al. 1979)

0.0013 (Worthing 1979)
 > 0.0133 (20–25°C, Weber et al. 1980)
 0.0020* (gas saturation-GC, measured range 25.4–45.1°C, Kim et al. 1984)
 $\log (P/\text{mmHg}) = 9.0935 - 4063.65/(T/K)$; temp range 25.4–45°C (gas saturation method, Kim et al. 1984)
 0.00084 (20°C, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984)
 $\log (P/\text{mmHg}) = 17.0502 - 6520.21/(T/K)$; temp range 25.4–34.3°C (gas saturation, Kim 1985)
 0.0013 (20°C, Hartley & Kidd 1987)
 0.0015 (22°C, selected, Seiber et al. 1989)
 0.023 (GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990)
 0.0024 (selected, Taylor & Spencer 1990)
 0.0002 (20°C, Worthing & Hance 1991; Tomlin 1994)
 0.002 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
 0.00041 (Tomlin 1994)
 0.00955 (gradient GC method; Tsuzuki 2000)
 9.77×10^{-3} ; 4.90×10^{-3} , 0.00389 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.0101 (Metcalf et al. 1980)
 0.0061 (estimated, Metcalf et al. 1980)
 0.0109 (calculated-P/C, Jury et al. 1987a; Jury & Ghodrati 1989)
 0.021 (20°C, calculated-P/C, Suntio et al. 1988)
 0.0101 (22°C, selected, Seiber et al. 1989)
 0.0062 (wetted wall column method-GC, Fendinger & Glotfelty 1990)
 0.0170 (calculated-bond contribution method, Meylan & Howard 1991)
 0.0062 (23°C, quoted, Schomburg et al. 1991)
 0.00383 (20°C, wetted wall column-GC, Rice et al. 1997b)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.04 (shake flask-GC, Jaglan & Gunther 1970)
 2.04 (shake flask, Leo et al. 1971)
 2.99 (shake flask, Mundy et al. 1978)
 2.68 (shake flask-HPLC, Moody et al. 1987)
 3.32 (Hansch & Leo 1979)
 3.32 (Rao & Davidson 1980)
 2.94 (shake flask-GC, Bowman & Sans 1983b)
 1.80 (shake flask-GC, Schimmel et al. 1983)
 2.86 (Hansch & Leo 1985)
 2.86 (recommended, Sangster 1993)
 2.71 (RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
 3.00 (Tomlin 1994)
 2.86 (recommended, Hansch et al. 1995)
 2.71 (RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, $\log \text{BCF}$:

0.778, 0.0 (carp/lipids, carp/muscle, Chigareva 1973)
 1.98 (fish in static water, Metcalf 1974)
 2.69 (bacteria, Smith et al. 1978)
 1.80, 2.89 (calculated-S; calculated- K_{oc} , Kenaga 1980)
 3.039 ± 0.005 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
 2.98 (guppy, calculated on an extractable lipid wt. basis, De Bruijn & Hermens 1991)
 3.04 (*Poecilia reticulata*, De Bruijn & Hermens 1991)
 1.85 (Pait et al. 1992)
 1.92 (paddy field fish, Tejada 1995)

Sorption Partition Coefficient, log K_{OC} :

- 3.99 (soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
- 1.699 (av. all sediments, Smith et al. 1978)
- 2.63 (av. of 3 soils, Rao & Davidson 1979)
- 2.67 (soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
- 3.71 (Rao & Davidson 1980)
- 3.02, 3.47, 2.93 (estimated-S, S and mp, K_{OW} , Karickhoff 1981)
- 3.71 (screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
- 3.84, 1.97 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
- 3.71–3.99 (soil, Carsel 1989)
- 3.00 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.71 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.68 (sediment, estimated, Paraiba et al. 1999)
- 3.27, 2.84 (soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
- 2.82, 2.74 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: volatilization rate $k < 0.01 \text{ kg ha}^{-1} \text{ d}^{-1}$ in a flooded rice field (Seiber et al. 1986; Seiber & McChesney 1987; quoted, Seiber et al. 1989)

Photolysis: lab. rate constant $k = 2.7 \times 10^{-7} \text{ s}^{-1}$ in early January with photolysis $t_{1/2} = 240 \text{ h}$, 850 h, 850 h and 170 h in river, pond, eutrophic lake and oligotrophic lake predicted by the one-compartment model (Smith et al. 1978; quoted, Howard et al. 1991);

$t_{1/2} = 8 \text{ d}$ in summer and $t_{1/2} = 38 \text{ d}$ in winter for direct sunlight photolysis in natural water (Smith et al. 1978; quoted, Howard 1991; Howard et al. 1991);

photolytic $t_{1/2} = 200 \text{ h}$ in aquatics (Haque et al. 1980);

photoreacted 390 times more rapidly when sorbed by algae than in distilled water (Zepp & Schlotzhauer 1983).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 3.0 \text{ M}^{-1} \text{ s}^{-1}$ (Smith et al. 1978)

photooxidation half-life of 3.6 d for the vapor-phase reaction with hydroxyl radical in the atmosphere (Atkinson 1985; quoted, Howard 1991);

photooxidation half-life of 1.0–10.5 h based on estimated rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis:

$k = .4 \times 10^{-2} \text{ mol min}^{-1}$ with $t_{1/2} = 125 \text{ h}$ for pH <11.0 at 15°C (Ketelaar & Gersmann 1958; quoted, Freed 1976)

$k = 1.1 \times 10^{-7} \text{ s}^{-1}$ with a half-life of 8.4 h at pH 6 buffer at 70°C in 20% ethanol aqueous solution (Ruzicka et al. 1967; quoted, Freed 1976; Smith et al. 1978)

$t_{1/2} = 1.7 \text{ wk}$ at pH about 6 and room temp. (Cowart et al. 1971; quoted, Smith et al. 1978)

$k = 1.1 \times 10^{-7} \text{ s}^{-1}$ with $t_{1/2} = 72 \text{ d}$ at pH 7 and 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991)

$k = 9 \times 10^{-7} \text{ s}^{-1}$ (Smith et al. 1978)

$k(\text{alkaline}) = 5.3 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 27°C and pH 10 (Smith et al. 1978; quoted, Wolfe 1980)

$t_{1/2} = 68 \text{ d}$ at pH 5, $t_{1/2} = 40 \text{ d}$ at pH 7, $t_{1/2} = 33 \text{ d}$ at pH 9 at 25°C (Tomlin 1994).

Biodegradation:

$k = 1.7 \times 10^{-7} \text{ -g cell}^{-1} \text{ h}^{-1}$ (Smith et al. 1978);

$t_{1/2}(\text{aq. aerobic}) = 360\text{--}1680 \text{ h}$, based on an unacclimated aerobic river die-away test data (Bourquin et al. 1979; Spain et al. 1980; quoted, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 24\text{--}168 \text{ h}$, based on unacclimated anaerobic soil and sediment grab sample data (Adhya et al. 1981; Wolfe et al. 1986; quoted, Howard et al. 1991);

$t_{1/2} = 15 \text{ d}$ for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983, 1987a, b; Jury & Ghodrati 1989);

$k = (0.003 \pm 0.0003) \text{ h}^{-1}$ with half-life of 220.9 h in surface aerobic soils at Williamsburg,

$k = (0.0017 \pm 0.00009) \text{ h}^{-1}$ with half-life of 410 h in subsurface aerobic soils at Sault Ste. Marie (Ward 1985)

$k = 0.30 \text{ d}^{-1}$ in river sediment, $k = 0.02 \text{ d}^{-1}$ in river water (Cripe et al. 1987; quoted, Battersby 1990)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$$k_1 = (2.59 \pm 0.88) \times 10^{-3} \text{ mL g}^{-1} \text{ d}^{-1} \text{ (guppy, De Bruijn \& Hermens 1991)}$$

$$k_2 = (2.38 \pm 0.14) \text{ d}^{-1} \text{ (guppy, De Bruijn \& Hermens 1991)}$$

$$k_2 = 1.71 \text{ d}^{-1} \text{ (guppy, calculated-} K_{OW} \text{, De Bruijn \& Hermens 1991)}$$

$$k_2 = (0.12 \pm 0.02) \times 10^{-3} \text{ (NADPH) min}^{-1} \text{ mg protein}^{-1} \text{ (rainbow trout, De Bruijn et al. 1993)}$$

$$k_2 = (0.11 \pm 0.03) \times 10^{-3} \text{ (GSH) min}^{-1} \text{ mg protein}^{-1} \text{ (rainbow trout, De Bruijn et al. 1993)}$$

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 3.6$ d for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard 1991);

photooxidation $t_{1/2} = 1.0$ – 10.5 h in air based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
reaction rate $k = 4.77 \times 10^{-4} \text{ min}^{-1}$ in air (Paraiba et al. 1999).

Surface water: persistence up to 4.0 wk in river water (Eichelberger & Lichtenberg 1971);

overall $t_{1/2} = 0.6$ h in river, $t_{1/2} = 15$ h in eutrophic pond, $t_{1/2} = 28.3$ h in eutrophic lake and $t_{1/2} = 157.5$ h oligotrophic lake (Smith et al. 1978);

$t_{1/2} = 8$ d in summer and $t_{1/2} = 38$ d in winter for direct sunlight photolysis in natural water (Howard 1991; Howard et al. 1991);

$t_{1/2} > 28$ d in 100 mL pesticide-seawater solution under indoor conditions, $t_{1/2} = 6.3$ d under outdoor light conditions and $t_{1/2} = 18$ d under outdoor dark conditions (Schimmel et al. 1983);

first-order biodegradation rate constant $k = 0.30 \text{ d}^{-1}$ in river sediment and $k = 0.02 \text{ d}^{-1}$ in river water (Cripe et al. 1987; quoted, Battersby 1990);

$t_{1/2} = 44$ h of dissipation from rice field water (Seiber & McChesney 1987; quoted, Seiber et al. 1989)

$t_{1/2} = 237$ d at 6°C , 46 d at 22°C in darkness for Milli-Q water at pH 6.1; $t_{1/2} = 95$ d at 0°C , 23 d at 22°C in darkness, $t_{1/2} = 11$ d under sunlight conditions for river water at pH 7.3; $t_{1/2} = 173$ d at 6°C , $t_{1/2} = 18$ d at 22°C in darkness for filtered river water at pH 7.3; $t_{1/2} = 233$ d at 6°C , $t_{1/2} = 30$ d at 22°C in darkness, $v = 34$ d under sunlight conditions for seawater at pH 8.1 (Lartiges & Garrigues 1995);

reaction rate $k = 3.80 \times 10^{-4} \text{ min}^{-1}$ in water (Paraiba et al. 1999).

Ground water: $t_{1/2} = 24$ – 1680 h based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} < 1.2$ d in 10 g sediment/100 mL pesticide-seawater solution under untreated conditions and $t_{1/2} > 28$ d under sterile conditions (Schimmel et al. 1983);

disappearance rate constants: $k = (3.5 \pm 0.6) \times 10^{-3} \text{ min}^{-1}$ in Beaver Dam sediments samples at pH 6.7, $k = (2.9 \pm 1.2) \times 10^{-3} \text{ min}^{-1}$ in Memorial Park sediments samples at pH 6.5 and $k = (2.8 \pm 2.4) \times 10^{-3} \text{ min}^{-1}$ in Hickory Hills sediments samples at pH 6.9 near Athens, Georgia (Wolfe et al. 1986);

reaction rate $k = 2.85 \times 10^{-5} \text{ min}^{-1}$ in sediment (Paraiba et al. 1999).

Soil: $t_{1/2} = 2,408,640$ h, based on unacclimated aerobic soil grab sample data (Davidson et al. 1980; Butler et al. 1981; quoted, Howard et al. 1991);

measured dissipation rate $k = 0.010$ – 0.034 d^{-1} (Baker & Applegate 1970; quoted, Nash 1988);

estimated dissipation rate $k = 0.029, 0.042 \text{ d}^{-1}$ (Nash 1988);

persistence of less than one month (Wauchope 1978);

non-persistent in soils with $t_{1/2} < 20$ d (Willis & McDowell 1982);

rate constant $k = 0.16 \text{ d}^{-1}$ with $t_{1/2} = 4$ d under laboratory conditions and rate constant $k = 0.046 \text{ d}^{-1}$ with $t_{1/2} = 15$ d under field conditions (Rao & Davidson 1980);

$t_{1/2} = 15$ d in screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989); selected field $t_{1/2} = 5.0$ d (Wauchope et al. 1992; quoted, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2} = 44$ d (Pait et al. 1992).

Biota: biochemical $t_{1/2} = 15$ d from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

TABLE 18.1.1.65.1

Reported vapor pressures of parathion-methyl at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Spencer et al. 1979		Kim et al. 1984	
gas saturation-GC		gas saturation-GC	
t/°C	P/Pa	t/°C	P/Pa
24.9	0.00229	25.4	0.00205
30.0	0.00529	30.1	0.00489
34.9	0.00960	34.3	0.00879
38.6	0.0148	38.5	0.0150
39.7	0.0164	41.7	0.0202
41.7	0.0207	45.1	0.0278
45.1	0.0291	20	0.00084#
		25	0.0020#
mp/°C	34.6		#extrapolated
eq. 1	P/mmHg	eq. 1	P/mmHg
A	14.37	A	9.9035
B	5700	B	4063.65

$$\Delta H_v = 109.2 \text{ kJ/mol}$$

above the melting point

eq. 1	P/mmHg
A	10.61
B	4543

$$\Delta H_v = 87.03 \text{ kJ/mol}$$

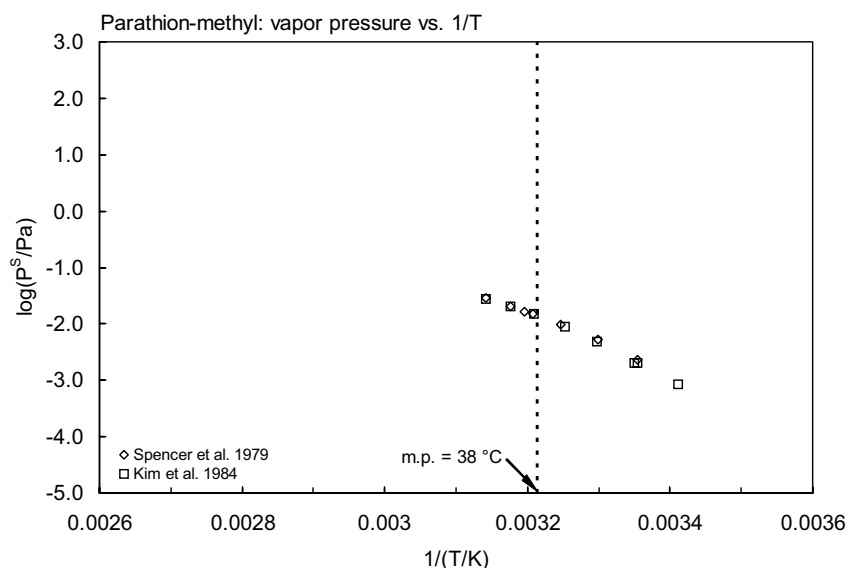
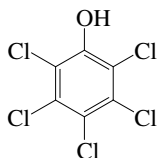


FIGURE 18.1.1.65.1 Logarithm of vapor pressure versus reciprocal temperature for parathion-methyl.

18.1.1.66 Pentachlorophenol

(See also [chapter 14](#). Phenolic Compounds)

Common Name: Pentachlorophenol

Synonym: chlorophen, PCP, penchlorol

Chemical Name: pentachlorophenol

Uses: insecticide/fungicide/herbicide; control of termites; as wood preservatives to protect against fungal rots and wood boring insects; as a pre-harvest defoliant in cotton; and also as a general pre-emergence herbicide.

CAS Registry No: 87-86-5

Molecular Formula: C_6Cl_5OH

Molecular Weight: 266.336

Melting Point ($^{\circ}C$):

191 (Firestone 1977; Weast 1982–83; Hartley & Kidd 1987)

187 (Schmidt-Bleek et al. 1982)

174 (Lide 2003)

Boiling Point ($^{\circ}C$):

310 (Verschueren 1977, 1983; Callahan et al. 1979)

309–310 (Hartley & Kidd 1987)

310 (dec, Lide 2003)

Density (20 $^{\circ}C$, g/cm³):

1.987 (Firestone 1977)

1.978 (Schmidt-Bleek et al. 1982; Verschueren 1983)

1.980 (22 $^{\circ}C$, Hartley & Kidd 1987)Dissociation Constant, pK_a :

4.80 (Blackman et al. 1955; Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)

5.0 (Farquharson et al. 1958; Renner 1990)

4.92 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)

4.74 (Drahonovsky & Vacek 1971; Callahan et al. 1979; Ugland et al. 1981; Könemann 1981; Könemann & Musch 1981; Dean 1985; Westall et al. 1985; Lagas 1988; Renner 1990; Lee et al. 1990,91)

4.71 (Cessna & Grover 1978; Saarikoski & Viluksela 1982; Saarikoski et al. 1986; Tratnyek & Hoigné 1991)

5.30 (Gebefügi et al. 1979; Xie 1983; Schellenberg et al. 1984)

4.70 (Crosby 1981; Hoigné & Bader 1983)

5.20 (Renberg 1981; Renner 1990; Larsson et al. 1993)

4.90 (Xie & Dryssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)

4.75 (Leuenberger et al. 1985)

4.60 (Nendza & Seydel 1988)

Molar Volume (cm³/mol):

207.9 (calculated-Le Bas method at normal boiling point)

134.3 (calculated-density)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.154 (Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K) F: 0.0345 (mp at 174 $^{\circ}C$)Water Solubility (g/m³ or mg/L at 25 $^{\circ}C$ or as indicated):

15.4 (gravimetric, Carswell & Nason 1938)

18 (27 $^{\circ}C$, gravimetric, Carswell & Nason 1938)

9.59 (shake flask-UV, at pH 5.1, Blackman et al. 1955)

14	(20°C, shake flask-UV, at pH 3.0, Bevenue & Beckman 1967)
10	(shake flask-gravimetric, at pH 5.0, Toyota & Kuwahara 1967)
14	(gravimetric at pH 5.0, Toyota & Kuwahara 1967)
20–25	(selected, Günther et al. 1968;)
20	(30°C, Firestone 1977)
14	(20°C, Verschueren 1977, 1983)
20	(20°C, Körte et al. 1978)
14	(Kenaga & Goring 1980; Geyer et al. 1982; McKim et al. 1985)
14, 20–25	(selected lit. values, Geyer et al. 1980, Geyer et al. 1984)
15	(23°C, Klöpffer et al. 1982)
20	(20°C, Schmidt-Bleek et al. 1982)
5–10	(at pH 5–6 in contaminated water, Goerlitz et al. 1985)
14	(recommended at pH 4.5–5.5, IUPAC 1985)
80	(20°C, Hartley & Kidd 1987)
41	(predicted-MCI χ , Nirmalakhandan & Speece 1988)
8 \pm 2	(shake flask-UV at pH 2.5, Valsaraj et al. 1991)
32 \pm 3	(shake flask-UV at pH 5.0, Valsaraj et al. 1991)
19	(quoted, Müller & Klein 1992)
18.4	(shake flask-HPLC/UV, at pH 4.8, Ma et al. 1993)

Vapor Pressure (Pa at 25°C or as indicated):

0.0227	(20°C, static method, Carswell & Nason 1938)
0.0147	(20°C, Bevenue & Beckman 1967)
0.231	(supercooled liq. extrapolated-Antoine eq., Weast 1976–77)
0.10	(Weast 1972–73)
0.0211	(Chiou & Freed 1977)
0.0213	(Firestone 1977)
0.0147–0.0227	(20°C, Goll 1954; Bevenue & Beckman 1967; Neumüller 1974)
0.0956	(supercooled liquid, Hamilton 1980; quoted, Bidleman & Renberg 1985)
0.00415	(23°C, OECD, Klöpffer et al. 1982)
0.0093	(20°C, Schmidt-Bleek et al. 1982)
0.0147	(20°C, Verschueren 1983; Howard 1991)
0.1153	(extrapolated-Antoine eq., Boublik et al. 1984)
0.50	(20°C, quoted, Crossland & Wolff 1985)
0.115	(capillary GC-RT correlation, Bidleman & Renberg 1985)
0.127	(extrapolated-Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol):

0.00248	(calculated-P/C, Hellmann 1987)
0.0127	(estimated-bond contribution, Hellmann 1987)
0.277	(calculated-P/C, Howard 1991)
0.079	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

5.01	(quoted unpublished result, Leo et al. 1971)
5.01	(Firestone 1977)
5.01, 5.12, 5.86, 3.81	(Hansch & Leo 1979)
5.01	(calculated, Veith et al. 1979b; McLeese et al. 1979)
2.97	(Veith et al. 1979)
3.69	(quoted from Kotzias 1980 unpublished result, Geyer et al. 1982)
4.16	(Rao & Davidson 1980)
5.10	(calculated-HPLC-k' correlation, Butte et al. 1981)
5.19	(calculated-f const., Könemann 1981; Könemann & Musch 1981)
4.00, 0.0	(at pH 4, 8, Renberg 1981)
5.08	(RP-HPLC-k' correlation, Miyake & Terada 1982)

- 5.15 (shake flask-GC, Saarikoski & Viluksela 1982; Saarikoski et al. 1986)
- 5.05 (Kaiser & Valdmanis 1982)
- 4.84 (shake flask-GC, apparent value at pH 1.2, Kaiser & Valdmanis 1982)
- 1.30 (shake flask-GC, apparent value at pH 10.5, Kaiser & Valdmanis 1982)
- 3.69 (Geyer et al. 1982, Schmidt-Bleek et al. 1982)
- 3.29 (shake flask average, OECD/EEC Lab. comparison tests, Harnisch et al. 1983)
- 5.01 (Verschuereen 1983)
- 5.85 (calculated as per Leo et al. 1971, Xie 1983)
- 5.11 ± 0.07 (exptl.-ALPM, Garst & Wilson 1984)
- 3.69, 3.81 (shake flask, OECD 1981 guidelines, Geyer et al. 1984)
- 5.24 (shake flask-HPLC/UV, Schellenberg et al. 1984)
- 5.04, 5.08, 5.85, 5.22 (shake flask-GC, HPLC-k', calculated- π const., calculated-f const., Xie et al. 1984; Bintein & Devillers 1994)
- 5.05 (calculated, Xie & Dryssen 1984; quoted, Lagas 1988)
- 5.24 (OECD 1981 guidelines, Leuenberger et al. 1985)
- 4.71 (RP-HPLC-RT correlation, Chin et al. 1986)
- 2.50 (at pH 4.7, Geyer et al. 1987)
- 4.47 (CPC-RV correlation, Terada et al. 1987)
- 4.07 (OECD 81 method, Kerler & Schönherr 1988)
- 5.04 (HPLC-RT correlation, Shigeoka et al. 1988; quoted, Saito et al. 1993)
- 5.00 (batch equilibration-UV, Beltrame et al. 1988)
- 5.06 (calculated-CLOGP, Müller & Klein 1992)
- 5.01, 5.38 (quoted, calculated-original UNIFAC, Chen et al. 1993)
- 5.24 (EPA CLOGP Data Base, Hulzebos et al. 1993)
- 5.18 (recommended, LOGKOW databank, Sangster 1993)
- 5.06, 5.12 (COMPUTOX databank, Kaiser 1993)
- 5.12 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 3.75 (fish, Statham et al. 1976)
- 3.04 (fish, Körte et al. 1978)
- 2.89 (fathead minnow, 32-d exposure, Veith et al. 1979)
- 2.89 (fathead minnow, calculated value, Veith et al. 1979b)
- 2.64 (algae, calculated, Geyer et al. 1981)
- 2.00 (trout, Hattula et al. 1981)
- 3.04, 3.10, 3.02 (activated sludge, algae, golden orfe, Freitag et al. 1982)
- 2.54 (mussel *Mytilus edulis*, quoted average, Geyer et al. 1982)
- 3.69 (calculated-K_{OW}, Mackay 1982)
- 1.60 (killifish, Trujillo et al. 1982)
- 1.86, 1.72, 1.60 (low-PCP flowing, high-PCP flowing, high-PCP static soft water; Brockway et al. 1984)
- 1.66, 1.62, 1.26 (low-PCP flowing, high-PCP flowing, high-PCP static hard water; Brockway et al. 1984)
- 3.10 (*alga chlorella fusca* in culture flasks, Geyer et al. 1984)
- 3.10, 2.72 (algae: exptl, calculated-K_{OW}, Geyer et al. 1984)
- 3.10, 3.02, 3.04 (algae, fish, sludge, Klein et al. 1984)
- 3.00 (quoted, LeBlanc 1984)
- 3.04, 3.10, 2.42 (activated sludge, algae, golden ide, Freitag et al. 1985)
- 0.57 (human fat, Geyer et al. 1987)
- 2.99 (zebrafish, Butte et al. 1987)
- 0.46 (15°C, initial concn. 1.0 mg/L uptake by *Allolobophora caliginosa* at 24 hours, Haque & Ebing 1988)
- 0.38 (15°C, initial concn. 10.0 mg/L uptake by *Allolobophora caliginosa* at 24 h, Haque & Ebing 1988)
- 0.80 (whole *Allolobophora caliginosa*/soil, uptake from soil after 131 d-exposure in outdoor lysimeters, Haque & Ebing 1988)
- 1.35 (whole *Lumbricus terrestris*/soil, uptake from soil after 131 d-exposure in outdoor lysimeters, Haque & Ebing 1988)
- 2.80, 2.63 (earthworm *E. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)

- 2.66 (daily intake/cow adipose tissue, Travis & Arms 1988)
- 4.10 (rainbow trout, field bioaccumulation, Thomann 1989)
- 4.38, 4.50, 4.53, 4.90 (earthworm system, Connell & Markwell 1990)
- 4.00, 5.30, 3.40, 8.00 (earthworm system, derived data, Connell & Markwell 1990)
- 2.97 (*P. hoyi*, Landrum & Dupuis 1990)
- 2.11 (*M. relictus*, Landrum & Dupuis 1990)
- 2.16–2.53 (soft tissue of freshwater mussel, Mäkelä & Oikari 1990)
- 2.33; 3.21 (flagfish: whole fish; fish lipid, Smith et al. 1990)
- 2.78, 2.11, 1.72 (goldfish at pH 7, pH 8, pH 9, Stehly & Hayton 1990)
- 2.89, 1.11 (fathead minnow, bluegill; Saito et al. 1992)
- 3.0, 3.4, 3.9, 4.0 (perch bile to water, Söderström et al. 1994)

Sorption Partition Coefficient, log K_{OC} :

- 2.95 (soil, calculated- K_{OW} , Kenaga & Goring 1980)
- 3.11–5.65 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a, b)
- 3.17–4.54 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a, b)
- 3.37–3.69 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a, b)
- 3.00–5.54 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a, b)
- 2.21–4.49 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a, b)
- 4.52 (sediment, Schellenberg et al. 1984)
- 2.95, 2.41 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
- 3.73 (quoted average of Kenaga & Goring 1980 and Schellenberg et al. 1984 values, Sabljic 1987a, b)
- 3.46 (soil, calculated-MCI χ , Sabljic 1987a, b)
- 2.95 (soil, calculated-MCI χ , Bahnick & Doucette 1988)
- 4.04 (estimated, HPLC- k' correlation, Hodson & Williams 1988)
- 4.40 (calculated, Lagas 1988)
- 3.10, 3.26 (totally dissociated as phenolate-calculated, Lagas 1988)
- 5.27, 5.71 (Bluepoint soil at pH 7.8, pH 7.4, Bellin et al. 1990)
- 5.58, 5.52 (Glendale soil at pH 7.3, pH 4.3, Bellin et al. 1990)
- 3.49, 3.57 (Norfolk soil at pH 4.3, pH 4.4, Bellin et al. 1990)
- 4.32–4.65 (Norfolk + lime soil at pH 6.9, Bellin et al. 1990)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization/evaporation: $t_{1/2} = 84$ h from the rate of loss experiment on watch glass for an exposure period of 192 h (Dobbs & Grant 1980);
- $k = 0.028$ d⁻¹ for nondissociated PCP, assuming diffusion coefficient in air to be 7×10^{-6} m²/s and in water 7×10^{-10} m²/s with wind speed 0.1 m above the pond is 2 m/s and the average temperature is 15°C for water depth of 1 m (Crossland & Wolff 1985);
- calculated rate constant $k = 5 \times 10^{-4}$ d⁻¹ to 1×10^{-7} d⁻¹ for total PCP (Crossland & Wolff 1985).
- Photolysis: calculated photolysis $t_{1/2} = 4.75$ h from observed rate $k = 3.4 \times 10^{-4}$ s⁻¹ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm² between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);
- photolysis $t_{1/2} = 1.5$ d was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);
- exposure of aqueous PCP solutions to either sunlight or laboratory ultraviolet light resulted in rapid degradation at pH 7.3 and slower degradation at pH 3.3 (Wong & Crosby 1981);
- photolytic $t_{1/2} = 10$ –15 d (Brockway et al. 1984);
- $k = 0.23$ to 0.46 d⁻¹ for direct photo-transformation, is the main loss process for PCP from ponds, with $t_{1/2} = 1.5$ to 3.0 d (Crossland & Wolff 1985);
- photo-transformation rate constant $k = 0.6$ h⁻¹ with $t_{1/2} = 1$ h for distilled water in summer (mean temperature 25°C) and $k = 0.37$ h⁻¹ with $t_{1/2} = 2$ h in winter (mean temperature 11°C); $k = 0.37$ h⁻¹ with $t_{1/2} = 2$ h for both poisoned estuarine water and estuarine water in summer and $k = 0.27$ h⁻¹ with $t_{1/2} = 3$ h in winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);
- photo-mineralization rate constant $k = 0.11$ h⁻¹ with $t_{1/2} = 6$ d for distilled water in summer (mean temperature 25°C) and $k = 0.049$ h⁻¹ with $t_{1/2} = 14$ d in winter (mean temperature 11°C); $k = 0.12$ h⁻¹ with $t_{1/2} = 6$ d

for poisoned estuarine water in summer and $k = 0.07 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ in winter; $k = 0.25 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ for estuarine water in summer and 0.10 h^{-1} with half-life of 7 d for winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);

phototransformation $t_{1/2} = 0.75 \text{ h}$ in Xenotest 1200 (Svenson & Björndal 1988);

aqueous photolysis $t_{1/2} = 1\text{--}110 \text{ h}$ (Hwang et al. 1986; Sugiura et al. 1984; selected, Howard et al. 1991);

$t_{1/2} = 7.43 \text{ d}$ assuming a linear rate of photolysis during 96-h period (Smith et al. 1987);

photodegradation rate constant $k = 0.60 \text{ h}^{-1}$ corresponding to $t_{1/2} = 1.0 \text{ h}$ (summer), $k = 0.37 \text{ h}^{-1}$ corresponding to $t_{1/2} = 2 \text{ h}$ (winter) in distilled water; and $k = 0.37 \text{ h}^{-1}$ corresponding to $t_{1/2} = 2 \text{ h}$ (summer), $k = 0.27 \text{ h}^{-1}$ corresponding to $t_{1/2} = 3.0 \text{ h}$ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).

Oxidation: rate constant $k \gg 3.0 \times 10^5 \text{ M}^{-1}\cdot\text{s}^{-1}$ for the reaction with ozone in water at pH 2.0 (Hoigné & Bader 1983);

photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reported reaction rate constants for reaction of OH and RO_2 radicals with phenol class in aqueous solution (Mill & Mabey 1985; Guesten et al. 1981; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 139.2\text{--}1392 \text{ h}$, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);

rate constant $k = (0.2 \pm 5.5) \times 10^6 \text{ M}^{-1}\cdot\text{s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $(27 \pm 1)^\circ\text{C}$ (Tratnyek & Hoigné 1991);

atmospheric $t_{1/2} < 24 \text{ h}$ at noon in mid-summer to $t_{1/2} = 216 \text{ h}$ in January at latitude of 41.79°N for reaction with OH radicals (Bunce et al. 1991).

Hydrolysis: is not expected to occur (Crossland & Wolff 1985).

Biodegradation: $t_{1/2} = 1800\text{--}2160 \text{ h}$ and $480\text{--}\infty \text{ h}$ to obtain 75% degradation in mineral medium and seawater, respectively (De Kreuk & Hanstveit 1981);

aqueous aerobic $t_{1/2} = 552\text{--}4272 \text{ h}$, based on unacclimated and acclimated aerobic sediment grab sample data (Delaune et al. 1983; Baker & Mayfield 1980; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 1008\text{--}36480 \text{ h}$, based on unacclimated anaerobic grab sample data for soil and ground water (Ide et al. 1972; Baker & Mayfield 1980; quoted, Howard et al. 1991);

aerobic degradation rate constant $k = 0.0017 \text{ L } \mu\text{g}^{-1}\cdot\text{d}^{-1}$ (Moos et al. 1983);

microbial degradation negligible in darkness (Hwang et al. 1986);

degradation rate constant $k = 0.12 \pm 0.01 \text{ h}^{-1}$ in the absence of light (Minero et al. 1993).

Biotransformation: degradation rate $k = 3 \times 10^{-14} \text{ mol}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 18.3 \text{ h}^{-1}$, 19 h^{-1} (at 1 mM buffer concn), 18.5 h^{-1} (at 10 mM buffer concn) at pH 8 (guppy *P. reticulata* Peters, Saarikoski et al. 1986)

$k_1 = 222 \text{ d}^{-1}$, 1677 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

$k_2 = 1.03 \text{ d}^{-1}$, 1.03 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

$k_2 = 1.03 \text{ d}^{-1}$, 0.95 d^{-1} (flagfish: BCF based, toxicity based, Smith et al. 1990)

$k_2 = 0.00195 \pm 0.00063 \text{ h}^{-1}$ (*M. relictus*, Landrum & Dupuis 1990)

$k_2 = 0.00330 \pm 0.00140 \text{ h}^{-1}$ (*P. hoyi*, Landrum & Dupuis 1990)

Half-Lives in the Environment:

Air: $t_{1/2} = 139.2\text{--}1392 \text{ h}$, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991);

photolysis $t_{1/2} = 6.5 \text{ h}$ in noonday summer sunshine (Howard 1991);

$t_{1/2} = 216 \text{ h}$ at latitude of 43.70°N at noon in January to $t_{1/2} < 24 \text{ h}$ in mid-summer for reaction with hydroxyl radicals (Bunce et al. 1991).

Surface water: calculated photolysis $t_{1/2} = 4.75 \text{ h}$ from a determined rate $k = 3.4 \times 10^{-4} \text{ s}^{-1}$ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm^2 between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);

photolysis $t_{1/2} = 1.5 \text{ d}$ was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);

photolytic $t_{1/2} = 10\text{--}15 \text{ d}$ (Brockway et al. 1984);

rate constant $k \gg 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 2.0 (Hoigné & Bader 1983);

$t_{1/2}$ = 1.5 to 3.0 d for direct photo-transformation from outdoor ponds (Crossland & Wolff 1985);

$t_{1/2}$ = 1 h in summer, $t_{1/2}$ = 2 h in winter for distilled water; $t_{1/2}$ = 2 h in summer, $t_{1/2}$ = 3 h in winter for estuarine water; $t_{1/2}$ = 2 h in summer, $t_{1/2}$ = 3 h in winter for poisoned estuarine water, based on photo-transformation rate constants (Hwang et al. 1986);

$t_{1/2}$ = 6 d in summer, $t_{1/2}$ = 14 d in winter for distilled water; $t_{1/2}$ = 3 d in summer, $t_{1/2}$ = 7 d in winter for estuarine water; $t_{1/2}$ = 6 d in summer, $t_{1/2}$ = 10 d in winter for poisoned estuarine water, based on photo-mineralization rate constants (Hwang et al. 1986);

$t_{1/2}$ = 0.75 h and 0.96 h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{1/2}$ = 1–110 h, based on aqueous photolysis half-life (Howard et al. 1991);

photodegradation half-lives ranging from hours to days, more rapid at the surface (Howard 1991);

photodegradation $t_{1/2}$ = 1.0 h in summer, 2.0 h in winter in distilled water and $t_{1/2}$ = 2.0 h in summer, 3.0 h in winter in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).

Ground water: $t_{1/2}$ = 1104–36,480 h, based on estimated unacclimated aqueous aerobic sediment grab sample data (Delaune et al. 1983; selected, Howard et al. 1991) and unacclimated anaerobic grab sample data for ground water (Baker & Mayfield 1980; selected, Howard et al. 1991).

Sediment:

Soil: disappearance $t_{1/2}$ = 23.2 d from Kooyenburg soil, $t_{1/2}$ = 47.9 d from Holten soil with earthworm *E. fetida andrei* and $t_{1/2}$ = 27.4 d from Kooyenburg soil, $t_{1/2}$ = 31.8 d from Holten soil with earthworm *L. rubellus* (van Gestel & Ma 1988);

$t_{1/2}$ = 552–4272 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2}$ = 12.0 d in an acidic clay soil with <1.0% organic matter and $t_{1/2}$ = 6.7 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab. microcosm experiments (Loehr & Matthews 1992).

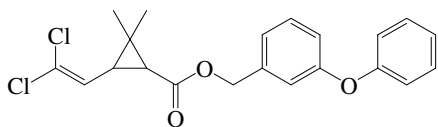
Biota: biological $t_{1/2}$ ~ 30 d in guppy *Lebistes reticulatus* (Landner et al. 1977);

elimination $t_{1/2}$ = 23, 9.3, 6.9, and 6.2 h for fat, liver muscle, and blood, respectively (rainbow trout, Call et al. 1980);

estimated $t_{1/2}$ = 7.0 d in trout (Niimi & Cho 1983; quoted, Niimi & Palazzo 1985);

clearance from flagfish: $t_{1/2}$ = 0.68 d from whole fish and $t_{1/2}$ = 0.68 d from fish lipid (Smith et al. 1990).

18.1.1.67 Permethrin



Common Name: Permethrin

Synonym: Ambush, Dragnet, Ectiban, Exmin, FMC 33297, FMC 41665, ICI-PP 557, Kafil, Kestrel, NDRC-143, NIA 33297, Niagara 33297, Outflank, Outflank-stockade, Perthrine, Picket, Pounce, Pramex, S 3151, SBP-1513, Talcord, WL 43479

Chemical Name: 3-phenoxybenzyl (1*RS*, 3*RS*; 1*RS*, 3*SR*)-3(2,2-dichlorovinyl)-2,2-dimethylcyclo-propanecarbo-xylate; 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid (3-phenoxyphenyl)methyl ester

Uses: insecticide to control overwintering forms of spider mites, aphids, and scale insects on fruit trees, vines, olives, bananas and ornamentals; used as herbicides to control grass and broadleaf weeds in umbelliferous crops, and in tree nurseries; also used as acaricide and surfactant.

CAS Registry No: 52645-53-1

Molecular Formula: C₂₁H₂₀Cl₂O₃

Molecular Weight: 391.288

Melting Point (°C):

liquid (tech. grade, Worthing & Hance 1991)
34 (Lide 2003)

Boiling Point (°C):

200 (at 0.01 mmHg, Hartley & Kidd 1987; Milne 1995)
200 (tech. grade at 0.1 mmHg, Worthing & Hance 1991; Tomlin 1994)
220 (at 0.05 mmHg, Montgomery 1993)
>290 (Tomlin 1994)

Density (g/cm³ at 20°C):

1.19–1.27 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994; Milne 1995)
1.214 (tech. grade at 25°C, Worthing & Hance 1991)

Molar Volume (cm³/mol):

431 (calculated-Le Bas method at normal boiling point)
318.1 (calculated-density)

Dissociation Constant, pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.816 (mp at 34°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

0.20 (Martin & Worthing 1977)
0.04 (shake flask-GC, Coats & O'Donnell-Jefferey 1979)
~ 0.2 (Spencer 1982)
0.05 (in seawater, Schimmel et al. 1983; Zaroogian et al. 1985; Clark et al. 1989)
0.20 (20°C, Hartley & Kidd 1987; Tomlin 1994)
0.20 (30°C, Worthing & Walker 1987, 1991)
0.006 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
0.2 (20°C, Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

4.8 × 10⁻⁶ (*cis* isomer, Barlow 1978)
4.9 × 10⁻⁶ (*cis* isomer, Wells et al. 1986)
3.7 × 10⁻⁶ (*trans* isomer, Barlow 1978)
3.1 × 10⁻⁶ (*trans* isomer, Wells et al. 1986)
4.5 × 10⁻⁵ (Hartley & Kidd 1987; Tomlin 1994)

1.0×10^{-5}	(<i>cis</i> isomer, GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990)
8.1×10^{-6}	(<i>trans</i> isomer, GC-RT correlation, supercooled liquid P_L , Hinckley et al. 1990)
1.3×10^{-6}	(tech. grade at 20°C, Worthing & Hance 1991)
2.5×10^{-6}	(pure <i>cis</i> isomer at 20°C, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)
1.5×10^{-6}	(pre <i>trans</i> isomer at 20°C, Worthing & Hance 1991; Tomlin 1994)
1.7×10^{-6}	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
$1.4 \times 10^{-5*}$	(<i>cis</i> isomer, Knudsen effusion, measured range 40–80°C, Goodman 1997)
8.71×10^{-6}	(solid P^S , converted from P_L determined by GC-RT correlation, Tsuzuki 2001)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.0867	(wetted wall column-GC, Fendinger & Glotfelty 1990)
2.50×10^{-5}	(calculated-bond contribution method, Meylan & Howard 1991)
0.00486	(20°C, calculated-P/C, Montgomery 1993)
0.0157	(20–25°C, calculated-P/C, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, log K_{OW} :

3.49	(shake flask-GC, Coats & O'Donnell-Jefferey 1979)
6.60	(calculated, Briggs 1981)
6.50	(shake flask-GC, Schimmel et al. 1983)
6.2 ± 0.9	(<i>cis</i> -form, HPLC-RT correlation, Muir et al. 1985)
5.7 ± 0.7	(<i>trans</i> -form, HPLC-RT correlation, Muir et al. 1985)
6.10	(tech. grade at 20°C, Worthing & Hance 1991; Tomlin 1994)
6.67	(HPLC-RT correlation, Hu & Leng 1992)
2.88–6.10	(Montgomery 1993)
6.50	(recommended, Sangster 1993)
6.10	(Milne 1995)
5.85	(RP-HPLC-RT correlation, Finizio et al. 1997)
5.73	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

3.18	(calculated-S, Kenaga 1980)
3.28	(Schimmel et al. 1983)
3.23, 3.49, 3.52	(<i>Pimephales promelas</i> , Spehar et al. 1983;)
1.49–1.84	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.08–2.13	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
0.95–1.70	(<i>trans</i> -form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
0.90–2.22	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in water, Muir et al. 1985)
1.46–2.62	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in sediment, Muir et al. 1985)
1.32–2.47	(<i>cis</i> -form on sediment, 24 h BCF for chironomid larvae in sediment/pore water, Muir et al. 1985)
4.71, 4.83	(oyster, calculated- K_{OW} & models, Zaroogian et al. 1985)
4.71, 4.83	(sheepshead minnow, calculated- K_{OW} & models, Zaroogian et al. 1985)
3.29, 3.39	(<i>Oncorhynchus mykiss</i> , Muir et al. 1994; quoted, Devillers et al. 1996)
2.79	(quoted, Pait et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

4.03	(calculated-S, Kenaga 1980)
2.76	(<i>cis</i> -form, silt, K_p on 34% DOC, Muir et al. 1985)
2.64	(<i>cis</i> -form, clay, K_p on 77% DOC, Muir et al. 1985)
2.64	(<i>trans</i> -form, silt, K_p on 23% DOC, Muir et al. 1985)
2.64	(<i>trans</i> -form, clay, K_p on 0% DOC, Muir et al. 1985)
5.25	(soil, calculated- χ and fragment contribution, Meylan et al. 1992)
5.00	(soil, 20–25°C, selected, Wauchope et al. 1992; Lohninger 1994; Hornsby et al. 1996)
1.32–2.79	(Montgomery 1993)
4.80	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
4.42, 4.35	(soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photodegradation rate constant $k = 1.73 \times 10^{-3} \text{ min}^{-1}$ and $t_{1/2} = 400 \text{ min}$ with TiO_2 as catalyst after 20 h irradiation at 222 nm (Hidaka et al. 1992).

Oxidation:

Hydrolysis:

Biodegradation:

$k = 1.24 \times 10^{-2} \text{ h}^{-1}$ by bacteria strain *A. sobria* with $t_{1/2} = 56 \text{ h}$, $k = 1.13 \times 10^{-2} \text{ h}^{-1}$ by *E. carotovora* with $t_{1/2} = 61 \text{ h}$, $k = 8.66 \times 10^{-3} \text{ h}^{-1}$ by *Y. frederiksenii* with $t_{1/2} = 80 \text{ h}$ and $k = 1.43 \times 10^{-3} \text{ h}^{-1}$ for the control, uninoculated solution with $t_{1/2} = 485 \text{ d}$ in aqueous soil-free phase (*cis*-permethrin, Lee et al. 2004)

$k = 1.50 \times 10^{-2} \text{ h}^{-1}$ by *A. sobria* with $t_{1/2} = 45 \text{ h}$, $k = 1.51 \times 10^{-2} \text{ h}^{-1}$ by *E. carotovora* with $t_{1/2} = 46 \text{ h}$, $k = 1.85 \times 10^{-2} \text{ h}^{-1}$ by *Y. frederiksenii* with $t_{1/2} = 37 \text{ h}$ and $k = 2.85 \times 10^{-3} \text{ h}^{-1}$ for the control, uninoculated solution with $t_{1/2} = 259 \text{ d}$ in aqueous soil-free phase (*trans*-permethrin, Lee et al. 2004)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 1.5\text{--}2.3 \text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

$k_1 = 1.50 \text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

$k_1 = 3.3\text{--}12.1 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system for *trans*-permethrin, 96-h exposure, Muir et al. 1983)

$k_1 = 4.9\text{--}14.7 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system for *trans*-permethrin, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)

$k_2 = 0.041 \text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system for *trans*-permethrin, calculated by concentration decay curve, Muir et al. 1983)

$k_2 = 0.021 \text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system for *trans*-permethrin, calculated by concentration decay curve, Muir et al. 1983)

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} > 21 \text{ d}$ in 100 mL pesticide-seawater solution under indoor conditions, $t_{1/2} = 14 \text{ d}$ under outdoor light conditions and $t_{1/2} > 14 \text{ d}$ under outdoor dark conditions (Schimmel et al. 1983);

biodegradation half-lives by bacteria strains: $t_{1/2} = 56 \text{ h}$ by *A. sobria*, $t_{1/2} = 61 \text{ h}$ by *E. carotovora*, $t_{1/2} = 80 \text{ h}$ by *Y. frederiksenii* and $t_{1/2} = 485 \text{ d}$ for the control, uninoculated solution for *cis*-permethrin; $t_{1/2} = 45 \text{ h}$ by *A. sobria*, $t_{1/2} = 46 \text{ h}$ by *E. carotovora*, $t_{1/2} = 37 \text{ h}$ by *Y. frederiksenii* and $t_{1/2} = 259 \text{ d}$ for the control, uninoculated solution for *trans*-permethrin (Lee et al. 2004)

Ground water:

Sediment: half-lives in 10 grams sediment/100 mL pesticide-seawater solution: $t_{1/2} < 2.5 \text{ d}$ for untreated sediment and $t_{1/2} > 28 \text{ d}$ for sterile sediment (Schimmel et al. 1983).

Soil: reported $t_{1/2} < 38 \text{ d}$ in soil containing 1.3–51.3% organic matter at pH 4.2–7.7 (Holmstead et al. 1978; quoted, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994);

selected field $t_{1/2} = 30 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996);

soil $t_{1/2} = 30 \text{ d}$ (Pait et al. 1992);

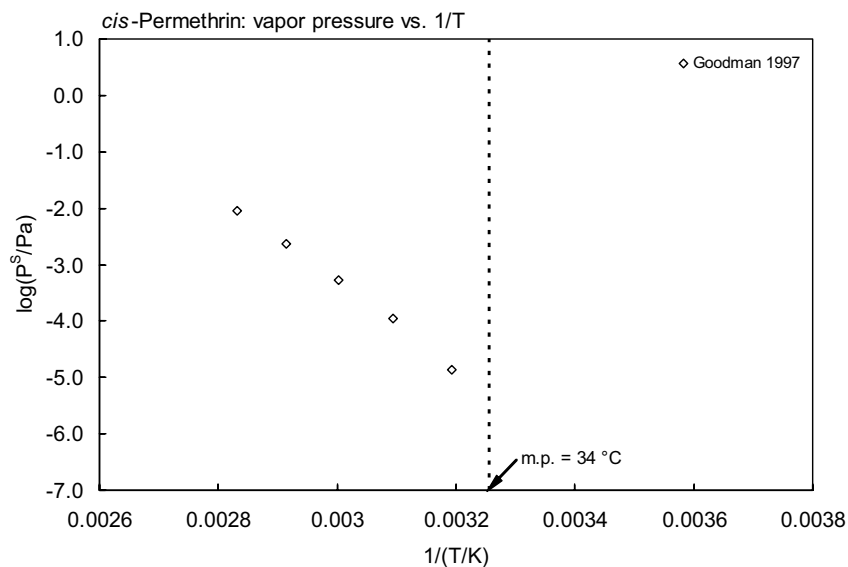
$t_{1/2} = 32 \text{ d}$ for forest soil (Dowd et al. 1993).

Biota: elimination $t_{1/2} \sim 16.7 \text{ h}$ in pond sediment-water, $t_{1/2} = 32.9 \text{ h}$ in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983)

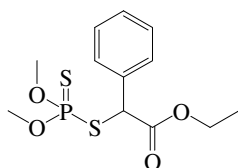
TABLE 18.1.1.67.1

Reported vapor pressures of *cis*-permethrin at various temperatures

Goodman 1997	
Knudsen effusion	
t/°C	P/Pa
40	1.4×10^{-5}
50	1.10×10^{-4}
60	5.30×10^{-4}
70	2.30×10^{-3}
80	8.90×10^{-3}
log P = A – B/(T/K)	
	P/Pa
A	18.70
B	7677

FIGURE 18.1.1.67.1 Logarithm of vapor pressure versus reciprocal temperature for *cis*-permethrin.

18.1.1.68 Phenthoate



Common Name: Phenthoate

Synonym: Cidial, Elsan

Chemical Name: ethyl 2-dimethoxyphosphinothioylthio(phenyl)acetate; ethyl 2-dimethoxy-thiophosphorylthio-2-phenylacetate; *S*- α -ethoxycarbonylbenzyl *O,O*-dimethyl phosphorodithioate; ethyl α -[(dimethoxy-phosphinothioyl)thio]benzeneacetate

Uses: insecticide to control aphids, scale insects, jassids, lepidopterous larvae, bollworms, mealybugs, psyllids, thrips, spider mites, etc. in citrus fruit, pome fruit, olives, cotton, cereals, rice, coffee, tea, sunflower, sugar cane, tobacco, ornamentals, and vegetables; also used as acaricide and for control of mosquito larvae.

CAS Registry No: 2597-03-7

Molecular Formula: $C_{12}H_{17}O_4PS_2$

Molecular Weight: 320.364

Melting Point ($^{\circ}C$):

17.5 (Khan 1980; Spencer 1982)

17–18 (Worthing & Hance 1991; Tomlin 1994)

Boiling Point ($^{\circ}C$): 78–80 (Spencer 1982)

Density (g/cm^3 at $20^{\circ}C$):

1.226 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Molar Volume (cm^3/mol):

261.3 (calculated from density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ K/ml K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

200 (Martin & Worthing 1977)

11 (20 – $25^{\circ}C$, shake flask-GC, Kanazawa 1981)

11 ($20^{\circ}C$, Khan 1980; Hartley & Kidd 1987)

11 ($24^{\circ}C$, Worthing & Walker 1987, 1991; Tomlin 1994)

11 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.005 ($40^{\circ}C$, Hartley & Kidd 1987)

0.0053 ($40^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

3.5×10^{-4} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

9.77×10^{-4} ; 2.45×10^{-4} ; 6.76×10^{-4} (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.01019 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.89 (shake flask-GC, Kanazawa 1981)

3.96 (shake flask/slow stirring-GC, De Bruijn et al. 1991)

3.69 (Worthing & Hance 1991; Tomlin 1994)

3.32 (RP-HPLC-RT correlation, Saito et al. 1993)

3.69 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 1.49 (calculated-S, Kenaga 1980)
- 1.56 (topmouth gudgeon *Pseudorasbora parva*, Kanazawa 1981)
- 2.85 (whole body willow shiner after 168 h exposure, Tsuda et al. 1992)
- 1.57, 1.43, 1.30, 1.51 (whole body carp: 24 h, 72 h, 120 h and 168 h; Tsuda et al. 1993)

Sorption Partition Coefficient, log K_{OC} :

- 2.38 (soil, calculated-S, Kenaga 1980)
- 3.00 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

- excretion rate constant $k = 0.05 \text{ h}^{-1}$ from whole body willow shiner (Tsuda et al. 1992);
- excretion rate constant $k = 0.52 \text{ h}^{-1}$ with $t_{1/2} = 1.3 \text{ h}$ (Tsuda et al. 1993).

Half-Lives in the Environment:

Air:

Surface water:

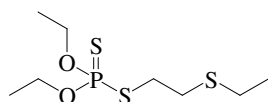
Ground water:

Sediment:

Soil: selected field $t_{1/2} = 11 \text{ d}$ (Augustijn-Beckers et al. 1994; Hornsby et al. 1996);
 $t_{1/2} = 10 \text{ d}$ in silty clay loam and other soils (Tomlin 1994).

Biota: excretion rate constant $k = 0.05 \text{ h}^{-1}$ from whole body willow shiner (Tsuda et al. 1992);
excretion rate constant $k = 0.52 \text{ h}^{-1}$ with $t_{1/2} = 1.3 \text{ h}$ (Tsuda et al. 1993).

18.1.1.69 Phorate



Common Name: Phorate

Synonym: AC 3911, American Cyanamid 3911, ENT 24042, Foraat, Gramitox, Granutox, Rampart, Thimate, Thimet, Timet, Vegfu, Vergfru foratox

Chemical Name: *O,O*-diethyl-*S*-(ethylthio)methyl phosphorodithioate; *O,O*-diethyl-*S*-ethylmercaptomethyl dithiophosphate; phosphorodithioic acid *O,O*-diethyl *S*-((ethylthio)methyl) ester

Uses: insecticide to control mites, chewing and sucking insects in fruits and vegetables, cotton, and some ornamentals; also used as acaricide and nematicide.

CAS Registry No: 298-02-2

Molecular Formula: $C_7H_{17}O_2PS_3$

Molecular Weight: 260.378

Melting Point ($^{\circ}C$):

−42.9 (Spencer 1982)

<−15 (Montgomery 1993; Lide 2003)

Boiling Point ($^{\circ}C$):

118–120 (at 0.8 mmHg, Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

125–127 (at 2 mmHg, Budavari 1989; Milne 1995)

118–120 (tech. grade at 0.8 mmHg, Worthing & Hance 1991)

Density (g/cm^3 at $20^{\circ}C$):

1.156 ($25^{\circ}C$, Merck Index 1989; Montgomery 1993; Milne 1995)

1.167 (tech. grade at $25^{\circ}C$, Spencer 1982; Worthing & Hance 1991)

Molar Volume (cm^3/mol):

259.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

19 ($26^{\circ}C$, 95% pure, shake flask-GC, Lord & Burt 1964)

14 ($15^{\circ}C$, shake flask-GC, Lord & Burt 1964)

85 (Günther et al. 1968)

70 (Melnikov 1971; Briggs 1981)

50 (Spencer 1973, 1982)

50 (Martin & Worthing 1977; Hartley & Kidd 1987)

80–85 (Wauchope 1978)

20 (shake flask-GC, Felsot & Dahm 1979)

17.9 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983b)

50 (room temp., Worthing & Walker 1987; Budavari 1989, Milne 1995)

50 (tech. grade at room temp., Worthing & Hance 1991)

22 (20 – $25^{\circ}C$, selected, Wauchope 1989; Wauchope et al. 1992; Hornsby et al. 1996)

20 ($24^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.112 ($20^{\circ}C$, Wolfdietrich 1965; Spencer 1973, 1982)

0.25 (Woolford 1975)

0.148 (gas saturation method, Sutherland et al. 1980)

0.074 (gas saturation-GC, Kim et al. 1984)

0.042 ($20^{\circ}C$, extrapolated-Clausius-Clapeyron eq., Kim et al. 1984)

0.0109	(20°C, GC-RT correlation, Kim et al. 1984; Kim 1985)
0.11	(20°C, Hartley & Kidd 1987)
0.112	(20°C, Budavari 1989; Montgomery 1993)
0.11	(GC-RT correlation method, Hinckley et al. 1990)
0.085	(tech. grade, Worthing & Hance 1991)
0.0853	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.769	(calculated-P/C, Jury et al. 1984, 1987a, 1990; Jury & Ghodrati 1989)
0.65	(20°C, calculated-P/C, Suntio et al. 1988)
0.648	(20–24°C, calculated-P/C, Montgomery 1993)
1.010	(calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

3.33	(shake flask-GC, Felsot & Dahm 1979)
2.92	(Rao & Davidson 1980)
4.26	(shake flask-UV, Lord et al. 1980)
4.26	(20°C, shake flask-GC, Briggs 1981)
3.83	(22°C, shake flask-GC, Bowman & Sans 1983b)
3.24	(shake flask, Log P Database, Hansch & Leo 1987)
3.92	(Worthing & Hance 1991)
2.91–3.92	(Montgomery 1993)
2.92	(recommended, Sangster 1993)
3.92	(Milne 1995)
3.56	(selected, Hansch et al. 1995)
4.25	(RP-HPLC-RT correlation, Finizio et al. 1997)
3.94	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.83, 2.34	(calculated-S, calculated-K _{OC} , Kenaga 1980)
3.34	(earthworms, Lord et al. 1980)
–1.70	(vegetation, correlated-K _{OW} , Travis & Arms 1988)

Sorption Partition Coefficient, log K_{OC}:

3.51	(soil, Hamaker & Thompson 1972; Kenaga 1980; Kenaga & Goring 1980)
2.71	(soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
2.82	(Rao & Davidson 1980; quoted, Jury et al. 1983, 1984, 1990)
2.82	(soil, sorption isotherm, converted form reported log K _{OM} of 2.82, Briggs 1981)
2.32–3.60	(reported as log K _{OM} , Mingelgrin & Gerstl 1983)
2.82	(screening model calculations, Jury et al. 1987a, b; Jury & Ghodrati 1989)
2.58, 2.88	(reported as log K _{OM} , estimated as log K _{OM} , Magee 1991)
2.73	(soil, Worthing & Hance 1991)
3.00	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
2.64	(estimated-QSAR & SPARC, Kollig 1993)
2.51–2.80	(Montgomery 1993)
2.82	(selected, Lohninger 1994)
2.70	(soil, calculated-MCI ¹ χ, Sabljic et al. 1995)
2.70; 2.98, 3.12	(soil, quoted exptl.; estimated-class-specific model, estimated-general model, Gramatica et al. 2000)
2.63	(soil: organic carbon OC -0.5%, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: neutral hydrolysis rate constant $k = 7.2 \times 10^{-3} \text{ h}^{-1}$ with a calculated $t_{1/2} = 96 \text{ h}$ at pH 7 (Ellington et al. 1987, 1988; quoted, Montgomery 1993);
calculated rate constant $k = 100 \times 10^{-12} \text{ cm}^3/\text{molecule}\cdot\text{s}$ for the vapor-phase reaction with hydroxyl radical in air (Winer & Atkinson 1990);

$t_{1/2} = 3.2 \text{ d}$ at pH 7 and $t_{1/2} = 3.9 \text{ d}$ at pH 9 (Worthing & Hance 1991);

rate constant $k = 62 \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993).

Biodegradation: $t_{1/2} = 82 \text{ d}$ for a 100 d leaching and screening test in 0–10 cm depth of soil (Rao & Davidson 1980; quoted, Jury et al. 1983);

$t_{1/2} = 82 \text{ d}$ in soil (Jury et al. 1984, 1987a, b, 1990; Jury & Ghorati 1989);

first-order rate constant $k = -0.0403 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.0209 \text{ h}^{-1}$ in sterile sediment by shake-tests at Range Point and first-order rate constant $k = -0.0206 \text{ h}^{-1}$ in nonsterile water and $k = -0.0186 \text{ h}^{-1}$ in sterile water by shake-tests at Range Point (Walker et al. 1988);

first-order rate constants $k = -0.0241 \text{ h}^{-1}$ in nonsterile sediment and $k = -0.0185 \text{ h}^{-1}$ in sterile sediment by shake-tests at Davis Bayou and first-order rate constants $k = -0.0262 \text{ h}^{-1}$ in nonsterile water and $k = -0.0185 \text{ h}^{-1}$ in sterile water by shake-tests at Davis Bayou (Walker et al. 1988).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

Sediment:

Soil: $t_{1/2} = 68 \text{ d}$ in a sandy soil (Way & Scopes 1968; quoted, Montgomery 1993);

estimated persistence of 2 wk (Kearney et al. 1969; Edwards 1973; quoted, Morrill et al. 1982; Jury et al. 1987a);

persistence of less than one month (Wauchope 1978);

biodegradation $t_{1/2} = 82 \text{ d}$ in soil (Jury et al. 1984, 1987a, b, 1990; Jury & Ghodrati 1989; quoted, Montgomery 1993);

$t_{1/2} = 2\text{--}14 \text{ d}$ (Worthing & Hance 1991);

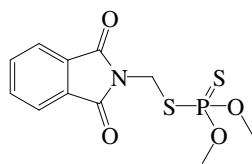
estimated field $t_{1/2} = 60 \text{ d}$ (Wauchope et al. 1992; quoted, Richards & Baker 1993; selected, Halfon et al. 1996; Hornsby et al. 1996);

soil $t_{1/2} = 25 \text{ d}$ (Pait et al. 1992).

Biota: $t_{1/2} = 1.4 \text{ d}$ half-lives in coastal Bermuda grass and alfalfa (Leuck & Bowman 1970; quoted, Montgomery 1993) and $t_{1/2} = 3.6 \text{ d}$ (Dobson et al. 1960; quoted, Montgomery 1993);

biochemical $t_{1/2} = 82 \text{ d}$ from screening model calculations (Jury et al. 1987a, b; Jury & Ghodrati 1989).

18.1.1.70 Phosmet



Common Name: Phosmet

Synonym: APPA, Decemthion, Decemthion p-6, ENT 25,705, Ftalophos, Imidan, Percolate, Phthalophos, Prolate, R 1504, Safidon, Smidan, Stauffer R-1504

Chemical Name: *O,O*-dimethyl *S*-phthalimidomethyl phosphorodithioate; *N*-dimethoxyphosphino-thioylthiome-thylphthalimide; *S*-[(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl] *O,O*-dimethyl phosphorodithioate; phospho-rodithioic acid, *S*-[(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl] *O,O*-dimethyl ester

Uses: nonsystemic acaricide and insecticide.

CAS Registry No: 732-11-6

Molecular Formula: $C_{11}H_{12}NO_4PS_2$

Molecular Weight: 317.321

Melting Point ($^{\circ}C$):

72.0–72.7, 66.5–69.5 (pure, technical grade, Montgomery 1993; Tomlin 1994)

72 (Lide 2003)

Boiling Point ($^{\circ}C$):

decompose rapidly $>100^{\circ}C$ (Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

263.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.96 (Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.346 (mp at $72^{\circ}C$)

0.3 ($20^{\circ}C$, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

25 (Bright et al. 1950, Melnikov 1971; Spencer 1982)

25 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

20 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

22–25 (Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

6.03×10^{-4} ($20^{\circ}C$, Freed et al. 1977)

0.133 ($50^{\circ}C$, Spencer 1982; Hartley & Kidd 1987)

6.53×10^{-5} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

6.03×10^{-5} , 0.133 (30, $50^{\circ}C$, Montgomery 1993)

6.50×10^{-5} (Tomlin 1994)

2.0×10^{-5} ; 5.90×10^{-5} (gradient GC method; quoted lit. value, Tsuzuki 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$):

9.50×10^{-4} (calculated-P/C, Suntio et al. 1988)

9.53×10^{-4} (calculated-P/C, Montgomery 1993)

7.62×10^{-4} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.83 ($20^{\circ}C$, shake flask-GC, Chiou et al. 1977)

2.83 (Rao & Davidson 1980)

2.78	(22°C, shake flask-GC, Bowman & Sans 1983)
2.81	(shake flask/slow stirring-GC, De Bruijn & Hermens 1991)
2.78–3.04	(Montgomery 1993)
2.78	(recommended, Sangster 1993)
2.95	(Tomlin 1994)
3.40	(Milne 1995)
2.78	(recommended, Hansch et al. 1995)
3.06	(RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

0.90	(bluegill sunfish/fathead minnows, Saito et al. 1992)
1.04	(channel catfish, Saito et al. 1992)
1.56	(av. whole body willow shiner after 24–168 h exposure, Tsuda et al. 1992)
0.23	(av. whole body carp after 24–168 h exposure, Tsuda et al. 1993)

Sorption Partition Coefficient, log K_{OC} :

2.91	(soil, Wauchope et al. 1992, Hornsby et al. 1996)
2.06, 2.34	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 53.25$ h for absorbance wavelength at 243 nm (Montgomery 1993).

Oxidation:

Hydrolysis: $t_{1/2} = 7.2$ d at pH 6.1 and $t_{1/2} = 7.1$ h at pH 7.4 at 20°C; $t_{1/2} = 1.1$ h at 37.5°C (Freed et al. 1979; quoted, Montgomery 1993);

$t_{1/2} = 13$ d at pH 4.5, $t_{1/2} < 12$ h at pH 7 and $t_{1/2} < 4$ h at pH 8.3 in buffered aqueous solution at 20°C (Montgomery 1993);

$t_{1/2} = 7.0$ d at pH 6.1, and $t_{1/2} = 7.1$ h at pH 7.4 at 20°C (Lartiges & Garrigues 1995).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.28$ h⁻¹ (whole body willow shiner, Tsuda et al. 1992)

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 33$ d at 6°C, $t_{1/2} = 5$ d at 22°C in darkness for Milli-Q water at pH 6.1 (Lartiges & Garrigues 1995).

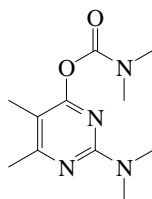
Ground water:

Sediment:

Soil: field $t_{1/2} = 10$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota: $t_{1/2} = 6.5$ d in Bermuda grass (Montgomery 1993).

18.1.1.71 Pirimicarb



Common Name: Pirimicarb

Synonym: Pirimor, Aphox, Abol, Aficida, Fernos, Rapid

Chemical Name: 2-dimethylamino-5,6-dimethylpyrimidin-4-yl dimethylcarbamate

CAS Registry No: 23103-98-2

Uses: insecticide

Molecular Formula: $C_{11}H_{18}N_4O_2$

Molecular Weight: 238.287

Melting Point ($^{\circ}C$):

90.5 (Spencer 1982; Hartley & Kidd 1987; Worthing 1987; Tomlin 1994; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.21 (Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.228 (mp at $90.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2700 (Kenaga 1980b; Spencer 1982; Hartley & Kidd 1987; Worthing & Walker 1987)

2000 (pH 4, $20^{\circ}C$, Tomlin 1994)

2700 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

0.004 ($30^{\circ}C$, Spencer 1982. Hartley & Kidd 1987; Worthing & Walker 1987)

0.00097 (Tomlin 1994)

0.004 (selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.70 (Tomlin 1994)

1.70 (recommended, Hansch et al. 1995)

1.70 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

0.845 (calculated-Solubility, Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{oc}$:

1.76 (soil, Kenaga 1980b)

1.57 (soil, estimated and selected value, Augustijn-Beckers et al. 1994)

1.36 (soil, estimated and selected, Hornsby et al. 1996)

1.90, 1.52 (soil: quoted, calculated-MCI χ , Meylan et al. 1992)

1.90 (soil, calculated-MCI χ , Sabljic et al 1995)

1.90; 2.30, 1.80 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: aqueous solutions are unstable to UV light with $t_{1/2} < 1$ d at pH 5.7 or 9 (Tomlin 1994).

Oxidation:

Hydrolysis:

Biodegradation: $t_{1/2} = 7\text{--}234$ d depending on soil type, organic matter ranging from 1.7–51.9% at pH 5.5–8.1 (Tomlin 1994).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: aqueous solutions are unstable to UV light with $t_{1/2} < 1$ d at pH 5.7 or 9 (Tomlin 1994).

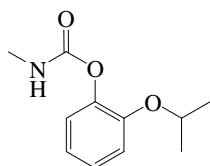
Ground water:

Sediment:

Soil: $t_{1/2} = 7\text{--}234$ d depending on soil type, organic matter ranging from 1.7–51.9% at pH 5.5–8.1 (Tomlin 1994);
field $t_{1/2} \sim 10$ d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

18.1.1.72 Propoxur



Common Name: Propoxur

Synonym: Baygon, Blattanex, Under, arprocarb, PHC, Sendran, Suncide, Aracarb, Tugon Fliegendugel

Chemical Name: 2-(1-methylethoxy)phenol methyl carbamate

CAS Registry No: 114-26-1

Uses: insecticide to control cockroaches, flies, fleas, mosquitoes, bugs, ants, millipedes and other insect pests in food storage areas, houses, animal houses, etc.; also to control sucking and chewing insects in fruits, vegetables, ornamentals, vines, maize, lucerne, soya beans, cotton, sugar cane, rice cocoa, forestry, etc.

Molecular Formula: $C_{11}H_{15}NO_3$

Molecular Weight: 209.242

Melting Point ($^{\circ}C$)

91.50 (Spencer 1982; Howard 1991; Kühne et al. 1995)

84–87 (Montgomery 1993)

87 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

244.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.246 (mp at $87^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2000 ($20^{\circ}C$, Spencer 1973; 1982)

2000 (Kenaga 1980; Kanazawa 1981)

2000 ($20^{\circ}C$, Worthing & Walker 1983, 1987, Worthing & Hance 1991)

1860 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983)

1800 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1740, 1930, 2440 (10, 20, $30^{\circ}C$, Montgomery 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.333 ($120^{\circ}C$, Melnikov 1971; Spencer 1973, 1982)

4.13×10^{-4} ($20^{\circ}C$, Hartley & Graham-Bryce 1980)

4.13×10^{-5} ($20^{\circ}C$, selected exptl. value from literature, Kim 1985)

0.0593, 0.0113 ($20^{\circ}C$, GC-RT correlation, GC-RT correlation with mp correction, Kim 1985)

4.00×10^{-4} ($20^{\circ}C$, Howard 1991)

1.69×10^{-3} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992, Hornsby et al. 1996)

1.30×10^{-3} ($20^{\circ}C$, Montgomery 1993; Siebers et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.1308 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

4.46×10^{-5} (calculated-P/C, Howard 1991)

1.32×10^{-4} (calculated-P/C, Montgomery 1993)

1.40×10^{-4} (calculated-P/C, Siebers et al. 1994)

1.98×10^{-6} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

1.52	(shake flask-UV, Fujita et al. 1974)
1.50	(Hansch & Leo 1979)
1.45	(Rao & Davidson 1980)
1.52	(Kenaga & Goring 1980; Kanazawa 1981)
1.552	(shake flask-GC, Bowman & Sans 1983)
1.52	(Hansch & Leo 1985)
1.75	(RP-HPLC-RT correlation, Trapp & Pussemier 1991)
1.45–1.56	(Montgomery 1993)
1.52	(recommended, Sangster 1993)
1.52	(recommended, Hansch et al. 1995)
1.99	(RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

0.924	(calculated, Howard 1991)
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Sorption Partition Coefficient, log K_{oc} :

1.67	(measurements for average of 2 soils, Kanazawa 1981, 1989)
1.86	(calculated, Howard 1991)
1.48	(soil, Wauchope et al. 1992; Hornsby et al. 1996)
0.48–1.97	(Montgomery 1993)
1.48	(estimated-chemical structure, Lohninger 1994)
1.67	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.63, 1.88	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric and/or aqueous photolysis $t_{1/2} = 62.5$ – 87.9 h, based on measured rate of photolysis on bean leaves in sunlight (Ivie & Casida 1971; quoted, Howard et al. 1991) and in aqueous solution under simulated sunlight (Jensen-Korte et al. 1987; quoted, Howard et al. 1991);
 photolyze in water with $t_{1/2} = 88$ h and decreased with humic material to 13–41 h; $t_{1/2} = 87.9$ h in water when irradiated with light >290 nm (Howard 1991).

Oxidation: photooxidation $t_{1/2} = 0.71$ – 7.1 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
 vapor-phase photooxidation $t_{1/2} = 4.3$ h for reaction with ambient OH radical (Howard 1991).

Hydrolysis: $t_{1/2} = 40$ min at pH 10 and 20°C , hydrolyzes at a rate of 1.5% d^{-1} in 1% aqueous solution at pH 7 (Spencer 1982);

$t_{1/2} = 16$, 1.6 and 0.17 d at pH 8, 9, 10, but stable between pH 3–7, $t_{1/2} = 40$ min at pH 10 (Howard 1991);

$t_{1/2} = 290$ d at pH 7, $t_{1/2} = 17.9$ d at pH 8 and $t_{1/2} = 48$ min at pH 10 (Montgomery et al. 1993);

hydrolysis $t_{1/2} = 16$ d, 1.6 d and 4.2 h in water at pH 8, 9 and 10 (Aly & El-Dib 1971; quoted, Montgomery 1993).

Biodegradation: aqueous aerobic $t_{1/2} = 168$ – 672 h, based on unacclimated aqueous aerobic screening test data (Gummer 1979; Kanazawa 1987; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ – 2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 44$ d under aerobic conditions and $t_{1/2} = 59$ d under anaerobic conditions in water used a combination of activated sludge, silt loam soil and sediment as an inoculum; $t_{1/2} = 78$ d under aerobic conditions and $t_{1/2} = 125$ d under anaerobic conditions at pH 6.9 (Howard 1991).

Biotransformation: metabolism rate $k = 3.70 \times 10^{-3} \text{ h}^{-1}$ leading to an irradiated moist soil $t_{1/2} = 180$ h (Graebing & Chib 2004)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.71$ – 7.1 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

$t_{1/2} \sim 4$ h reacting with photochemically produced hydroxyl radical in air (Howard 1991).

Surface water: $t_{1/2} = 38\text{--}672$ h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 1$ d to 1 wk by degradation, photolyze rapidly with $t_{1/2} = 13$ to 88 h (Howard 1991).

Ground water: $t_{1/2} = 38\text{--}1344$ h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

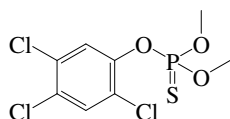
Soil: $t_{1/2} = 38\text{--}672$ h, based on estimated hydrolysis half-life at pH 9 (Aly & El-Dib 1971; quoted, Howard et al. 1991) and estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Field $t_{1/2} = 14\text{--}50$ d (Wauchope et al. 1992)

On sandy loam soil: first-order rate constants for photolytic decline, $k = 1.65 \times 10^{-3} \text{ h}^{-1}$ irradiated in moisture-maintained soil, $k = 0.91 \times 10^{-3} \text{ h}^{-1}$ irradiated in air-dried soil, $k = 0.91 \times 10^{-3} \text{ h}^{-1}$ in dark control moist soil and $k = 0.23 \times 10^{-3} \text{ h}^{-1}$ in dark control air-dried sandy loam soil from Madia, CA. The initial metabolism rate $k = 3.70 \times 10^{-3} \text{ h}^{-1}$ leading to an irradiated moist soil $t_{1/2} = 180$ h; in the dark $t_{1/2} = 380$ h in moist soil Graebing & Chib 2004)

Biota:

18.1.1.73 Ronnel



Common Name: Ronnel

Synonym: Blitex, Dermafos, Dermaphos, dimethyl trichlorophenyl thiophosphate, Dow ET 14, Dow ET 57, Ectoral, ENT 23284, Etrolene, Fenchlorfos, Fenchlorphos, Gesektin K, Karlan, Korlan, Nanchor, Nanker, Nankor, OMS 123, Phenchlorfos, Remelt, Rovon, trichlorometafos, Trolen, Trolene, Viozene

Chemical Name: *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl)thiophosphate; *O,O*-dimethyl *O*-2,4,5-trichlorophenyl phosphorothioate; phosphoric acid *O,O*-dimethyl *O*-(2,4,5-trichlorophenyl)ester

Uses: insecticide.

CAS Registry No: 299-84-3

Molecular Formula: $C_8H_8Cl_3O_3PS$

Molecular Weight: 321.546

Melting Point ($^{\circ}C$):

40–42 (Spencer 1982)

41 (Montgomery 1993; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.48 ($25^{\circ}C$, Montgomery 1993)

Molar Volume (cm^3/mol):

257.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.85 (Plato & Glasgow 1969)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.697 (mp at $41^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

44 (Günther et al. 1968; Melnikov 1971)

1.08 ($20^{\circ}C$, shake flask-GC, Chiou et al. 1977)

1.08 (20 – $25^{\circ}C$, shake flask-GC/ECD, Freed et al. 1979)

2.5 ($20^{\circ}C$, Spencer 1982)

0.60 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1979, 1983)

0.98 ($20^{\circ}C$, corrected supercooled liq. value, shake flask-GC, Bowman & Sans 1979,83)

6.0 (Dow Chemical unpublished data, Kenaga 1980a, b; Kenaga & Goring 1980)

40 ($22^{\circ}C$, Khan 1980)

1.0 ($20^{\circ}C$, shake flask-HPLC, Ellgehausen et al. 1981)

1.61 ($20^{\circ}C$, selected, Suntio et al. 1988)

40 (Montgomery 1993; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0533 ($20^{\circ}C$, Eichler 1965; Melnikov 1971)

0.0071 (20 – $25^{\circ}C$, Freed et al. 1979)

1.067 (Spencer 1982)

0.0017 ($20^{\circ}C$, GC-RT correlation without mp correlation, Kim et al. 1984; Kim 1985)

0.0011 ($20^{\circ}C$, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)

0.016 ($20^{\circ}C$, selected, Suntio et al. 1988)

0.0045 ($20^{\circ}C$, Montgomery 1993)

Henry's Law Constant (Pa· m^3/mol at $25^{\circ}C$ or as indicated):

3.22 ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

0.857 (20 – $25^{\circ}C$, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$ at 25°C or as indicated:

4.88	(20°C, shake flask-GC, Chiou et al. 1977)
4.67	(Kenaga 1980b; Kenaga & Goring 1980)
4.88	(20–25°C, shake flask-GC/ECD, Freed et al. 1979)
5.34	(shake flask-HPLC, Ellgehausen et al. 1981)
4.81	(20°C, shake flask-GC, Bowman & Sans 1983)
5.068 ± 0.004	(shake flask/slow-stirring method, De Bruijn et al. 1989)
4.67–5.068	(Montgomery 1993)
4.88	(recommended, Sangster 1993)
5.07	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.35	(calculated-S, Kenaga 1980a, b)
–1.38	(average beef fat diet, Kenaga 1980b)
4.64	(guppy <i>Poecilia reticulata</i> , lipid wt basis, De Bruijn & Hermens 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

3.20	(soil, calculated-S as per Kenaga & Goring 1978, Kenaga 1980a, b)
2.90	(soil, calculated-MCI χ , Gerstl & Helling 1987)
2.76	(calculated, Montgomery 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: estimated $t_{1/2} \sim 3$ d at pH 6 (Montgomery 1993).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

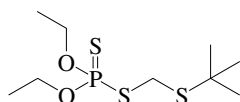
$k_1 = 0.01337 \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, 0.5–420 h exposure, De Bruijn & Hermens 1991)

$k_2 = 0.38 \text{ d}^{-1}$ (guppy, De Bruijn & Hermens 1991)

$k_2 = 0.14 \text{ d}^{-1}$ (calculated- K_{ow} , De Bruijn & Hermens 1991)

Half-Lives in the Environment:

18.1.1.74 Terbufos



Common Name: Terbufos

Synonym: AC 92100, Counter, ST-100

Chemical Name: *S*-((*tert*-butylthio)methyl) *O,O*-diethyl phosphorodithioate; *S*-[[[(1,1-dimethylethyl)thio]methyl] *O,O*-diethyl phosphorodithioate; phosphorodithioic acid *S*-((*tert*-butylthio)methyl) *O,O*-diethyl ester

Uses: insecticide in soil to control insects and also used as nematocide to control nematodes in beet, maize, cotton, sorghum, onions, cabbage, and bananas.

CAS Registry No: 13071-79-9

Molecular Formula: $C_9H_{21}O_2PS_3$

Molecular Weight: 288.431

Melting Point ($^{\circ}C$):

-29.2 (Worthing & Hance 1991; Howe et al. 1994; Montgomery 1993; Tomlin 1994; Milne 1995)

Boiling Point ($^{\circ}C$):

69 (at 0.01 mmHg, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

312 (Brecken-Folse et al. 1994; Howe et al. 1994)

Density (g/cm^3 at $20^{\circ}C$):

1.105 ($24^{\circ}C$, Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

261 ($24^{\circ}C$, calculated from density)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

12 (Martin & Worthing 1977)

5.07 (shake flask-GC, Felsot & Dahm 1979)

≤ 10 (Spencer 1982)

5.5 ($19^{\circ}C$, shake flask-GC, Bowman & Sans 1983a, b)

10–15 (Worthing & Hance 1991)

5 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

15 (calculated, Pait et al. 1992)

4.5 ($27^{\circ}C$, Montgomery 1993; quoted, Tomlin 1994; Majewski & Capel 1995)

0.10 (Howe et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0346 (Worthing & Hance 1991; Tomlin 1994)

0.0427 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0351 ($20^{\circ}C$, Montgomery 1993)

0.0174; 0.0346 (liquid P_L , GC-RT correlation; quoted lit., Donovan 1996)

0.0148; 0.00912, 0.0151 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

2.229 (20 – $27^{\circ}C$, calculated-P/C, Montgomery 1993)

2.463 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

3.68 (shake flask-LSC, Felsot & Dahm 1979)

2.22 (Rao & Davidson 1980)

4.477	(shake flask-GC, Bowman & Sans 1983b)
4.52	(Worthing & Hance 1991; Tomlin 1994)
2.22–4.70	(Montgomery 1993)
4.48	(recommended, Sangster 1993)
3.54	(22°C, shake flask, Brecken-Folse et al. 1994)
0.832	(12°C in reconstituted test water at pH 7.5, Howe et al. 1994)
4.52	(Milne 1995)
4.48	(recommended, Hansch et al. 1995)
4.86	(RP-HPLC-RT correlation, Finizio et al. 1997)
4.51	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.73	(topmouth gudgeon, Metcalf & Sanborn 1975)
2.18	(calculated-S, Kenaga 1980; quoted, Pait et al. 1992)
1.0	(<i>Triaenodes tardus</i> , Belluck & Felsot 1981)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

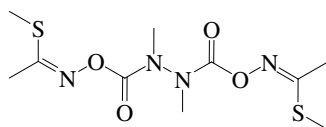
3.04	(soil, calculated-S per Kenaga & Goring 1978, Kenaga 1980)
2.76, 3.29	(quoted, calculated-MCI χ , Gerstl & Helling 1987)
2.70	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.46–3.03	(Montgomery 1993)
2.82	(soil, calculated-MCI χ , Sabljic et al. 1995)
2.80, 3.30	(soil, estimated-class-specific model, estimated-general model, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: $t_{1/2}$ = 9–27 d in soil (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994);
 selected field $t_{1/2}$ = 5.0 d (Wauchope et al. 1992; quoted, Richards & Baker 1993; Hornsby et al. 1996);
 soil $t_{1/2}$ = 5 d (Pait et al. 1992).

18.1.1.75 Thiodicarb



Common Name: Thiodicarb

Synonym: Bismethomyl thioether, Dicarbosulf

Chemical Name: dimethyl *N,N'*-(thiobis(methylimino)carbonyloxy)bis(ethanimidothioate)

CAS Registry No: 59669-26-0

Uses: insecticide/molluscicide

Molecular Formula: $C_{10}H_{18}N_4O_4S_3$

Molecular Weight: 354.470

Melting Point ($^{\circ}C$):

168–172 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

173–174 (Tomlin 1994)

173 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.40 (Montgomery 1993)

Molar Volume (cm^3/mol):

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0353 (mp at $173^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

35 (Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

19.1 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0043 ($20^{\circ}C$, Hartley & Kidd 1987; Montgomery 1993)

1.33×10^{-5} (20 – $25^{\circ}C$, Wauchope et al. 1992; Hornsby et al. 1996)

0.0054 ($20^{\circ}C$, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.044 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.70 (shake flask-HPLC, Drabel & Bachmann 1983)

1.2–1.6 (Montgomery 1993)

1.70 (recommended, Sangster 1993)

1.70 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

1.81–3.07; 2.54 (quoted range of reported data; mean, Wauchope et al. 1992)

2.54 (soil, selected, Wauchope et al. 1992; Hornsby et al. 1996)

3.06; 2.25; 2.10–2.69; 2.32–2.52; 2.57 (various soils: clay; loam; sand; sandy loam; silty loam (quoted, Montgomery 1993)

1.81–3.07 (various soils, Montgomery 1993)

2.54; 1.68, 2.57 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} \sim 9$ d at pH 3 (Montgomery 1993);

stable at pH 6, rapidly hydrolyzed at pH 9 and slowly at pH 3, $t_{1/2} \sim 9$ d (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} \sim 9$ d at pH 3 (Montgomery 1993);

stable at pH 6, rapidly hydrolyzed at pH 9 and slowly at pH 3, $t_{1/2} \sim 9$ d (Tomlin 1994).

Ground water:

Sediment:

Soil: $t_{1/2} = 3$ –8 d in various soils (Hartley & Kidd 1987)

field $t_{1/2} = 7$ d (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

18.1.1.76 Toxaphene

Common Name: Toxaphene

Synonym: Agricide maggot killer, Alltex, Alltox, Camphochlor, Chem-Phene, chlorinated Camphene, Chloro-camphene, Coopertox, Crestoxo, Cristoxo, ENT 9735, Estonox, Fasco terpene, Geniphene, Gy-phene, Hercules 3956, Huilex, Kamfochlor, Melipax, Motox, NA 2761, NCI-C00259, Octachlorcamphene, Polychlorocamphene, Strobane-T, Texadust, Toxakil, Toxon 63

Chemical Name: mixtures of chlorinated camphene and bornane

Uses: pesticide used primarily on lettuce, cotton, corn, tomatoes, peanuts, wheat and soybean.

CAS Registry No: 8001-35-2

Molecular Formula: $C_{10}H_{16}Cl_8$

Molecular Weight: 413.812

Note: A large number of isomers exist, thus the commercial product is a mixture and the properties below should be regarded as average values for the specific mixture. Considerable variability in properties is thus expected.

Melting Point (°C):

65–90 (Howard 1991; Montgomery 1993; Milne 1995)
35 (dec., Milne 1995)

Boiling Point (°C):

246, 351, 360 (estimated from structure, Tucker et al. 1983)

Density (g/cm³ at 20°C):

1.65 (25°C, Spencer 1982; Montgomery 1993)

Molar Volume (cm³/mol):

358.8 (calculated-Le Bas method at normal boiling point)
366.8 (calculated-Le Bas method)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 20°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:

0.30 (Mackay et al. 1986)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and the reported temperature dependence equations):

3.0 (Brooks 1974)
0.74 (generator column-GC/ECD, Weil et al. 1974)
0.40 (Leonard et al. 1976; Wauchope 1978)
0.40 (Sanborn et al. 1976; Weber et al. 1980)
0.40 (Martin & Worthing 1977)
0.50 (shake flask-GC, Paris et al. 1977)
3.0 (22°C, Khan 1980; Spencer 1982)
0.3–3.0 (U.S. EPA 1984; McLean et al. 1988)
3.0 (Worthing & Walker 1987)
0.50 (20°C, selected, Suntio et al. 1988)
0.55 (20°C, Montgomery 1993)
0.63 (calculated from vapor pressure and HLC, Wania & Mackay 1993)
 $\log [C/(\text{mol/m}^3)] = 0.77 - 1071/(T/K)$ (Wania & Mackay 1993)
3.0 (20–25°C, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

4.0×10^{-5} (20°C, Spencer 1973)
27–53 (Brooks 1974; Khan 1980)
 1.3×10^{-4} (Leonard et al. 1976)
 1.3×10^{-4} (20–25°C, Weber et al. 1980)
 1.3×10^{-4} (30°C, Seiber et al. 1981)
 2.0×10^{-5} , 4.5×10^{-5} , 0.667 (estimated-bp, Tucker et al. 1983)

- 27.0 (U.S. EPA 1984; quoted, McLean et al. 1988)
 8.92×10^{-4} (20°C, estimated, Murphy et al. 1987)
 0.0005 (20°C, selected, Suntio et al. 1988)
 27–54 (20°C, Montgomery 1993)
 0.0016 (calculated from the eq. below, Wania & Mackay 1993)
 $\log(P/\text{Pa}) = 12.25 - 4487/(T/K)$ (Wania & Mackay 1993)
 5.3×10^{-4} (20–25°C, selected, Hornsby et al. 1996)
 $(2.3\text{--}7.10) \times 10^{-4}$ (supercooled P_L , capillary GC-RT correlation, for 21 toxaphene components-chlorinated bornane and camphene congeners, Bidleman et al. 2003)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 490 (gas stripping-GC, Warner et al. 1980)
 6380 (calculated-P/C, Kavanaugh & Trussel 1980)
 45.59 (estimated-group method per Hine & Mookerjee 1975, Tucker et al. 1983)
 0.0238 (calculated-P/C, Mackay et al. 1986)
 496 (gas stripping-GC, Warner et al. 1987)
 0.608 (20°C, estimated, Murphy et al. 1987; quoted, Howard 1991)
 0.62 (20°C, average value for toxaphene complex mixture, Murphy et al. 1987)
 520 (quoted from WERL Treatability Database, Ryan et al. 1988)
 0.42 (20°C, calculated-P/C, Suntio et al. 1988)
 3097 (calculated-P/C, Jury et al. 1990)
 0.067 (0°C, selected, Cotham & Bidleman 1991)
 6382 (Montgomery 1993)
 1.054 (calculated-temp dependence eq., Wania & Mackay 1993)
 $\log[H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 11.48 - 3416/(T/K)$ (Wania & Mackay 1993)
 0.36* (technical toxaphene, gas stripping-GC, measured range 10–40°C, Jantunen & Bidleman 2000)
 $\log[H/(\text{Pa}\cdot\text{m}^3/\text{mol})] = 10.42 - 3209/(T/K)$; temp range 10–40°C (technical toxaphene, gas stripping-GC, Jantunen & Bidleman 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.52 (shake flask-GC, Paris et al. 1977)
 5.30 (HPLC-RT correlation, Veith et al. 1979)
 3.23 (Rao & Davidson 1980)
 5.28 (Veith & Kosian 1983)
 4.83 (from Veith's personal communication, Zaroogian et al. 1985)
 5.50 (Garten & Trabalka 1983)
 3.85 (Ryan et al. 1988)
 5.50 (Isnard & Lambert 1988, 1989; Travis & Arms 1988; Wania & Mackay 1993)
 4.63 (estimated-QSAR & SPARC, Kollig 1993)
 3.23–5.50 (Montgomery 1993)
 4.77–6.64 (range for 36 toxaphene components/congeners, shake flask/slow stirring-GC/ECD, Fisk et al. 1999)

Bioconcentration Factor, $\log BCF$:

- 2.79 (beef biotransfer factor $\log B_b$, correlated- K_{ow} , Radeleff et al. 1952; Claborn et al. 1953,60)
 –3.20 (milk biotransfer factor $\log B_m$, correlated- K_{ow} , Saha 1969)
 3.53 (*Bacillus subtilis*, Paris et al. 1975, 1977)
 3.72 (*Flavobacterium harrisonii*, Paris et al. 1975, 1977)
 4.23 (*Aspergillus sp.*, Paris et al. 1975, 1977)
 4.04 (*Chlorella prenioidosa*, Paris et al. 1975, 1977)
 3.63 (*Gambusia*, Sanborn et al. 1976)
 4.84 (fathead minnows, Mayer et al. 1977)
 3.51–4.23 (microorganisms, Paris et al. 1977)
 3.59 (pinfish, 4-d exposure, Schimmel et al. 1977; Veith & Kosian 1983)
 3.64 (sheepshead minnow, 4-d exposure, Schimmel et al. 1977)

- 3.49–4.52, 2.60–3.08 (fish, shrimp, Reish et al. 1978)
 4.42, 3.63 (fish: flowing water, static water; Kenaga & Goring 1980)
 4.42, 3.02 (fish, calculated-solubility, Kenaga 1980)
 3.59 (pinfish, Veith & Kosian 1983)
 3.64 (sheepshead minnow, Veith & Kosian 1983)
 3.81, 3.72 (fish: flowing system, microcosm, Garten & Trabalka 1983)
 3.84, 3.98 (algae: snail, Garten & Trabalka 1983)
 3.44, 3.41 (oyster, calculated- K_{OW} and models, Zaroogian et al. 1985)
 3.44, 3.41 (pinfish, calculated- K_{OW} and models, Zaroogian et al. 1985)
 3.44, 3.41 (sheepshead minnow, calculated- K_{OW} & models, Zaroogian et al. 1985)
 4.52, 6.44 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.57, 6.50 (oyster, flow-through 6 months: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.84, 6.06 (fathead minnow, flow-through 96-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
 4.80, 5.80 (fathead minnow, flow-through 150-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
 >4.73, >5.84 (channel catfish, flow-through 100-d: wet wt basis, lipid wt basis, Geyer et al. 2000)
 3.04, 3.204 (human, fat: wet wt basis, lipid wt basis, Geyer et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.86 (calculated-S, Kenaga 1980; quoted, Howard 1991)
 4.99 (soil, McDowell et al. 1981; quoted, Nash 1988)
 4.32 (soil, screening model calculations, Jury et al. 1987a, b, 1990; Jury & Ghodrati 1989)
 5.32 (sediment, Bomberger et al. 1983; quoted, Howard 1991)
 3.17 (calculated- K_{OW} as per Kenaga & Goring 1980, Chapman 1989)
 4.31 (estimated-QSAR and SPARC, Kollig 1993)
 3.18 (calculated, Montgomery 1993)
 5.00 (20–25°C, selected, Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} = 2650$ d from chemical below soil surface (Jury et al. 1990).

Photolysis:

Hydrolysis: estimated $t_{1/2} > 10$ yr at pH 5–8 and 25°C (Callahan et al. 1979; quoted, Howard 1991)

$k = (8.0 \pm 2.2) \times 10^{-6} \text{ h}^{-1}$ at pH 7 with a calculated $t_{1/2} = 10$ yr (Ellington et al. 1987, 1988)

$k = 7.0 \times 10^{-2} \text{ yr}^{-1}$ at pH 7.0 and 25°C (Kollig 1993).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$t_{1/2} = 4\text{--}5$ d for the vapor-phase reaction with hydroxyl radicals (Howard 1991)

$k(aq.) = 8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 1.9 ± 0.1 and at $24 \pm 1^\circ\text{C}$ (Buxton et al. 1988; quoted, Faust & Hoigné 1990; Haag & Yao 1992)

$k(aq.) < 1.3 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 5.6 and 21°C , with $t_{1/2} > 7$ h at pH 7 (Yao & Haag 1991).

$k(aq.) = (1.2\text{--}8.1) \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction (Fenton with reference to lindane) with hydroxyl radical in aqueous solutions at pH 1.9 ± 0.1 and at $24 \pm 1^\circ\text{C}$ (Haag & Yao 1992)

Biodegradation: very resistant to degradation in soils with reported from $t_{1/2} = 0.8$ yr (Adams 1967; quoted, Howard 1991) to 14 yr (Nash & Woolson 1967; quoted, Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.016 \text{ d}^{-1}$ with $t_{1/2} = 43$ d and $k_2 = 0.022 \text{ d}^{-1}$ with $t_{1/2} = 32$ d for food concn of 21 ng/g and 136 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for a C_7 -CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.007 \text{ d}^{-1}$ with $t_{1/2} = 95$ d and $k_2 = 0.016 \text{ d}^{-1}$ with $t_{1/2} = 43$ d for food concn of 18 ng/g and 121 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for a C_8 -CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.008 \text{ d}^{-1}$ with $t_{1/2} = 83 \text{ d}$ and $k_2 = 0.017 \text{ d}^{-1}$ with $t_{1/2} = 42 \text{ d}$ for food concn of 17 ng/g and 134 ng/g, respectively, in a 30-d uptake followed by 160-d depuration studies for C₉-CHB toxaphene congener (juvenile rainbow trout, Fisk et al. 1998)

$k_2 = 0.068 \text{ yr}^{-1}$, 0.093 yr^{-1} , 0.160 yr^{-1} in Lake Michigan, Lake Huron and Lake Ontario, respectively, in lake trout (lipid-adjusted, Glassmeyer et al. 2000)

$k_2 = 0.085 \text{ yr}^{-1}$, 0.086 yr^{-1} , 0.165 yr^{-1} in Lake Michigan, Lake Huron and Lake Ontario, respectively, in lake trout (wet weight, Glassmeyer et al. 2000)

Half-Lives in the Environment:

Air: $t_{1/2} = 4\text{--}5 \text{ d}$ for the vapor-phase reaction with hydroxyl radicals (GEMS 1986; quoted, Howard 1991).

Surface water: measured $k < 1.3 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 21°C, with $t_{1/2} > 7 \text{ h}$ at pH 7 (Yao & Haag 1991);

half-lives in lake water: $t_{1/2} = 18\text{--}31 \text{ yr}$ in Lake Superior, $t_{1/2} = 5\text{--}8 \text{ yr}$ in Lake Michigan, $t_{1/2} \sim 8.5 \text{ yr}$ in Lake Huron and $t_{1/2} \sim 6 \text{ yr}$ in Lake Ontario (Glassmeyer et al. 2000).

Ground water:

Sediment:

Soil: very persistent with reported half-life from $t_{1/2} = 0.8 \text{ yr}$ (Adams 1967; quoted, Howard 1991) to 14 yr (Nash & Woolson 1967; quoted, Howard 1991);

$t_{1/2} > 50 \text{ d}$ when subject to plant uptake via volatilization (Callahan et al. 1979; quoted, Ryan et al. 1988) measured dissipation rate $k = 0.010 \text{ d}^{-1}$ (Seiber et al. 1979; quoted, Nash 1988);

$t_{1/2} = 9 \text{ d}$ in screening model calculations (Jury et al. 1987b);

estimated dissipation rate $k = 0.0011$ and 0.013 d^{-1} (Nash 1988);

$t_{1/2} = 3650 \text{ d}$ for volatilization to atmosphere from chemical below soil surface (Jury et al. 1990);

field $t_{1/2} = 9 \text{ d}$ (20–25°C, selected, Hornsby et al. 1996)

$t_{1/2} = 0.8\text{--}14 \text{ yr}$ in soil, $t_{1/2} = 10\text{--}18 \text{ yr}$ in the environment (Geyer et al. 2000)

Biota: field $t_{1/2} = 15.6 \text{ d}$ in fruit tree leaves (Decker et al. 1950; quoted, Nash 1983);

microagroecosystem $t_{1/2} = 19 \text{ d}$ in cotton leaves (Nash & Harris 1977; quoted, Nash 1983);

field $t_{1/2}$ ca. 6.3 d in cotton canopy (Willis et al. 1980; quoted, Nash 1983);

$t_{1/2} = 524 \text{ d}$ for white suckers, and $t_{1/2} = 232$ to 322 d for lake trout (total toxaphene, Delorme et al. 1993);

average fish half-lives in the Great Lakes. $t_{1/2} = 9.1 \text{ yr}$ in Lake Michigan, $t_{1/2} = 7.7 \text{ yr}$ in Lake Huron and $t_{1/2} = 4.3 \text{ yr}$ in Lake Ontario (lake trout, Glassmeyer et al. 2000)

Depuration $t_{1/2} = 32\text{--}96 \text{ d}$ for a 30-d uptake and 160-d depuration studies (Juvenile rainbow trout, Fisk et al. 1998)

TABLE 18.1.1.76.1
Reported Henry's law constants of toxaphene at various temperatures

Jantunen et al. 2000

air stripping-GC

$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$
10	0.10
20	0.36
30	0.69
35	0.86
40	1.50
$\log H = A - B/(T/K)$	
	$H/(\text{Pa m}^3/\text{mol})$
A	10.42 ± 0.54
B	3209 ± 162

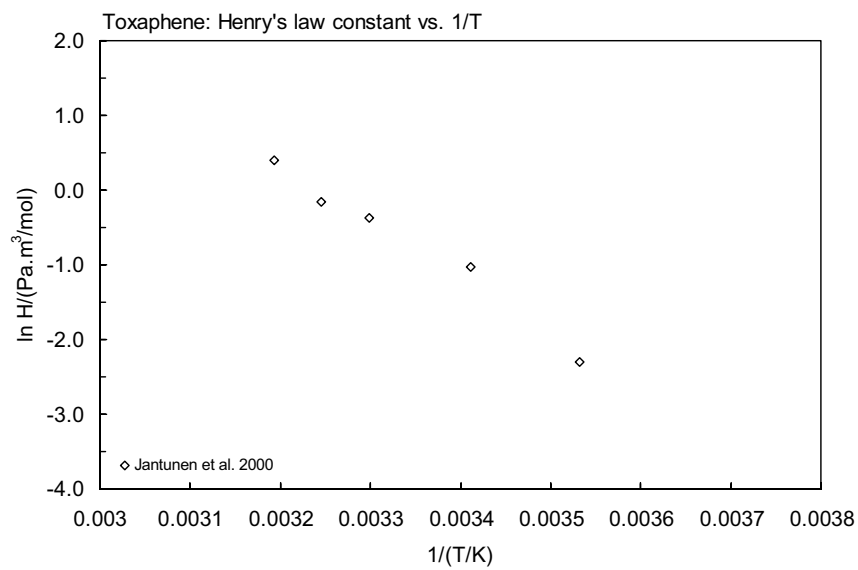
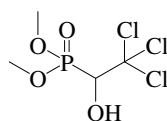


FIGURE 18.1.1.76.1 Logarithm of Henry's law constant versus reciprocal temperature for toxaphene.

18.1.1.77 Trichlorfon



Common Name: Trichlorfon

Synonym: Aerol 1, Agroforotox, Anthion, Bay 15922, Bayer 15922, Bilarcil, Bovinox, Britten, Britton, Cekufon, Chlorak, Chlorfos, Chlorphos, Chloroftalm, Chloroxyphos, Ciclosom, Combat, Comboto, Danex, DEP, Dephton, DETF, Dimetox, Dipterax, Diptevur, Ditrifon, Dylox, Dyrex, Dyvon, ENT 19763, Equino-acid, Flibol E, Forotox, Foschlor, Hypodermacid, Leivasom, Loisol, Masoten, Mazoten, Methyl chlorophos, Metifonate, Metrifonate, Metriphonate, NA 2783, NCI-C54831, Neguvon, Phoschlor, Proxol, Ricifon, Ritsifon, Soldep, Sotipox, Trichlorphon, Trichlorophene, Trinex, Tugon, Volfartol, Votexit, Wotexit

Chemical Name: dimethyl 2,2,2-trichloro-hydroxyethylphosphorothioate; 2,2,2-trichloro-hydroxy-ethylphosphoric acid dimethyl ester

Uses: insecticide to control flies and roaches.

CAS Registry No: 52-68-6

Molecular Formula: $C_4H_8Cl_3O_4P$

Molecular Weight: 257.437

Melting Point ($^{\circ}C$):

77 (Lide 2003)

Boiling Point ($^{\circ}C$):

100 (at 0.1 mmHg, Spencer 1973; Montgomery 1993; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.73 (Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

194.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.309 (mp at $77^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

154000 (Spencer 1973, 1982; Martin & Worthing 1977; Worthing 1979)

> 5000 ($20^{\circ}C$, shake flask-GC, Bowman & Sans 1983a)

150000 (Davies & Lee 1987)

120000 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

120000 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

154000 (Montgomery 1993; Milne 1995)

90000 (Brecken-Folse et al. 1994)

9000 (Howe et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.00095 ($20^{\circ}C$, vapor density, MacDougall 1964)

0.00104 ($20^{\circ}C$, Eichler 1965; Melnikov 1971; Spencer 1973; Hartley & Graham-Bryce 1980)

0.0640 ($20^{\circ}C$, GC-RT correlation without mp correction, Kim et al. 1984; Kim 1985)

0.0187 ($20^{\circ}C$, GC-RT correlation with mp correction, Kim et al. 1984; Kim 1985)

0.00021 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

0.00027 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.00104 ($20^{\circ}C$, Montgomery 1993)

0.00051 (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

1.7×10^{-6} ($20^{\circ}C$, calculated-P/C, Suntio et al. 1988)

1.7×10^{-6} (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.48 (Dow Chemical data, Kenaga & Goring 1980)

0.431	(shake flask-GC, Bowman & Sans 1983b)
0.76	(HPLC-RT correlation, Kawamoto & Urano 1989)
0.43–0.76	(Montgomery 1993)
0.51, 0.72	(shake flask, RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
1.70	(22°C, shake flask, Brecken-Folse et al. 1994)
0.304	(12°C in reconstituted test water at pH 7.5, Howe et al. 1994)
0.51	(recommended, Sangster 1993)
0.43	(Tomlin 1994)
0.51	(recommended, Hansch et al. 1995)
0.72	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

–0.155 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

0.778 (calculated-S as per Kenaga & Goring 1978, Kenaga 1980)
 1.90 (correlated, Kawamoto & Urano 1989)
 1.73 (soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
 1.00 (soil, 20–25°C, selected, Wauchope et al. 1992; quoted, Dowd et al. 1993; Lohninger 1994; Hornsby et al. 1996)
 0.99–1.58 (Montgomery 1993)
 1.90 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 1.30 (sediment, estimated, Paraiba et al. 1999)
 1.90; 1.87, 2.25 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 1$ –101 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: first-order hydrolysis $t_{1/2} = 68$ h, based on first-order rate constant at pH 7 and 25°C (Chapman & Cole 1982; quoted, Howard et al. 1991);

$t_{1/2} = 510$ d at 22°C and at pH 4, $t_{1/2} = 46$ h at pH 7, and $t_{1/2} < 30$ min at pH 9 (Tomlin 1994).

Biodegradation: $k(\text{aerobic}) = 0.28 \text{ d}^{-1}$ with $t_{1/2} = 2.5$ d at 20°C by aerobic activated sludge cultivated by an artificial sewage (batch contacting method, Kawamoto & Urano 1990)

aqueous aerobic $t_{1/2} = 24$ –1080 h, based on unacclimated soil grab sample data (Guirguis & Shafik 1975; Kostovetskii et al. 1976; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 96$ –4320 h, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 1$ –101 h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);

reaction rate $k = 1.90 \times 10^{-4} \text{ min}^{-1}$ in air (Paraiba et al. 1999).

Surface water: $t_{1/2} = 22$ –588 h, based on aqueous hydrolysis half-lives at pH 6 and 8 and 25°C (Chapman & Cole 1982; quoted, Howard et al. 1991);

$t_{1/2} = 2.5$ d at 20°C by aerobic activated sludge (Kawamoto & Urano 1990)

reaction rate $k = 1.90 \times 10^{-4} \text{ min}^{-1}$ in water (Paraiba et al. 1999).

Ground water: $t_{1/2} = 22$ –588 h, based on aqueous hydrolysis half-lives at pH 6 and 8 and 25°C (Chapman & Cole 1982; quoted, Howard et al. 1991).

Sediment: reaction rate $k = 1.90 \times 10^{-5} \text{ min}^{-1}$ in sediment (Paraiba et al. 1999).

Soil: $t_{1/2} = 24$ –1080 h, based on unacclimated soil grab sample data (Guirguis & Shafik 1975; Kostovetskii et al. 1976; quoted, Howard et al. 1991);

selected field $t_{1/2} = 10$ d (Wauchope et al. 1992; Dowd et al. 1993; Hornsby et al. 1996).

Biota:

18.2 SUMMARY TABLES

TABLE 18.2.1

Common names, chemical names and physical properties of insecticides

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, Fat 25°C	pK _a
Acephate [30560-19-1]	Orthene	<i>O,S</i> -dimethyl acetylphosphoramidothioate	C ₄ H ₁₀ NO ₃ PS	183.166	88	0.241	
Aldicarb [116-06-3]	Temik	2-methyl-2-(methylthio)-propionaldehyde <i>O</i> -(methylcarbamoyl) oxime	C ₇ H ₁₄ N ₂ O ₂ S	190.263	99	0.188	
Aldrin [309-00-2]	Aldrec, Aldrex, Aldrite, Octalene	1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4-endoexo-5,8-dimethano-naphthalene	C ₁₂ H ₈ Cl ₆	364.910	104	0.168	
Aminocarb [2032-59-9]	Matacil	4-dimethylamino- <i>m</i> -tolyl methylcarbamate	C ₁₁ H ₁₆ N ₂ O ₂	208.257	94	0.210	
Azinphos-methyl [86-50-0]	Guthion	<i>O,O</i> -dimethyl- <i>S</i> -[4-oxo-1,2,3-benzotriazin-3(4 <i>H</i>)-yl)methyl]phosphorodithioate	C ₁₀ H ₁₂ N ₃ O ₃ PS ₂	317.324	73	0.338	
Bendiocarb [22781-23-3]	Bencarbate, Dycarb, Garvox, Multamat	2,2-dimethyl-1,3-benzodioxol-4-yl-methylcarbamate	C ₁₁ H ₁₃ NO ₄	223.226	130	0.0933	8.8
Bromophos [2104-96-3]	Nexion, S-1942, Omexan, Brofene	<i>O</i> -4-bromo-2,5-dichlorophenyl- <i>O,O</i> -dimethyl phosphorothioate	C ₈ H ₈ BrCl ₂ PS	317.999	54	0.519	
Bromophos-ethyl [4824-78-6]	Nexagen, Filariol	<i>O</i> -(4-bromo-2,5-dichlorophenyl) <i>O,O</i> -diethyl phosphorothioate	C ₁₀ H ₁₂ Cl ₂ O ₃ PS	394.049			
Carbaryl [63-25-2]	Sevin	1-naphthyl- <i>N</i> -methyl carbamate	C ₁₂ H ₁₁ NO ₂	201.221	145	0.0665	
Carbofuran [1563-66-2]	Furadan, Yaltox	2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate	C ₁₂ H ₁₅ NO ₃	221.252	151	0.0580	
Carbophenothion [786-19-6]	Carbofenotion, Acarithion, Akarithion	<i>S</i> -chlorophenylthio methyl <i>O,O</i> -diethyl phosphorothioate	C ₁₁ H ₁₆ ClO ₂ PS ₃	342.866	liquid	1	
Carbosulfan [55285-14-8]	Marshal, Advantage Posse, FMC 35001	2,3-dihydro-2,2-dimethylbenzofuran-7-yl(dibutylaminothio) methylcarbamate	C ₂₀ H ₃₂ N ₂ O ₃ S	380.544	liquid	1	
Chlordane [57-74-9]	Aspon-chlordane, Chlorindan, Octachlor	1,2,4,5,7,8,8-octachloro-3 <i>a</i> ,4,7,7 <i>a</i> -tetrahydro-4,7-methanoindane	C ₁₀ H ₆ Cl ₈	409.779	106	0.160	
	cis- or α-chlordane [5103-71-9]		C ₁₀ H ₆ Cl ₈	409.799	107–109	0.153	
	trans- or β-chlordane [5103-74-2]		C ₁₀ H ₆ Cl ₈	409.799	103–105	0.168	
	γ-chlordane [5564-34-7]		C ₁₀ H ₆ Cl ₈	409.799	131	0.0912	
	technical grade ^a [12789-03-6]						
Chlorfenvinphos [470-90-6]	Birlane, Sapecron	2-chloro-1-(2,4-dichlorophenyl) vinyl diethyl phosphate	C ₁₂ H ₁₄ Cl ₃ O ₄ P	359.569	B19	1	
Chlorpyrifos [2921-88-2]	Brodan, Dursban, Dowco 179	<i>O,O</i> -diethyl <i>O</i> -3,5,6-trichloro 2-pyridyl phosphorothioate	C ₉ H ₁₁ Cl ₃ NO ₃ PS	350.586	42	0.681	
Chlorpyrifos-methyl [5598-13-0]	Reldan, Dowco 214	<i>O,O</i> -dimethyl <i>O</i> -3,5,6-trichloro-2-pyridyl phosphorothioate	C ₇ H ₇ Cl ₃ NO ₃ PS	322.534	43	0.666	

Crotoxyphos [7700-17-6]	Ciodrin	dimethyl(<i>E</i>)-1-methyl-2-(1-phenyl-ethoxycarbonyl)vinyl phosphate	C ₁₄ H ₁₉ O ₆ P	314.271	liquid	1
Cyhalothrin [68085-85-8]	Cyhalothrin	(<i>RS</i>)- α -cyano-3-phenoxybenzyl(<i>Z</i>)-(1 <i>RS</i> ,3 <i>RS</i>)-2-chloro-3,3,3-trifluoropropanyl)-2,2-dimethylcyclopropanecarboxylate	C ₂₃ H ₁₉ ClF ₃ NO ₃	449.850		
lambda-Cyhalothrin [91465-08-6]			C ₂₃ H ₁₉ ClF ₃ NO ₃	449.850	49.2	0.579
Cypermethrin [52315-07-8]	Polytrin, Ambush C, Kakfil Super, BSI, draft E-ISO	(<i>RS</i>)- α -cyano-3-phenoxybenzyl (1 <i>RS</i> ,3 <i>RS</i> ; 1 <i>RS</i> ,3 <i>RS</i>)-3-(2,2-dichlorovinyl)-2,2=dimethylcyclopropanecarboxylate	C ₂₂ H ₁₉ Cl ₂ NO ₃	416.297	70	0.362
	α -cypermethrin [67375-30-8]		C ₂₂ H ₁₉ Cl ₂ NO ₃	416.297	78-81	0.292
	β -cypermethrin [65731-84-2]		C ₂₂ H ₁₉ Cl ₂ NO ₃	416.297	64-71	
	ζ -cypermethrin [52315-07-8]		C ₂₂ H ₁₉ Cl ₂ NO ₃	416.297	-22.4	1
DDD						
<i>p,p'</i> -DDD [72-54-8]	<i>p,p'</i> -TDE	1,1-Dichloro-2,2-bis (4-chlorophenyl)ethane	C ₁₄ H ₁₀ Cl ₄	320.041	109.5	0.148
<i>o,p'</i> -DDD [53-10-0]		1,1-dichloro-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	C ₁₄ H ₁₀ Cl ₄	320.041	112	0.140
DDE						
<i>p,p'</i> -DDE [72-55-9]	<i>p,p'</i> -DDE	1,1-dichloro-2,2-bis-(<i>p</i> -chlorophenyl)-ethylene	C ₁₄ H ₈ Cl ₄	318.026	89	0.236
<i>o,p'</i> -DDE [3424-82-6]	<i>o,p'</i> -DDE	1,1-Dichloro-2(2-chlorophenyl)-2-(4-chlorophenyl)ethylene	C ₁₄ H ₈ Cl ₄	318.026	88-90	0.236
DDT	Agritan		C ₁₄ H ₉ Cl ₅	354.486	108.5	0.152
<i>p,p'</i> -DDT [50-29-3]		1,1,1-trichloro-2,2-bis-(4-chlorophenyl)-ethane				
<i>o,p'</i> -DDT [789-02-6]		1,1,1-trichloro-2-(chlorophenyl)-2-(4-chlorophenyl)-ethane	C ₁₄ H ₉ Cl ₅	354.486		
Deltamethrin [62918-63-5]	Decis, K-Othrine Butox, Butoflin	(<i>S</i>)- α -cyano-3-phenoxybenzyl(1 <i>R</i> ,3 <i>R</i>)-3-(2,2-dibromovinyl)-2,2-dimethylcyclo-propanecarboxylate	C ₂₂ H ₁₉ Br ₂ NO ₃	505.199	98-101	0.186
Demeton [8065-48-3]	Systox	<i>O,O</i> -diethyl <i>O</i> -2-ethylthioethyl phosphorothioate	C ₈ H ₁₉ O ₃ PS ₂	258.339	liquid	1
Demeton-S-methyl [919-86-8]	Metasystoxi	<i>S</i> -2-ethylthioethyl <i>O,O</i> -dimethyl phosphorothioate	C ₆ H ₁₅ O ₃ PS ₂	230.285	liquid	1
Dialifor [10311-84-9]	Torak	<i>S</i> -2-chloro-1-phthalimidoethyl <i>O,O</i> -diethylphosphorodithioate	C ₁₄ H ₁₇ ClNO ₄ PS ₂	393.846	68	0.379
Diamidaphos [1754-58-1]	Nellite	phenyl <i>N,N'</i> -dimethylphosphoro-diamidate	C ₈ H ₁₃ N ₂ O ₂ P	200.175	103.5	0.170
Diazinon [333-41-5]	Basudin, Diazide, Spectracide	<i>O,O</i> -diethyl <i>O</i> -2-isopropyl-6-methyl-pyrimidin-4-yl phosphorothioate	C ₁₂ H ₂₁ N ₂ O ₃ PS	304.345	liquid	1
Dicapthon [2463-84-5]	Dicaptan	<i>O</i> -(2-chloro-4-nitrophenyl)- <i>O,O</i> -dimethyl phosphorothioate	C ₈ H ₉ ClNO ₅ PS	297.653	53	0.531
Dichlofenthion [97-17-6]	Mobilawn	<i>O</i> -2,4-dichlorophenyl <i>O,O</i> =diethyl phosphorothioate	C ₁₀ H ₁₃ Cl ₂ O ₃ PS	315.153	liquid	1

(Continued)

TABLE 18.2.1 (Continued)

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, Fat 25°C	pK _a
Dichlorvos [62-73-7]	Vapona, Nuvan, DDVP, Dede vap	2,2-dichlorovinyl- <i>O,O</i> -dimethyl phosphate	C ₄ H ₇ Cl ₂ O ₄ P	220.976	liquid	1	
Dicrotophos [141-66-2]	Carbicon, Ektafos, Bidrin	(<i>E</i>)-2-dimethylcarbamoyl-1-methylvinyl dimethyl phosphate	C ₈ H ₁₆ NO ₅ P	237.191	liquid	1	
Dieldrin [60-57-1]	HEOD	1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro- <i>exo</i> -1,4- <i>endo</i> -5,8-dimethanonaphthalene	C ₁₂ H ₈ Cl ₆ O	380.909	175.5	0.0334	
Diflubenzuron [35367-38-5]	Deflubenzon, Dimilin	1-(4-chlorophenyl)-3-(2,6-difluoro-benzol) urea	C ₁₄ H ₉ ClF ₂ N ₂ O ₂	310.683	239	0.00795	
Dimethoate [60-51-5]	Cygon	<i>O,O</i> -dimethyl- <i>S</i> -(<i>N</i> -methyl-carbamoyl-methyl phosphorodithioate	C ₅ H ₁₂ NO ₃ PS ₂	229.258	52	0.543	
Dinoseb [88-85-7]	Antox, Aretit, BNP 30, DNBP	2- <i>sec</i> -butyl-4,6-dinitrophenol	C ₁₀ H ₁₂ N ₂ O ₅	240.212	40	0.713	
Disulfoton [298-04-4]	Di-Syston, Dithiosystox	<i>O,O</i> -diethyl- <i>S</i> -(ethylthio)-ethyl phosphorodithioate	C ₈ H ₁₉ O ₂ PS ₃	274.405	-25	1	
Endosulfan [115-29-7]	Thiodan, Cyclo dan, Malix, Thifor	5-norbornene-2,3-dimethanol-1,4,5,6,7,7-hexachlorocyclic sulfite	C ₉ H ₆ Cl ₆ O ₃ S	406.925	106	0.160	
	α-Endosulfan [959-98-8]		C ₉ H ₆ Cl ₆ O ₃ S	406.925	106	0.160	
	β-Endosulfan [33213-65-9]		C ₉ H ₆ Cl ₆ O ₃ S	406.925	207-209	0.0160	
Endosulfan sulfate [1031-07-8]			C ₉ H ₆ Cl ₆ O ₄ S	422.925	181	0.0295	
Endrin [72-20-8]	endrine, nendrin	1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro- <i>exo</i> -1,4- <i>exo</i> -5,8-dimethanonaphthalene	C ₁₂ H ₈ Cl ₆ O	380.909	dec 245	0.00694	
Ethiofencarb [29973-13-5]	Croneton, Bay-Hox-1901	α-ethylthio- <i>o</i> -tolyl methylcarbamate	C ₁₁ H ₁₅ NO ₂ S	225.307	33.4	0.827	
Ethion [563-12-2]	Nialate, diethion	<i>O,O,O',O'</i> -tetraethyl- <i>S,S'</i> -methylene bis(phosphorodithioate)	C ₉ H ₂₂ O ₄ P ₂ S ₄	384.476	-13	1	
Ethoprophos [13194-48-4]	Mocap, ethoprop	<i>O</i> -ethyl- <i>S,S</i> -dipropyl-phosphorodithioate	C ₈ H ₁₉ O ₂ PS ₂	242.340	liquid	1	
Fenitrothion [122-14-5]	Sumithion, Folithion Cyfen	<i>O,O</i> -dimethyl <i>O</i> -4-nitro- <i>m</i> -tolyl phosphorothioate	C ₉ H ₁₂ NO ₅ PS	277.234	liquid	1	
Fenoxycarb [79127-80-3]	Logic, Pictyl, Varodo	ethyl 2-(4-phenoxyphenoxy)ethyl-carbamate	C ₁₇ H ₁₉ NO ₄	301.338	53	0.531	
Fenpropathrin [64257-84-7]	Rody, Danitol, Meothrin, S-3206	(<i>R,S</i>)- <i>O</i> -cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate	C ₂₂ H ₂₃ NO ₃	349.423	47	0.608	
Fensulfothion [115-90-2]	Dassnit, Terracur	<i>O,O</i> -diethyl <i>O</i> -4-methylsulphinylphenyl phosphorothioate	C ₁₁ H ₁₇ O ₄ PS ₂	308.354			

Fenthion [55-38-9]	Baytex, Baycid, Mercaptophos,	<i>O,O</i> -dimethyl- <i>O</i> -(3-methyl-4-(methylthio)phenyl) phosphorothioate	C ₁₀ H ₁₅ O ₃ PS ₂	278.328	liquid	1
Fenvalerate [51630-58-1]	Sumicidin, Belmark, Pydrin	(<i>RS</i>)- α -cyano-3-phenoxybenzyl (<i>RS</i>)-2-(4-chlorophenyl)-3-methylbutyrate	C ₂₅ H ₂₂ ClNO ₂	419.901	liquid	1
Flucythrinate [70124-77-5]	Cybolt, Cythrin, Pay-Off	(<i>RS</i>)- α -cyano-3-phenoxybenzyl (<i>S</i>)-2-(4-difluoromethoxyphenyl)-3-methylbutyrate	C ₂₆ H ₂₃ F ₂ NO ₄	451.463	liquid	1
Fonofos [944-22-9]	Dyfonate, Fonophos	<i>O</i> -ethyl- <i>S</i> -phenyl (<i>RS</i>)-ethyl-phosphorodithioate	C ₁₀ H ₁₅ OPS ₂	246.329	liquid	1
Heptachlor [76-44-8]	Methanoindene	1,4,5,6,7,8,8-heptachloro-3a-4,7-7a-tetrahydro-4,7- <i>endo</i> -methanoindene	C ₁₀ H ₅ Cl ₇	373.318	95.5	0.203
Heptachlor epoxide [1024-57-3]		1,4,5,6,7,8-heptachloro-2,3-epoxy-2,3,3a-4,7,7a-tetrahydro-4,7-methanoindene	C ₁₀ H ₅ Cl ₇ O	389.317	160	0.0474
Hexachlorocyclohexane	BHC, HCH	1,2,3,4,5,6-Hexachlorocyclohexane	C ₆ H ₆ Cl ₆	290.830		
α -HCH'[319-84-6]	α -BHC	1,2,3,4,5,6-Hexachlorocyclohexane		290.830	158	0.0496
β -HCH'[319-85-7]	β -BHC	1,2,3,4,5,6-Hexachlorocyclohexane		290.830	309	0.00164
γ -HCH (Lindane)	Gammexane	1,2,3,4,5,6-hexachlorocyclohexane	C ₆ H ₆ Cl ₆	290.830	112.5	0.139
δ -HCH'[319-86-8]	Δ -BHC	1,2,3,4,5,6-hexachlorocyclohexane	C ₆ H ₆ Cl ₆	290.830	141.5	0.0719
Iodofenphos [25311-71-1]	Nuvanol N	<i>O</i> -2,5-dichloro-4-iodophenyl <i>O,O</i> -dimethyl phosphorothioate	C ₈ H ₈ Cl ₂ IO ₃ PS	345.395	oil	1
Isophorone [78-59-1]	Isooctaphenone	3,5,5-trimethyl-2-cyclohexene-1-one	C ₉ H ₁₄ O	138.206	-8.1	1
Kepone [143-50-0]	Chlordecone	decachlorooctahydro-1,3,4-metheno-2 <i>H</i> -cyclobuta[<i>cd</i>]pentalen-2-one	C ₁₀ H ₁₀ O	490.636	350 dec	0.00065
Leptophos [21609-90-5]	Phosvel	<i>O</i> -(4-bromo-2,5-dichlorophenyl) <i>O</i> -methyl phenylphosphorothioate	C ₁₃ H ₁₀ BrCl ₂ O ₂ P S	412.066	71	0.345
Lindane [58-89-9]	γ -BHC, γ -HCH	1,2,3,4,5,6-hexachlorocyclohexane	C ₆ H ₆ Cl ₆	290.830	112.5	0.139
Malathion [121-75-5]	Karbofos, Cythion, mercaptothion	<i>S</i> -[1,2-bis(ethoxycarbenyl)ethyl]- <i>O,O</i> -dimethyl phosphorodithioate	C ₁₀ H ₁₉ O ₆ PS	330.358	1.4	1
Mecarbam [2595-54-2]	Afos	<i>S</i> -(<i>N</i> -ethyoxycarbonyl- <i>N</i> -methyl-carbamoylmethyl) <i>O,O</i> -diethyl	C ₁₀ H ₂₀ NO ₃ PS ₂	329.374	oil	1
Methamidophos [10265-92-6]	Monitor, Tamaron	<i>O,S</i> -dimethylphosphoramidothioate	C ₂ H ₈ NO ₂ PS	141.130	46	0.622
Methiocarb [2032-65-7]	Mesuroil, Draza	4-methylthio-3,5-xylyl methylcarbamate	C ₁₁ H ₁₅ NO ₂ S	225.308	120	0.117
Methomyl [16752-77-5]	Lannate	<i>S</i> -methyl- <i>N</i> -(methylcarbamoyl-oxy)-thioaceticimide	C ₅ H ₁₀ N ₂ O ₂ S	162.210	78	0.302
Methoxychlor [72-43-5]	Marlate	1,1,1-trichloro-2,2-bis(4-methoxy-phenyl)ethane	C ₁₆ H ₁₅ Cl ₃ O ₂	345.648	87	0.246
Mevinphos [7786-34-7]	Apavinfos, Duraphos	2-carbomethoxy-1-methylvinyl dimethyl phosphate	C ₇ H ₁₃ O ₆ P	224.148	-56.1	1
Mirex [2385-85-5]	Dechlorane	1,1a,2,2,3a,4,5,5,5a,5b,6-dodeca-chlorooctahydro-1,3,4-metheno-1 <i>H</i> -cyclobuta(<i>cd</i>)pentalene	C ₁₀ Cl ₁₂	545.543	485 dec	0.000031
Monocrotophos [6923-22-4]	Nuvacron, Azodrin	dimethyl (<i>E</i>)-1-methyl-2-(methyl-carbamoyl)vinyl phosphate	C ₇ H ₁₄ NO ₅ P	223.164	55	0.508

(Continued)

TABLE 18.2.1 (Continued)

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C	pK _a
Naled [300-76-5]	Arthodibrom, Dibrom, Bromex, Bromchlophos	1,2-dibromo-2,2-dichloroethyl dimethyl phosphate	C ₄ H ₇ Br ₂ Cl ₂ O ₄ P	380.784	27	0.956	
Oxamyl [23135-22-0]	Vydate	<i>N,N'</i> -dimethyl-2-methylcarbamoyloxyimino-2-(methylthio)acetamine	C ₇ H ₁₃ N ₃ O ₃ S	219.261	109	0.150	
Parathion [56-38-2]	Folidol, Bladan, Niran	<i>O,O</i> -diethyl <i>O</i> -4-nitrophenyl phosphorothioate	C ₁₀ H ₁₄ NO ₅ PS	291.261	6.1	1	
Parathion-methyl [298-00-0]	Dalf, Nitrox	<i>O,O</i> -dimethyl <i>O</i> -(<i>p</i> -nitrophenyl) phosphorothioate	C ₈ H ₁₀ NO ₅ PS	263.208	38	0.746	
Pentachlorophenol [87-86-5]	PCP	pentachlorophenol	C ₆ H ₅ OH	266.336	174	0.0345	4.74
Pentachlorophenol sodium salt (Pentacon)							
Permethrin [52645-53-1]	Ambush, Kafil, Picket, Pramex	3-phenoxybenzyl(1 <i>RS</i> ,3 <i>RS</i> ;1 <i>RS</i> ,3 <i>RS</i>)-3(2,2-dichlorovinyl)-2,2=dimethylcyclo-prapanecarboxylate	C ₂₁ H ₂₀ Cl ₂ O ₃	391.288	34	0.816	
<i>cis</i> -Permethrin					63-65	0.414	
<i>trans</i> -Permethrin					44-47	0.629	
technical grade							
Phenthoate [2597-03-7]	Cidial, Elsan	ethyl 2-dimethoxythiophosphorythio-2-phenylacetate	C ₁₂ H ₁₇ O ₄ PS ₂	320.364	17-18	1	
Phorate [298-02-2]	Forsaath, Gramitox	<i>O,O</i> -diethyl- <i>S</i> -(ethylthio)methyl phosphordithioate	C ₇ H ₁₇ O ₂ PS ₃	260.378	<-15	1	
Phorate-sulfone				292.3			
Phorate-sulfoxide				276.4			
Phosmet [732-11-6]	Imidan	<i>S</i> -[(1,3-dihydro-1,3-dioxo-2 <i>H</i> -isoindol-2-yl)methyl]	C ₁₁ H ₁₂ NO ₄ PS ₂	317.321	72	0.346	
Phosphamidon [13171-21-6]	Dimecron	2-chloro-2-diethylcarbamoyl-1-methylvinyl dimethyl phosphate	C ₁₀ H ₁₉ ClNO ₅ P	299.689	-45	1	
Pirimicarb [23103-98-2]	Pirimor, Aphox	2-dimethylamino-5,6-dimethyl-pyrimidin-4-yl dimethylcarbamate	C ₁₁ H ₁₈ N ₄ O ₂	238.287	90.5	0.228	
Profenofos [41198-08-7]	Selecron	<i>O</i> -4-bromo-2-chlorophenyl <i>O</i> -ethyl <i>S</i> -propyl phosphorothioate	C ₁₁ H ₁₅ BrClO ₃ PS	373.631	liquid	1	
Propoxur [114-26-1]	Baygon	2-(1-Methylethoxy)phenol methyl carbamate	C ₁₁ H ₁₅ NO ₃	209.242	87	0.246	
Ronnel [299-84-3]	Fenchlorphos, Korlan, Etrolene, Trolene	<i>O,O</i> -dimethyl <i>O</i> -2,4,5-trichlorophenyl-phosphorothioate	C ₈ H ₈ Cl ₃ O ₃ PS	321.546	41	0.697	
Sulfotep [3689-24-5]	dithio, thiotep, ENT, Bladafum	<i>O,O,O',O'</i> -tetraethyl dithiopyrophosphate	C ₈ H ₂₀ O ₅ P ₂ S ₂	322.320	liquid	1	
Terbacil [5902-51-2]	Sinbar, Turbacil	5-chloro-3-(1,1-dimethyl)-6-methyl-2,4-(1 <i>H</i> ,3 <i>H</i>)-pyrimidine-dione	C ₉ H ₁₃ Cl ₂ N ₂ O ₃	216.664	176	0.0330	9.0

Terbufos [13071-79-9]	Contraven, Counter	<i>S-tert</i> -butylthiomethyl <i>O,O</i> -diethyl phosphorodithioate	$C_9H_{21}O_2PS_3$	288.431	liquid	1
Terbufos sulfone				320.41		
Terbufos sulfoxide				304.41		
Tetramethrin [7696-12-0]	Neo-Pynamin, phthalthrin	cyclohex-1-ene-1,2-dicarboximidomethyl (1 <i>RS</i> ,3 <i>RS</i> ;1 <i>RS</i> ,3 <i>SR</i>)-2,2-dimethyl-3-methylprop-1-enyl)cyclopropanecarboxylate	$C_{19}H_{25}NO_4$	331.407	65-80	
Thiobencarb [28249-77-6]	Benthiocarb, Bolero, Saturno	<i>S</i> -(4-chlorophenyl)methyl diethyl-carbamothioate	$C_{12}H_{16}ClNOS$	257.779	1.7	1
Thiodicarb [59669-26-0]	Cicarbosulf, Larvin, Lepicron	dimethyl <i>N,N'</i> -thiobis(methylimino)-carbonyloxy bisethanimidothioate	$C_{10}H_{18}N_4O_4S_3$	354.470	173	0.0353
Toxaphene [8001-35-2]	Camphechlor	chlorinated camphene (67–69% Cl content) - mixture	$C_{10}H_{10}Cl_8$	413.812	65-90	
Trichlorfon [52-68-6]	Tugon, Chlorophos, Dipterex, Neguvon	dimethyl 2,2,2-trichloro-1-hydroxy-ethylphosphonate	$C_4H_8Cl_3O_4P$	257.437	77	0.309
Zinophos [297-92-2]	Thionazin, Namafos Cynem	<i>O,O</i> -diethyl- <i>O</i> -pyrazin-2-yl phosphorothioate	$C_8H_{13}N_2O_3PS$	248.239	–1.69	1

TABLE 18.2.2
Summary of selected physical-chemical properties of insecticides at 25°C

Compound	Selected properties					log K _{OW}	Henry's law constant H/(Pa·m ³ /mol) calcd P/C	log K _{OC} reported
	Vapor pressure		Solubility					
	P ^s /Pa	P _L /Pa	S/(g/m ³)	C ^s /(mol/m ³)	C _L /(mol/m ³)			
Acephate	2.26 × 10 ⁻⁴	8.96 × 10 ⁻⁴	818000	4465	17710	-1	5.06 × 10 ⁻⁸	0.301
Aldicarb	0.004	0.0216	6000	31.54	170	1.1	1.27 × 10 ⁻⁴	1.48
Aldrin	0.005	0.0302	0.02	5.48 × 10 ⁻⁵	3.31 × 10 ⁻⁴	3.01	91.23	2.61
Aminocarb	0.00227	0.0109	915	4.39	21.1	1.73	5.17 × 10 ⁻⁴	2.00
Azinphos-methyl	3.0 × 10 ⁻⁵	9.05 × 10 ⁻⁵	30	0.0945	0.285	2.7	3.17 × 10 ⁻⁴	2.61
Bendiocarb	6.6 × 10 ⁻⁴	7.21 × 10 ⁻³	40	0.179	1.96		3.68 × 10 ⁻³	2.76
Carbaryl	2.67 × 10 ⁻⁵	3.83 × 10 ⁻⁴	120	0.596	8.56	2.36	4.48 × 10 ⁻⁵	2.36
Carbofuran	8.0 × 10 ⁻⁵	1.41 × 10 ⁻³	351	1.59	28.0	2.32	5.04 × 10 ⁻⁵	2.02
Chlordane								
<i>cis</i> - or α-chlordane	4.0 × 10 ⁻⁴	2.65 × 10 ⁻³	0.056	1.37 × 10 ⁻⁴	9.07 × 10 ⁻⁴	6.0	0.342	5.5
<i>trans</i> - or β-chlordane	5.2 × 10 ⁻⁴	3.15 × 10 ⁻³	0.056	1.37 × 10 ⁻⁴	8.30 × 10 ⁻⁴	6.0	0.262	5.5
Chlorfenvinphos	1.0 × 10 ⁻⁴	1.0 × 10 ⁻⁴	124	0.345	0.345	3.82	2.90 × 10 ⁻⁴	2.47
Chlorpyrifos	0.00227	3.34 × 10 ⁻³	0.73	2.08 × 10 ⁻³	3.07 × 10 ⁻³	4.92	1.09	3.78
Chlorpyrifos-methyl	0.006	9.68 × 10 ⁻³	4.76	0.0148	0.0238		0.407	3.48
Crotoxyphos	0.0019	1.90 × 10 ⁻³	1000	3.18	3.18	2.23	5.97 × 10 ⁻⁴	2.23
Cypermethrin#	1.87 × 10 ⁻⁷	6.62 × 10 ⁻⁷	0.004	9.61 × 10 ⁻⁶	3.40 × 10 ⁻⁵	6.6	0.0195	2.59
α-cypermethrin	2.30 × 10 ⁻⁷	8.21 × 10 ⁻⁷	0.01	2.40 × 10 ⁻⁵	8.41 × 10 ⁻⁵	6.94*	0.0098	
β-cypermethrin	1.80 × 10 ⁻⁷	5.13 × 10 ⁻⁷	0.0934	2.24 × 10 ⁻⁴	6.4 × 10 ⁻⁴	4.70*	8.02 × 10 ⁻⁷	
ζ-cypermethrin	2.50 × 10 ⁻⁷	2.5 × 10 ⁻⁷	0.045	1.08 × 10 ⁻⁴	1.08 × 10 ⁻⁴		2.31 × 10 ⁻³	
DDD								
<i>p,p'</i> -DDD	1.30 × 10 ⁻⁴	6.93 × 10 ⁻⁴	0.05	1.56 × 10 ⁻⁴	1.08 × 10 ⁻³	5.5	0.640	5.0
<i>o,p'</i> -DDD	2.0 × 10 ⁻⁴ *	1.39 × 10 ⁻³	0.10*			6.0		
DDE								
<i>p,p'</i> -DDE	8.66 × 10 ⁻⁴	3.72 × 10 ⁻³	0.04	1.26 × 10 ⁻⁴	5.40 × 10 ⁻⁴	5.7	7.95	5.0
<i>o,p'</i> -DDE	8.0 × 10 ⁻⁴	3.44 × 10 ⁻³	0.1	3.14 × 10 ⁻⁴	1.35 × 10 ⁻³	5.8	2.54	
DDT								
<i>p,p'</i> -DDT	2.0 × 10 ⁻⁵	1.35 × 10 ⁻⁴	0.0055	1.55 × 10 ⁻⁵	1.11 × 10 ⁻⁴	6.19	2.36	5.4
<i>o,p'</i> -DDT	2.53 × 10 ⁻⁵	1.72 × 10 ⁻⁴	0.026	7.33 × 10 ⁻⁵	4.96 × 10 ⁻⁴		0.347	
Deltamethrin	1.0 × 10 ⁻⁵	5.52 × 10 ⁻⁵	0.002	3.96 × 10 ⁻⁶	2.18 × 10 ⁻⁵		2.53	5.66
Demeton	0.0347	0.0347	60	0.232	0.232		0.15	1.85
Demeton-S-methyl	0.04	0.040	3300	14.3	14.3		2.79 × 10 ⁻³	
Dialifor	6.50 × 10 ⁻⁵	1.73 × 10 ⁻⁴	0.18	4.57 × 10 ⁻⁴	1.22 × 10 ⁻³	4.7	0.14	

Diamidaphos			50000					
Diazinon	0.008	8.0×10^{-3}	60	0.197	0.197	3.3	0.0406	2.76
Dicapthon	5.0×10^{-4}	1.19×10^{-3}	6.25	0.021	0.05	3.6	0.0238	
Dichlofenthion	25	25.0	0.25	7.93×10^{-4}	7.93×10^{-4}	5.1	31646	
Dichlorvos	7.02	7.02	8000	36.20	36.20	1.45	0.194	1.45
Dicrotophos	0.0213	0.0213	1000000	4216	4216		5.05×10^{-6}	1.88
Dieldrin	0.0005	0.016	0.17	4.46×10^{-4}	0.0142	5.20	1.120	4.08
Diflubenzuron	1.20×10^{-7}	1.31×10^{-5}	0.08	2.57×10^{-4}	0.0281	0.78	4.66×10^{-4}	3.01
Dimethoate	0.01	0.019	20000	87.23	163.2	0.8	1.15×10^{-4}	1.3
Dinoseb	10	14.07	47	0.196	0.275		51.11	2.09
Disulfoton	0.02	0.132	25	0.0911	0.603	4.02	0.220	3.25
DNOC	0.011	0.044	150	1.013	4.063		0.0109	
Endosulfan	0.0013		0.5	1.23×10^{-3}		3.6	1.06	4.09
α -Endosulfan	0.0013	0.008	0.5	1.23×10^{-3}	0.008	3.62		3.4
β -Endosulfan	0.0061	0.394	0.45	1.11×10^{-3}	0.071	3.83		3.5
Endrin	2.0×10^{-5}	1.32×10^{-3}	0.23	6.04×10^{-4}	0.0399	5.2	0.0331	4
Ethion	1.5×10^{-4}	1.50×10^{-4}	1.8	4.68×10^{-3}	4.68×10^{-3}	5.7	0.0320	4.19
Ethoprophos	0.0507	0.0507	750	3.095	3.095	3.59	0.0164	1.85
Fenitrothion	1.3×10^{-4}	1.30×10^{-4}	30	0.108	0.108	3.4	1.20×10^{-3}	3.3
Fenoxycarb	1.70×10^{-6}	3.29×10^{-6}	6	0.0199	0.039	4.3	8.54×10^{-5}	3.0
Fenthion	0.004	4.0×10^{-3}	50	0.180	0.180	4.1	0.0223	3.18
Fenvalerate	4.27×10^{-6}	4.27×10^{-6}	0.085	2.02×10^{-4}	2.02×10^{-4}	6.2	0.0211	4.0
Flucythrinate	$1.20 \times 10^{-6*}$	1.20×10^{-6}	0.5*	1.11×10^{-3}	1.11×10^{-3}	6.2	1.08×10^{-3}	5.0
Fonofos	0.045	0.045	16	0.0650	0.065	3.9	0.693	2.94
Heptachlor	0.053	0.267	0.056	1.50×10^{-4}	7.56×10^{-4}	5.27	353.4	4.38
Heptachlor epoxide			0.35	8.99×10^{-4}	0.0190	5.0		4.0
Hexachlorocyclohexane								
α -BHC	0.003	0.10	1	3.44×10^{-3}	0.115	3.81	0.872	3.81
β -BHC	4.0×10^{-5}	0.0264	0.1	3.44×10^{-4}	0.227	3.8	0.116	3.36
δ -BHC	0.002	0.0268	8	0.0275	0.369	4.14	0.0727	
Iodofenphos	4.4×10^{-4}	4.4×10^{-4}	18	0.0521	0.0521	4.04	8.45×10^{-3}	
Isophorone	50	50.0	12000	86.83	86.83	1.7	0.576	
Kepone	2.93×10^{-5}	0.05	3	0.0061	10.02	5.4	0.005	4.74
Leptophos	3.0×10^{-6}	6.08×10^{-6}	0.005	1.21×10^{-5}	2.46×10^{-5}	5.9	0.247	3.97
Lindane	0.00374	0.0274	7.3	0.0251	0.184	3.7	0.149	3.0
Malathion	0.001	0.001	145	0.439	0.439	2.8	2.28×10^{-3}	3.26
Mecarbam	negligible		< 1000					
Methamidophos	0.0023	3.59×10^{-3}	200000	142	2210			

(Continued)

TABLE 18.2.2 (Continued)

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol) calcd P/C	log K _{oc} reported
	Vapor pressure		Solubility			log K _{ow}		
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)			
Methiocarb	0.016*	0.130	30	0.133	1.082	2.92	0.120	2.48
Methomyl	0.0067	0.0229	58000	358	1223	0.60	1.87 × 10 ⁻⁵	
Methoxychlor	0.00013	5.46 × 10 ⁻⁴	0.045*	1.30 × 10 ⁻⁴	5.47 × 10 ⁻⁴	5.08	0.999	4.9
Mevinphos	0.017	0.0170	600000	268	2677	0.5	6.35 × 10 ⁻⁶	1.64
Mirex	0.0001	3.545	6.5 × 10 ⁻⁵	1.19 × 10 ⁻⁷	4.22 × 10 ⁻³	6.9	839.4	6.0
Monocrotophos	0.00933	0.0185	1000000	448	8870	B0.20	2.08 × 10 ⁻⁶	
Oxamyl	0.0306	0.173	282000	1290	7261	B0.47	2.38 × 10 ⁻⁵	1.4
Parathion	6.0 × 10 ⁻⁴	6.0 × 10 ⁻⁴	12.4	0.0426	0.0426	3.8	0.0141	4.02
Parathion methyl	0.002	2.69 × 10 ⁻³	25	0.095	0.128	3.0	0.0211	3.7
Pentachlorophenol	0.00415	0.12	14	0.053	1.565	5.05	0.79	4
Permethrin	1.70 × 10 ⁻⁶	2.34 × 10 ⁻⁶	0.006	1.53 × 10 ⁻⁵	2.11 × 10 ⁻⁵	6.1	0.111	4.8
Phenthoate	3.5 × 10 ⁻⁴	3.50 × 10 ⁻⁴	11	0.0343	0.034	3.69	0.0102	3.00
Phorate	0.085	0.085	22	0.0845	0.084	3.56	1.01	2.82
Phosmet	6.0 × 10 ⁻⁵	1.75 × 10 ⁻⁴	25	0.0788	0.229	2.8	7.62 × 10 ⁻⁴	2.8
Phosphamidon	0.003	0.003	2.5	8.34 × 10 ⁻³	0.0083		0.360	0.845
Pirimicarb	0.003	0.0133	2200	9.232	41.03		3.25 × 10 ⁻⁴	
Profenofos	1.2 × 10 ⁻⁴	1.20 × 10 ⁻⁴	28	0.0749	0.075		1.60 × 10 ⁻³	3.34
Propoxur	1.70 × 10 ⁻⁵	7.73 × 10 ⁻⁵	1800	8.603	39.12	1.5	1.98 × 10 ⁻⁶	1.48
Pyrethrins	1.33 × 10 ⁻⁶		0.001	3.05 × 10 ⁻⁶			0.437	5
Ronnel (Fenchlorofos)	0.107	0.154	0.6	1.87 × 10 ⁻³	2.69 × 10 ⁻³	5.07	57.35	2.9
Sulfotep	0.0227	0.0227	25	0.0776	0.0776		0.293	
Terbacil	4.13 × 10 ⁻⁵	1.29 × 10 ⁻³	710	3.276	102.06		1.26 × 10 ⁻⁵	1.74
Terbufos	0.0427	0.0427	5	0.0173	0.017	4.48	2.463	2.70
Thiobencarb	0.00293		19.2	0.0745			0.0393	2.95
Thiodicarb	0.00431	0.117	35	0.0987	2.68		0.0437	
Toxaphene	0.0009		0.5	1.21 × 10 ⁻³		5.50	0.745	5
Trichlorfon	0.001	3.83 × 10 ⁻³	154000	598	2290	0.51	1.67 × 10 ⁻⁶	1.00
Zinophos	0.4	0.40	1000	4.029	4.03		0.0993	

isomer not specified

* The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to a large error.

TABLE 18.2.3

Suggested half-life classes of insecticides in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aldicarb	1	5	6	8
Aldrin	4	8	8	9
Carbaryl	3	4	5	6
Carbofuran	1	4	5	6
Chlordane	4	8	8	9
Chloropyrifos	2	4	4	6
DDE	4	9	9	9
<i>p,p'</i> -DDT	4	7	8	9
Diazinon	5	6	6	7
Dieldrin	4	8	8	9
Heptachlor	3	5	6	7
γ -HCH (lindane)	5	8	8	9
Malathion	2	3	3	5
Methoxychlor	2	4	6	7
Mirex	4	6	9	9
Parathion	2	5	5	6
Parathion-methyl	2	5	5	6
Propoxur	1	5	5	6
Toxaphene	4	9	9	9

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

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19 Fungicides

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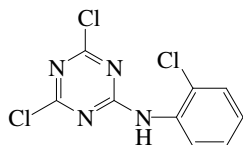
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19.1 LIST OF CHEMICALS AND DATA COMPILATIONS

19.1.1 ANILAZINE



Common Name: Anilazine

Synonym: Botrysan, Direz, Dyrene, Kemate, Triasyn, triazine, Zinochlor

Chemical Name: 2-chloro-*N*-(4,6-dichloro-1,3,5-triazin-2-yl)aniline; 2,4-dichloro-6-(*o*-chloro-anilino)-*s*-triazine; 4,6-dichloro-*N*-(2-chlorophenyl)-1,3,5-triazin-2-amine

Uses: as fungicide to control early and late blights of potatoes and tomatoes; anthracnose in cucurbits; leaf spot diseases in many crops; glume blotch of wheat; also used on vegetables, ornaments, berry fruits, melons, coffee and tobacco, etc.

CAS Registry No: 101-05-3

Molecular Formula: $C_9H_5Cl_3N_4$

Molecular Weight: 275.522

Melting Point ($^{\circ}C$):

160 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.80 (Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm^3/mol):

252.8 (calculated-Le Bas method at normal boiling point)

153.1 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0474 (mp at $160^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

8.00 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

8.00 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

8.00 (selected, Lohninger 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

negligible ($20^{\circ}C$, Hartley & Kidd 1987)

8.20×10^{-7} ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

8.26×10^{-7} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

2.82×10^{-5} ($20^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

4.39 (calculated, Chiou 1981)

3.79 (calculated-CLOGP program, Biagi et al. 1991)

3.01 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

3.88 (RP-HPLC-RT correlation, Saito et al. 1993)

1.91 (at pH 7, Milne 1995)

3.00 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.28 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, $\log K_{oc}$:

- 3.00 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.00 (estimated-chemical structure, Lohninger 1994)
- 3.14 (calculated-S as per Kenaga 1980, this work)
- 3.00, 2.53, 3.30 (soil, quoted obs.; estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: stable in neutral and slightly acidic media, $t_{1/2} = 730$ h at pH 4, $t_{1/2} = 790$ h at pH 7, $t_{1/2} = 22$ h at pH 9, 22°C (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

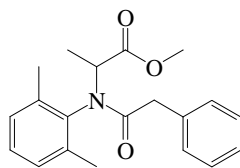
Sediment:

Soil: $t_{1/2} \sim 12$ h in damp soil (Hartley & Kidd 1987; Tomlin 1994);

field $t_{1/2} = 1$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

19.1.2 BENALAXYL



Common Name: Benalaxyl

Synonym: Galben, M 9834, Tairel

Chemical Name: methyl *N*-phenylacetyl-*N*-2,6-dimethylphenyl-*DL*-alaninate; methyl *N*-(2,6-dimethylphenyl)-*N*-(phenylacetyl)-*DL*-alaninate

CAS Registry No: 71626-11-4

Uses: as fungicide to control late blights of potatoes and tomatoes; downy mildews of hops, vines, lettuce, onions, soybeans and other crops; many diseases in flowers and ornamentals; and often used in combination with other fungicides, etc.

Molecular Formula: $C_{20}H_{23}NO_3$

Molecular Weight: 325.402

Melting Point ($^{\circ}C$):

79 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.27 ($25^{\circ}C$, Hartley & Kidd 1987; Milne 1995)

Molar Volume (cm^3/mol):

390.8 (calculated-Le Bas method at normal boiling point)

256.2 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.295 (mp at $79^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

37.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

37.0 (20 – $25^{\circ}C$, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

6.7×10^{-4} (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

1.33×10^{-3} (20 – $25^{\circ}C$, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.0117 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.40 (Worthing & Hance 1991; Milne 1995)

3.40 (Tomlin 1994)

3.40 (selected, Hansch et al. 1995)

3.24 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log BCF$:

1.91 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, $\log K_{oc}$:

3.44–3.86 (soil, Tomlin 1994)

3.00 (soil, estimated, Augustin-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} = 86$ d at pH 9, 25°C, but stable in aqueous solutions at pH 4–9 (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

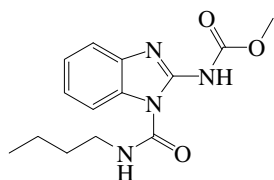
Sediment:

Soil: $t_{1/2} = 20$ –71 d in soil (Tomlin 1994);

field $t_{1/2} = 30$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.3 BENOMYL



Common Name: Benomyl

Synonym: Arilate, BBC, Benex, Benlate, Benosan, Fibenzo, Fundazol

Chemical Name: methyl *N*-(1-butylcarbamoyl-2-benzimidazole)carbamate; methyl 1-(butyl-carbamoyl)benzimidazol-2-ylcarbamate; methyl 1-[(butylamino)carbonyl]-1*H*-benz-imidazol-2-ylcarbamate

Uses: as fungicide to control a wide range of diseases of fruit, nuts, vegetables, mushrooms, field crops, ornamentals, turf and trees; also provides secondary acaricidal control, principally as an ovicide, etc.

CAS Registry No: 17804-35-2

Molecular Formula: C₁₄H₁₈N₄O₃

Molecular Weight: 290.318

Melting Point (°C):

140 (dec., Tomlin 1994)

dec (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

320.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0744 (mp at 140°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

3.8 (Austin et al. 1976; quoted, Kenaga 1980; Howard 1991)

18.2, 4.0, 3.6, 2.8, 3.0, 1.9, 1.8, 8.8, 4.5 (pH 1, 3, 5, 7, 8, 9, 10, 11, 12, room temperature, shake flask-HPLC/UV, Singh & Chiba 1985)

2.8 (shake flask-HPLC/UV at pH 7, Singh & Chiba 1985; quoted, Howard 1991)

2.0 (Hartley & Kidd 1987; Milne 1995)

4.0 (pH 3–10, Worthing & Hance 1991)

2.0 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

2.0 (stable only at pH 7, Montgomery 1993)

4.0 (selected, Lohninger 1994)

4.0 (pH 3–10, very soluble at pH 1, decomposes at pH 13, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated):

< 1.00 × 10⁻⁵ (20°C, Hartley & Kidd 1987)

< 1.33 × 10⁻⁸ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

< 4.90 × 10⁻⁶ (Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

< 1.93 × 10⁻⁶ (calculated-P/C)

Octanol/Water Partition Coefficient, log K_{ow}:

2.12 (20°C, shake flask-UV, Austin & Briggs 1976)

2.42 (Rao & Davidson 1982; Hansch & Leo 1985; 1987)

3.11 (Garten & Trabalka 1983; Travis & Arms 1988)

2.12 (Hansch & Leo 1985)

- 2.42 (Sangster 1993)
1.40–3.11 (Montgomery 1993)
2.12 (recommended, Hansch et al. 1995)
1.33 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 2.46 (estimated-S, Kenaga 1980; quoted, Howard 1991)
–0.47 (vegetation, Popov & Sboeva 1974; Jalali & Anderson 1976)

Sorption Partition Coefficient, log K_{OC} :

- 3.32 (estimated-S, Kenaga 1980; quoted, Howard 1991)
3.28 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
3.28 (soil, calculated, Montgomery 1993)
3.28 (selected, Lohninger 1994)
3.28 (soil, Tomlin 1994)
2.71 (soil, calculated-MCI χ , Sabljic et al. 1995)
2.73, 1.92 (soil, estimated-class-specific model, estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2}$ = 1.6 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).

Hydrolysis: very significant in water with $t_{1/2}$ < 1 wk (Howard 1991).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2}$ ~ 1.6 h, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).

Surface water: $t_{1/2}$ = 2 h (Tomlin 1994).

Groundwater:

Sediment:

Soil: degradation occurred within 15 d in unsterilized soil (Hine et al. 1969);

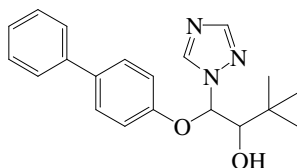
$t_{1/2}$ = 6–12 months (Hartley & Kidd 1987);

field $t_{1/2}$ = 67 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2}$ = 19 h in soil (Tomlin 1994).

Biota: $t_{1/2}$ = 3–7 d on foliage (quoted, Montgomery 1993).

19.1.4 BITERTANOL



Common Name: Bitertanol

Synonym: Baycor, Baymat, Biloxazol, Sibutol

Chemical Name: 1-(biphenyl-4-yloxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butan-2-ol; β -([1,1'-biphenyl]-4-yloxy)- α -(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol

Uses: as fungicide to control scab on apples and pears; rusts and powdery mildews on ornamentals; black spot on roses; and leaf spot and other diseases of vegetables, cucurbits, cereals, deciduous fruit, bananas, groundnuts, soy beans, etc.

CAS Registry No: 70585-38-5 (diastereoisomer A), 55179-31-2 (diastereoisomer B)

Molecular Formula: $C_{20}H_{23}N_3O_2$

Molecular Weight: 337.415

Melting Point ($^{\circ}C$):

139.8	(diastereoisomer A, Hartley & Kidd 1987)
146.3	(diastereoisomer B, Hartley & Kidd 1987)
118.0	(eutectic mixture of the two diastereoisomers, Hartley & Kidd 1987; Worthing & Hance 1991)
136.7	(diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
145.2	(diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

399.7	(calculated-Le Bas method at normal boiling point)
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Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.122 (eutectic mixture, mp at $118^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

5.0	($20^{\circ}C$, eutectic mixture; Hartley & Kidd 1987; Worthing & Hance 1991)
2.9	($20^{\circ}C$, diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
1.6	($20^{\circ}C$, diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.0×10^{-6}	($20^{\circ}C$, Hartley & Kidd 1987)
0.0038	($100^{\circ}C$, diastereoisomer A, Worthing & Hance 1991)
0.0032	($100^{\circ}C$, diastereoisomer B, Worthing & Hance 1991)
2.2×10^{-10}	($20^{\circ}C$, diastereoisomer A, Tomlin 1994)
2.5×10^{-10}	($20^{\circ}C$, diastereoisomer B, Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

8.45×10^{-5}	($20^{\circ}C$, eutectic mixture, calculated-P/C, this work)
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Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.10	($20^{\circ}C$, diastereoisomer A, Worthing & Hance 1991; Tomlin 1994)
4.40	($20^{\circ}C$, diastereoisomer B, Worthing & Hance 1991; Tomlin 1994)
4.16	(Schreiber & Schönherr 1992)
4.16	(selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.40 (20°C, eutectic mixture, calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC} :

2.25 (20°C, eutectic mixture, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: stable in neutral, acidic and alkaline media, hydrolytic $t_{1/2} > 1$ yr at 25°C and pH 4, 7 and 9 (Tomlin 1994).

Biodegradation: degradation in soil is rapid (Tomlin 1994).

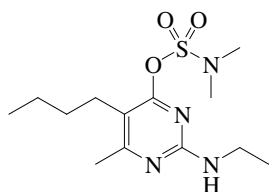
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: environmental $t_{1/2} = 1$ month to 1 yr (Tomlin 1994).

19.1.5 BUPIRIMATE



Common Name: Bupirimate

Synonym: Nimrod, PP 588

Chemical Name: 5-butyl-2-ethylamino-6-methylpyrimidin-4-yl dimethylsulfamate; 5-butyl-2-(ethylamino)-6-methyl-4-pyrimidinyl dimethylsulfamate

Uses: as fungicide to control powdery mildews of apples and pears, stone fruit, strawberries, gooseberries, vines, roses and other ornamentals, cucurbits, hops, beet, and other crops, etc.

CAS Registry No: 41483-43-6

Molecular Formula: $C_{13}H_{24}N_4O_3S$

Molecular Weight: 316.419

Melting Point ($^{\circ}C$):

50–51 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

368.9 (calculated-Le Bas method at normal boiling point, this work)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

22.0 (Martin & Worthing 1977)

22.0 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

23.0 (at pH 5.2, Worthing & Hance 1991)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

6.7×10^{-5} ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991)

1.0×10^{-4} (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

9.64×10^{-3} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.70 (shake flask, pH 7, Stevens et al. 1988)

3.70 (Worthing & Hance 1991)

3.90 (Tomlin 1994)

2.70 (selected, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.02 (calculated-S, Kenaga 1980)

2.56 (calculated- K_{ow} as per Kenaga 1980, this work)

Sorption Partition Coefficient, $\log K_{oc}$:

2.90 (calculated-S, Kenaga 1980)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rapidly decomposed by ultraviolet irradiation in aqueous solutions (Tomlin 1994).

Oxidation:

Hydrolysis: stable in dilute alkalis, but readily hydrolyzed by dilute acids (Tomlin 1994).

Biodegradation:

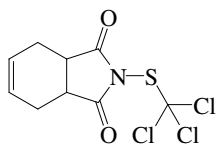
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} = 35\text{--}90$ d for nonsterile flooded or non-flooded soil, pH 5.1 to pH 7.3 (Tomlin 1994).

19.1.6 CAPTAN



Common Name: Captan

Synonym: Aacaptan, Amercide, Captab, Captaf, Captane, Captex, Flit 406, Glyodex 37-22, Malipur, Merpan, Orthocide, Pillarcap, Vondcaptan

Chemical Name: *N*-(trichloromethylthio)cyclohex-4-ene-1,2-dicarboximide; 1,2,3,6-tetrahydro-*N*-(trichloromethylthio)phthalimide; 3a,4,7,7a-tetrahydro-[(trichloromethylthio)-1*H*-isoindole-1,3(2*H*)-dione

CAS Registry No: 133-06-2

Uses: as fungicide to control a wide range of fungal diseases; also used as seed treatment on maize, ornamentals, vegetables, oilseed rape, and other crops.

Molecular Formula: C₉H₈Cl₃NO₂S

Molecular Weight: 300.590

Melting Point (°C):

178	(Hartley & Kidd 1987; Howard 1991; Worthing & Hance 1991; Tomlin 1994; Milne 1995)
172.5	(Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.74	(Hartley & Kidd 1987; Tomlin 1994; Milne 1995)
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Molar Volume (cm³/mol):

250.5	(calculated-Le Bas method at normal boiling point)
172.8	(calculated-density)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

44.35	(DSC method, Plato 1972)
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Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0357 (mp at 172.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

8.70	(colorimetric, Burchfield 1959)
< 0.5	(Martin & Worthing 1977)
0.50	(Briggs 1981)
3.30	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.50	(20°C, selected, Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
5.10	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
1.44	(calculated, Patil 1994)

Vapor Pressure (Pa at 25°C or as indicated):

< 0.0013	(Khan 1980)
< 0.0013	(Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)
0.0010	(20°C, selected, Suntio et al. 1988; quoted, Howard 1991; Majewski & Capel 1995)
1.1 × 10 ⁻⁵	(20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

0.60	(20°C, calculated-P/C, Suntio et al. 1988)
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Octanol/Water Partition Coefficient, log K_{ow} :

2.35	(Leo et al. 1971)
1.52	(Rao & Davidson 1980)
2.54	(shake flask-UV, Lord et al. 1980; Briggs 1981)
2.35	(Hansch & Leo 1985)
2.79	(Worthing & Hance 1991; Milne 1995)
2.35	(RP-HPLC-RT correlation, Saito et al. 1993)
2.60	(RP-HPLC-RT correlation, Sicbaldi & Finizio 1993)
2.35	(recommended, Sangster 1993)
2.35	(recommended, Hansch et al. 1995)
2.60	(RP-HPLC-RT correlation, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

> 2.96	(estimated-S, Kenaga 1980a; quoted, Howard 1991)
2.67	(earthworms, Lord et al. 1980)
1.30	(activated sludge, Freitag et al. 1984, 1985)
1.30	(algae, Freitag et al. 1984, 85)
1.00	(golden ide, Freitag et al. 1985)
1.56	(regression-log K_{ow} , Hansch & Leo 1985)

Sorption Partition Coefficient, log K_{oc} :

2.30	(soil, converted from K_{om} multiplied by 1.724, Briggs 1981)
2.29	(Lyman et al. 1982; quoted, Howard 1991)
1.52	(estimated, Jury et al. 1987)
1.52	(screening model calculations, Jury et al. 1987b)
2.30	(soil, quoted exptl., Meylan et al. 1992)
2.94	(soil, calculated-MCI χ and fragments contribution, Meylan et al. 1992)
2.30	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.30	(selected, Lohninger 1994)
2.30	(soil, quoted or calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolysis $t_{1/2}$ = 37 min in isopropanol, $t_{1/2}$ = 420 min in cyclohexene and $t_{1/2}$ = 380 min in cyclohexane by UV-irradiation ($\lambda > 280$ nm): (Schwack & Flöber-Müller 1990).

Oxidation: photooxidation $t_{1/2}$ = 3.2–32 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991)

Hydrolysis: pseudo-first-order hydrolysis $t_{1/2}$ = 0.1 d (Burchfield 1959; quoted, Freed 1976);

$t_{1/2}$ = 1.8 h, based on first-order rate constant $k = 6.5 \times 10^{-3} \text{ s}^{-1}$ at pH 7.1 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{1/2}$ = 10.3 h, based on first-order rate constant $k = 1.87 \times 10^{-5} \cdot \text{s}^{-1}$ at pH 5.2 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{1/2}$ = 10.5 minutes, based on first-order rate constant $k = 1.10 \times 10^{-3} \cdot \text{s}^{-1}$ at pH 8.3 and 28°C (Wolfe et al. 1976; quoted, Howard et al. 1991);

$t_{1/2}$ = 170 min in a river water sample at pH 7 and 28°C (Wolfe et al. 1976; quoted, Howard 1991);

over rate constant $k = 6.5 \times 10^{-5} \text{ s}^{-1}$ with $t_{1/2}$ = 3 h at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2}$ = 7 h in Lake Superior water at pH 7.6 and 12°C, $t_{1/2}$ = 1 h at pH 7.6 and 25°C, $t_{1/2}$ = 40 h at pH 6.7 and 12°C, and $t_{1/2}$ = 8 h at pH 6.7 and 23°C (Wolfe et al. 1976; quoted, Howard 1991).

Biodegradation: unacclimated aqueous aerobic degradation $t_{1/2}$ = 48–1440 h, based on unacclimated and acclimated soil grab sample data (Agnihotri 1970; Foschi et al. 1970; quoted, Howard et al. 1991); unacclimated aqueous anaerobic degradation $t_{1/2}$ = 192–5760 h, based on unacclimated aqueous aerobic half-life (Howard et al. 1991);

rate constant $k = 0.231 \text{ d}^{-1}$ with a biodegradation $t_{1/2}$ = 3 d in soil (Rao & Davidson 1980).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 2.6 h and 1.4 h for the vapor-phase reaction with photochemically produced hydroxyl radicals and ozone (Atkinson 1985; quoted, Howard 1991);

photooxidation $t_{1/2}$ = 3.2–32 h in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: hydrolysis $t_{1/2}$ = 170 min in a river water sample at pH 7 and 28°C (Wolfe et al. 1976; quoted, Howard 1991);

$t_{1/2}$ = 7 h in Lake Superior water at pH 7.6 and 12°C, $t_{1/2}$ = 1 h at pH 7.6 and 25°C, $t_{1/2}$ = 40 h at pH 6.7 and 12°C, and $t_{1/2}$ = 8 h at pH 6.7 and 23°C (Wolfe et al. 1976; quoted, Howard 1991).

Groundwater: $t_{1/2}$ = 10.5 min at pH 8.3 to $t_{1/2}$ = 10.3 h at pH 5.2, based on first-order hydrolysis rate constants in surface waters (Wolfe et al. 1976; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 48–1440 h, based on unacclimated and acclimated soil grab sample data (Agnihotri 1970; Foschi et al. 1970; quoted, Howard et al. 1991);

rate constant k = 0.231 d⁻¹ with a biodegradation $t_{1/2}$ = 3 d (Rao & Davidson 1980);

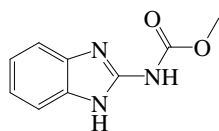
$t_{1/2}$ = 2.5 d in soil (Halfon et al. 1996);

field $t_{1/2}$ = 2.5 d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2}$ = 1 d at pH 7.2 (Tomlin 1994).

Biota: biochemical $t_{1/2}$ = 3 d from screening model calculations (Jury et al. 1987b).

19.1.7 CARBENDAZIM



Common Name: Carbendazim

Synonym: Bavistin, BCM, BMK, Carbendazime, Carbendazol, Carbendazym, G 665, Kemdazin, Mecarzole

Chemical Name: carbamic acid, methyl 1*H*-benzimidazol-2-yl, methyl ester; methyl benzimidazole-2-ylcarbamate; methyl 1*H*-benzimidazol-2-ylcarbamate

Uses: as fungicide for control of a wide range of fungal diseases in cereals, fruit, vines, hops, ornamentals, vegetables, rice coffee, cotton, mushrooms, and other crops; also used by trunk injection to give some control of Dutch elm disease.

CAS Registry No: 10605-21-7

Molecular Formula: C₉H₉N₃O₂

Molecular Weight: 191.186

Melting Point (°C):

302–307 (with dec., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

300 (dec, Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.45 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm³/mol):

194.8 (calculated-Le Bas method at normal boiling point)

131.9 (calculated-density)

Dissociation Constant pK_a:

4.48 (Austin & Briggs 1976)

4.24 (Sangster 1993)

4.20 (Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.002 (mp at 300°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

8.0 (24°C at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

29, 8.0, 7.0 (24°C, at pH 4, 7, 8, Tomlin 1994)

8.0 (20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

6.50 × 10⁻⁸ (20°C, Hartley & Kidd 1987)

< 9.0 × 10⁻⁵ (20°C, Worthing & Hance 1991)

9.0 × 10⁻⁵, 1.5 × 10⁻⁴, 0.0013 (20, 25, 50°C, quoted, Tomlin 1994)

< 1.0 × 10⁻⁷ (20°C, quoted, Tomlin 1994)

6.50 × 10⁻⁸ (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at 25°C):

1.55 × 10⁻⁶ (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW}:

1.52 (shake flask, Austin & Briggs 1976)

1.40 (shake flask-UV, Lord et al. 1980)

1.34 (shake flask at pH 5, Barak et al. 1983)

- 1.56 (Worthing & Hance 1991; Milne 1995)
- 1.43 (recommended, Sangster 1993)
- 1.38, 1.505, 1.49 (pH 5, 7, 9, Tomlin 1994)
- 1.56, 1.77 (pH 6, 7, Tomlin 1994)
- 1.52 (recommended, Hansch et al. 1995)
- 1.80 (Pomona-database, Müller & Kördel 1996)
- 1.35 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 2.28 (calculated-S, Kenaga 1980)
- 1.57 (earthworms, Lord et al. 1980; quoted, Connell & Markwell 1990)

Sorption Partition Coefficient, log K_{OC} :

- 3.14 (soil, calculated-S, Kenaga 1980)
- 2.35 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
- 2.30–2.40 (soil, Tomlin 1994)
- 2.35 (soil, calculated-MCI χ , Sabljic et al. 1995)
- 2.69 (soil, 20–25°C at pH 7, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)
- 2.35; 2.25 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
- 4.00, 2.09, 2.41, 2.28, 2.83 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 2.318, 2.346, 2.091, 2.198 (second generation Eurosoils ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Hydrolysis: $t_{1/2} > 35$ d (pH 5 and 7 at 22°C, Worthing & Hance 1991);
- slowly decomposed in alkaline solution, $t_{1/2} > 350$ d at pH 5, 7, 124 d at pH 9 (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 2$ and 25 months in water under aerobic and anaerobic conditions, respectively (Tomlin 1994).

Groundwater:

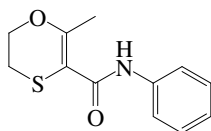
Sediment:

Soil: $t_{1/2} = 8$ –32 d under outdoor conditions, decomposes with $t_{1/2} = 6$ –12 months on bare soil, $t_{1/2} = 3$ to 6 months on turf (Tomlin 1994);

field $t_{1/2} = 120$ d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.8 CARBOXIN



Common Name: Carboxin

Synonym: Carbothiin, D 735, Kemikar, Kisvax, Vitavax

Chemical Name: 5,6-dihydro-2-methyl-1,4-oxathi-ine-3-carboxanilide; 2,3-dihydro-6-methyl-5-phenylcarbamo-yl-1,4-oxathi-ine

CAS Registry No: 5234-68-4

Uses: as fungicide in seed treatment for control of seed diseases of barley, wheat, oats, rice, groundnuts, soybeans, cotton, vegetables, maize, and other crops, etc.

Molecular Formula: $C_{12}H_{13}NO_2S$

Molecular Weight: 235.302

Melting Point ($^{\circ}C$):

91.5–92.5 (Spencer 1982; Harley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

98.0–100 (dimorphic, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

94 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.30 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

246.6 (calculated-Le Bas method at normal boiling point)

173.0 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.175 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.210 (mp at $94^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

170 (Martin & Worthing 1977)

170 (Spencer 1982; Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

199 (Worthing & Hance 1991; Tomlin 1994)

215 (calculated-group contribution fragmentation method, Kühne et al. 1995)

195 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

195 (selected, Lohninger 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

$< 1.0 \times 10^{-3}$ ($20^{\circ}C$, Hartley & Kidd 1987)

2.5×10^{-5} (Worthing & Hance 1991; Tomlin 1994)

1.3×10^{-5} (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

2.5×10^{-5} ($20^{\circ}C$, Montgomery 1993)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.45×10^{-5} (calculated-P/C, Montgomery 1993)

1.57×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.17 (Worthing & Hance 1991; Montgomery 1993; Milne 1995)

2.18 (Tomlin 1994)

2.14 (selected, Hansch et al. 1995)

2.60 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

1.53 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{oc} :

2.41 (soil, calculated-S, Kenaga 1980)

2.41 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

2.41 (calculated, Montgomery 1993)

2.41 (estimated-chemical structure, Lohninger 1994)

2.57 (soil, Tomlin 1994)

Environmental Fate Rate Constants, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} < 3$ h when exposed to light in aqueous solutions at pH 7 (Tomlin 1994).

Oxidation:

Hydrolysis: hydrolysis $t_{1/2} < 3$ d when exposed to light (Montgomery 1993).

Biodegradation:

Biotransformation:

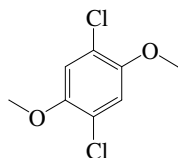
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} \sim 24$ h (Worthing & Hance 1991; quoted, Montgomery 1993; Tomlin 1994);

field $t_{1/2} = 3$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.9 CHLORONEB



Common Name: Chloroneb

Synonym: Demosan; Tersan SP

Chemical Name: 1,4-dichloro-2,5-dimethoxybenzene

CAS Registry No: 2675-77-6

Uses: as fungicide applied to soil or used as seed treatment for control of seedling diseases of beans, cotton, soybeans, and beet; also used for control of snow mold (*Typhula* spp.) and Pythium blight on turf grass.

Molecular Formula: $C_8H_8Cl_2O_2$

Molecular Weight: 207.055

Melting Point ($^{\circ}C$):

134 (Lide 2003)

Boiling Point ($^{\circ}C$):

268 (Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.66 (Spencer 1982)

Molar Volume (cm^3/mol):

200.4 (calculated-Le Bas method at normal boiling point)

124.8 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

71.91 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

30.54 (DSC method, Plato & Glasgow 1969)

29.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

72.0 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0852 (mp at $134^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

8 (Martin & Worthing 1977; Spencer 1982)

8 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

8 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.40 (Spencer 1982)

0.40 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

0.017, 0.43, 6.90, 77.0, 630 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 16.452 - 5436/(T/K)$; measured range 32.5 – $135^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 12.303 - 3757.8/(T/K)$; measured range 136 – $151^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

0.40 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc} :

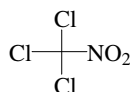
- 3.06 (soil, Hamaker & Thompson 1972)
- 3.10 (soil, quoted exptl., Meylan et al. 1992)
- 2.36 (calculated-MCI χ and fragments contribution, Meylan et al. 1992)
- 3.22 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.22 (selected, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

- Soil: $t_{1/2} \sim 24$ h (Worthing & Hance 1991);
field $t_{1/2} = 130$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.10 CHLOROPICRIN



Common Name: Chloropicrin

Synonym: Acquinite, Nemax, Nitrochloroform, Picfume

Chemical Name: Trichloronitromethane

CAS Registry No: 76-06-2

Uses: fungicide/herbicide/insecticide/nematicide/rodenticide; used as a soil disinfectant for control of nematodes, soil insects, soil fungi, and weed seeds; also used for fumigation of stored grain to control insects and rodents, for glasshouse and mushroom-house fumigation, etc.

Molecular Formula: CCl_3NO_2

Molecular Weight: 164.376

Melting Point ($^{\circ}\text{C}$):

-64.0 (Spencer 1982; Hartley & Kidd 1987; Tomlin 1994; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

112.4 (Spencer 1982; Hartley & Kidd 1987; Tomlin 1994)

Density (g/cm^3 at 20°C):

1.65659, 1.64756 (20°C , 25°C , Dreisbach 1961)

1.656 (20°C , Spencer 1982; Tomlin 1994)

1.6558, 1.6483 (20°C , 25°C , Montgomery 1993)

Molar Volume (cm^3/mol):

113.9 (calculated-Le Bas method at normal boiling point)

99.3 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.40, 33.12 (25°C , bp, Dreisbach 1961)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.68 (Dreisbach 1961)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F: 1.0)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

2270 (Martin & Worthing 1977; Kenaga 1980; Montgomery 1993; Lohninger 1994)

2270 (0°C , Spencer 1982; quoted, Howard 1991; Tomlin 1994)

2270, 1620 (0, 25°C , Hartley & Kidd 1987)

2300 (Davies & Lee 1987)

1621 (Howard 1991)

2270 (20 – 25°C , selected, Wauchope et al. 1992; Hornsby et al. 1996)

1620 (Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

3174* (gas saturation, measured range 0 – 35°C , Baxter et al. 1920)

$\log(P/\text{mmHg}) = 8.2424 - 2045.1/(273 + t/^{\circ}\text{C})$; temp range 0 – 35°C (gas saturation, Baxter et al. 1920)

2666* (20°C , summary of literature data, temp range -25.5 to 111.9°C , Stull 1947)

3324 (calculated by formula, Dreisbach 1961)

$\log(P/\text{mmHg}) = 7.03335 - 1369.70/(218.0 + t/^{\circ}\text{C})$, temp range 28 – 176°C , (Antoine eq. for liquid state, Dreisbach 1961)

760, 3173 (0, 25°C , Spencer 1982)

3200 (Hartley & Kidd 1987)

3173 (Howard 1991)

2253, 3173, 4400 (20, 25, 30°C , Montgomery 1993)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

208.0 (Kawamoto & Urano 1989)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

1.03 (HPLC-RT correlation, Kawamoto & Urano 1989)

2.09 (shake flask, Hansch & Leo 1987)

2.07 (Howard 1991)

1.03, 2.09 (Montgomery 1993)

2.09 (selected, Sangster 1993; Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

0.90 (calculated, Kenaga 1980; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{\text{oc}}$:

1.79 (calculated, Kenaga 1980)

1.91 (soil, correlated-Freundlich Isotherm, Kawamoto & Urano 1989)

1.79 (soil, Wauchope et al. 1992; Hornsby et al. 1996)

1.79 (selected, Lohninger 1994)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 4.3$ h for evaporation from a body of water 1 m deep with a current of 1 m/s and a wind of 3 m/s (Howard 1991).

Photolysis: $t_{1/2} = 20$ d in simulated atmosphere, $t_{1/2} = 3$ d in aqueous solution with sunlight irradiation (Montgomery 1993).

Oxidation:

Hydrolysis:

stable in neutral aqueous solution and with a minimum $t_{1/2} = 11$ yr (Howard 1991).

Biodegradation: rate constant $k(\text{aerobic}) = 1.5 \text{ d}^{-1}$ with $t_{1/2} = 0.46$ d at 20°C by aerobic activated sludge and $k(\text{anaerobic}) = 1.5 \text{ d}^{-1}$ with $t_{1/2} = 0.46$ d at 20°C by anaerobic microorganisms cultivated on artificial sewage (Kawamoto & Urano 1990)

$k(\text{anaerobic}) = 12 \text{ d}^{-1}$ and $t_{1/2} = 0.058$ d (corrigendum, Kawamoto & Urano 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 20$ d by photodegradation (Howard 1991).

Surface water: biodegradation $t_{1/2} = 0.46$ d at 20°C by aerobic activated sludge or anaerobic microorganisms (Kawamoto & Urano 1990)

volatilization $t_{1/2} = 4.3$ h from a model river and photodegradation $t_{1/2} = 3$ d in the surface layer of water (Howard 1991).

Groundwater:

Sediment:

Soil: field $t_{1/2} \sim 1$ d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

TABLE 19.1.10.1

Reported vapor pressures of chloropicrin at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Baxter et al. 1920	Stull 1947	Spencer 1982	Montgomery 1993				
gas saturation	summary of literature data	handbook	handbook				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
-20	200	-25.5	133.3	0	760	20	2253
-19	226.6	-3.30	666.6	25	3173	25	3173
-18	253.3	7.80	1333			30	4400
0	760.3	20.0	2666	Dreisbach eq.2			
10	1383	33.8	5333	A	7.03335		
15	1843	42.3	7999	B	1369.7		
20	2441	53.8	13332	C	218		
25	3174	71.8	26664	temp range 28–176°C			
30	4146	91.8	53329				
35	5352	111.9	101325				
eq. 2	P/mmHg	mp/°C	-64				
A	8.2424						
B	2045.1						
C	273						

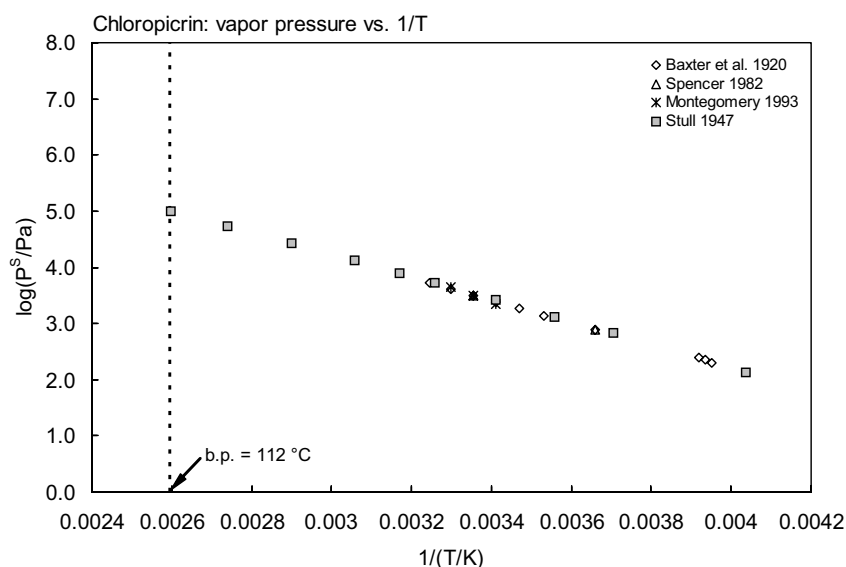
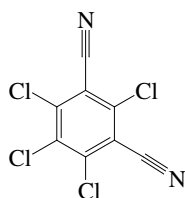


FIGURE 19.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for chloropicrin.

19.1.11 CHLOROTHALONIL



Common Name: Chlorothalonil

Synonym: Bravo, chlorthalonil, Daconil, DAC 2787, Exotherm, Forturf, Nopocide N 96, TPN

Chemical Name: tetrachloroisophthalonitrile; 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile; 2,4,5,6-tetrachloro-1,3-dicyanobenzene

CAS Registry No: 1897-45-6

Uses: fungicide, fumigant, soil insecticide

Molecular Formula: $C_6Cl_4N_2$

Molecular Weight: 265.911

Melting Point ($^{\circ}C$):

250 (Lide 2003)

Boiling Point ($^{\circ}C$):

350 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$): 1.80 (Montgomery 1993; Tomlin 1994)

Molar Volume (cm^3/mol):

233.0 (calculated-Le Bas method at normal boiling point)

147.7 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0062 (mp at $250^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.60 (Martin & Worthing 1977; Kenaga 1980; Spencer 1982; Hartley & Kidd 1987; Worthing 1987, 1991)

0.30 (Davies & Lee 1987)

0.50 (calculated-group contribution fragmentation method, Kühne et al. 1995)

0.60 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.90 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

< 1.30 ($40^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991)

232 (Worthing & Walker 1987; quoted, Majewski & Capel 1995)

0.133 (20 – $25^{\circ}C$, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

1.3×10^{-3} ($40^{\circ}C$, Montgomery 1993)

8.1×10^{-3} (selected, Brouwer et al. 1994)

7.6×10^{-5} (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

576 (calculated-P/C as per Worthing 1987, Majewski & Capel 1995)

0.0194 ($20^{\circ}C$, Kawamoto & Urano 1989)

0.0151 ($20^{\circ}C$, calculated-bond contribution method, Meylan & Howard 1991)

0.02 (Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.14 (screening model calculations, Jury et al. 1987b)

2.64	(HPLC-RT correlation, Kawamoto & Urano 1989)
2.64	(recommended, Sangster 1993)
2.89	(RP-HPLC-RT correlation, Saito et al. 1993)
2.90	(recommended, Hansch et al. 1995)
3.80	(RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

1.92	(calculated-S, Kenaga 1980)
1.66	(calculated- K_{ow} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{oc} :

3.76	(soil, calculated, Kenaga 1980)
3.14	(soil, screening model calculations, Jury et al. 1987b)
3.14	(soil, Gustafson et al. 1989)
3.26	(soil, correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
3.14	(soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.76, 3.14	(soil, Montgomery 1993)
3.00	(sand, quoted, Montgomery 1993)
3.14	(estimated-chemical structure, Lohninger 1994)
3.20, 4.15	(sand, silt, Tomlin 1994)
3.26	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: biochemical $t_{1/2} = 70$ d (Jury et al. 1987b);

first-order rate constants in biotic and abiotic shake-flask tests $k = -0.0161$ and -0.0155 d⁻¹ in nonsterile sediment/estuarine water and $k = -0.00574$ d⁻¹ in sterile sediment/estuarine water and $k = -0.00355$ and -0.00329 d⁻¹ in nonsterile estuarine water and $k = -0.00283$ d⁻¹ in sterile estuarine water both at Davis Bayou (Walker et al. 1988);

rate constant $k(\text{aerobic}) = 1.7$ d⁻¹ with $t_{1/2} = 0.41$ d at 20°C by aerobic activated sludge and $k(\text{anaerobic}) = 1.7$ d⁻¹ with $t_{1/2} = 0.41$ d at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: biodegradation $t_{1/2} = 0.41$ d at 20°C by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)

Groundwater:

Sediment:

Soil: $t_{1/2} = 70$ d from screening model calculations (Jury et al. 1987b);

$t_{1/2} \sim 1.5$ –3 months (Hartley & Kidd 1987; Worthing & Hance 1991);

soil $t_{1/2} = 68$ d (Gustafson 1989);

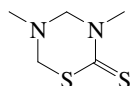
field $t_{1/2} = 30$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 4.1$ d and 1.5–3 months (Montgomery 1993);

$t_{1/2} = 5$ –35 d in aerobic and anaerobic soil studies and from a few hours to a few days in aerobic and anaerobic aquatic soil studies (Tomlin 1994).

Biota: biochemical $t_{1/2} = 70$ d from screening model calculations (Jury et al. 1987b).

19.1.12 DAZOMET



Common Name: Dazomet

Synonym: tiazon, Mylone, Crag Fungicide 974, Salvo, Basamid, Fongosan

Chemical Name: 3,5-dimethyl-1,3,5-thiadiazinane-2-thione

Uses: soil fumigant, nematocide, fungicide, herbicide, insecticide

CAS Registry No: 533-74-4

Molecular Formula: $C_5H_{10}N_2S_2$

Molecular Weight: 162.276

Melting Point ($^{\circ}C$):

106 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3): 1.37 (Montgomery 1993; Tomlin 1994)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.160 (mp at $106^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1200 (Spencer 1982)

3000 ($20^{\circ}C$, Worthing & Walker 1983, 1987; Hartley & Kidd 1987; Montgomery 1993; Tomlin 1994)

2000 (Herbicide Handbook 1989, quoted, Augustijn-Beckers et al. 1994)

3000 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

3.7×10^{-4} ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1983, 1987; Montgomery 1993; Tomlin 1994)

4.0×10^{-4} , 3.73×10^{-4} ($20^{\circ}C$, quoted, Augustijn-Beckers et al. 1994)

4.0×10^{-4} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

2.03 ($20^{\circ}C$, calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.15 (Montgomery 1993)

1.40 (at pH 7, Tomlin 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

0.48 (calculated, Montgomery 1993)

–0.046 at pH 9, 0.778 (quoted values, Augustijn-Beckers et al. 1994)

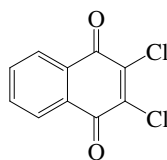
1.0 (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: field $t_{1/2} = 7$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.13 DICHLONE



Common Name: Dichlone

Synonym: Algistat, Compound 604, Ent 3776, Phygon, Quintar, Sanquinon

Chemical Name: 2,3-dichloro-1,4-naphthoquinone; 2,3-dichloro-1,4-naphthalenedione

CAS Registry No: 117-80-6

Uses: fungicide/algicide; as fungicide for control of blossom blights, scab on apples and pears and brown spot on stone fruit, etc.; also used to control blue-green algae in ponds, lakes, and swimming pools.

Molecular Formula: $C_{10}H_4Cl_2O_2$

Molecular Weight: 227.044

Melting Point ($^{\circ}C$):

195 (Lide 2003)

Boiling Point ($^{\circ}C$):

275 (at 2 mmHg, Hartley & Kidd 1987; Howard 1991; Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

196.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.30 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.0 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

58 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0215 (mp at $195^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ as indicated):

0.10 (Kenaga 1980)

8.00 ($20^{\circ}C$, Hodnett et al. 1983)

0.10 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

1.00 (Montgomery 1993)

0.10 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence):

3.30×10^{-4} , 8.80×10^{-3} , 0.15, 1.70, 14.0 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 14.965 - 5500.9/(T/K)$; measured range 40.4 – $191^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_l/Pa) = 13.396 - 4803.6/(T/K)$; measured range 40.4 – $191^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

1.47×10^{-4} (calculated from S and Henry's law constant, Howard 1991)

10930 (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.51×10^{-5} (Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.16 (estimated, Hodnett et al. 1983)

5.62 (calculated, Montgomery 1993)

Bioconcentration Factor, log BCF:

3.35 (estimated-S, Kenaga 1980; quoted, Howard 1991)

Sorption Partition Coefficient, log K_{OC} :

4.19 (estimated-S, Kenaga 1980; quoted, Howard 1991)

4.00 (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

4.19 (calculated, Montgomery 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: estimated photooxidation $t_{1/2} = 3.87$ d in air, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).

Hydrolysis: $t_{1/2} = 5$ d at pH 7 (Howard 1991).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 3.87$ d, based on the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard 1991).

Surface water:

Groundwater:

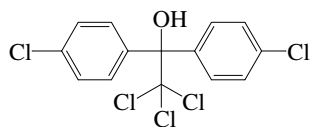
Sediment:

Soil: $t_{1/2} = 1$ d in moist and slightly under three months in dry silt loam soil at pH 6.2–6.4 and 29°C, respectively (Burchfield 1959; quoted, Howard 1991);

field $t_{1/2} = 10$ d (20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.14 DICOFOL



Common Name: Dicofol

Synonym: kelthane, kelthan

Chemical Name: 2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethanol, 4-chloro- α -(4-chlorophenyl)- α -(trichloromethyl)-benzenemethanol

Uses: acaricide

CAS Registry No: 115-32-2

Molecular Formula: $C_{14}H_9Cl_5O$

Molecular Weight: 370.485

Melting Point ($^{\circ}C$):

77.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

180 (0.1 mmHg, Hartley & Kidd 1987)

193 (360 mmHg, tech., Tomlin 1994)

Density (g/cm^3): 1.45 (Worthing & Walker 1987; Tomlin 1994)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

Enthalpy of Vaporization, ΔH_v (kJ/mol):

104.0 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.8 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

57 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.305 (mp at $77.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.32 (generator column-GC/ECD, Weil et al. 1974)

1.20 ($24^{\circ}C$, 99% purity, Verschueren 1983)

0.80 ($20^{\circ}C$, in distilled water, Verschueren 1983)

0.80 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.80 (Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.40×10^{-5} , 1.20×10^{-3} , 0.032, 0.56, 68.0 (25, 50, 70, 100, $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_g/Pa) = 17.084 - 6470.1/(T/K)$; measured range 85.5 – $145^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 14.104 - 5354.8/(T/K)$; measured range 85.5 – $145^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

5.33×10^{-5} (selected, Wauchope et al. 1992; Hornsby et al. 1996)

5.30×10^{-5} (tech., Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.66×10^{-5} (calculated-bond contribution method, Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.54 (Rao & Davidson 1980)

3.54 (Nigg et al. 1986)

4.28 (Tomlin 1994)

3.54 (Hansch & Leo 1987; quoted, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

- 4.18–4.27 (fathead minnow, Howard 1991)
- 3.98–4.16 (in presence of suspended clay, Howard 1991)
- 2.75, 3.54 (calculated-S, calculated- K_{OW} , Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.60, 3.30 (estimated-S, calculated- K_{OW} , Howard 1991)
- 3.46–3.91 (range of reported data, Wauchope et al. 1992)
- 3.70 (soil, recommended, Wauchope et al. 1992; Hornsby et al. 1996)
- 3.92, 3.91, 3.79, 3.77 (sand, sandy loam, silty loam, clay loam, Tomlin 1994)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photolysis $t_{1/2} = 2.92$ d in the atmosphere for reaction with OH radicals; $t_{1/2} = 6$ d for exposure of thin film of dicofol to sunlight at 300 nm (Howard 1991).

Photooxidation:

Hydrolysis: $t_{1/2} = 60$ min at pH 8.2 and 3 min at pH 10.2 with an initial concn of 0.4 mg/L (Verschuereen 1983); stable to acids, but unstable in alkaline media, $t_{1/2} = 85$ d at pH 5, 64–99 h at pH 7, 26 min at pH 9 (Tomlin 1994).

Biodegradation: degradation in anaerobic sewage to 4,4'-dichlorobenzophenone (DBP); 88–94% conversion to DBP for filtered river water, 47–56% for unfiltered river water of pH 7.5 in a 24-h expt. (Verschuereen 1983); $t_{1/2} = 61$ d and 16 d under aerobic and anaerobic conditions in silt loam (Tomlin 1994).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: vapor phase $t_{1/2} \sim 2.92$ s life in the atmosphere for reaction with OH radicals (estimated, Howard 1991)

Surface water: hydrolysis $t_{1/2} = 60$ min at pH 8.2 and 3 min at pH 10.2 with an initial concn of 0.4 mg/L; degradation in anaerobic sewage to 4,4'-dichlorobenzophenone (DBP); 88–94% conversion to DBP for filtered river water, 47–56% for unfiltered river water of pH 7.5 in a 24-h expt. (Verschuereen 1983)

aqueous photodegradation $t_{1/2} = 1$ –4 d at pH 5 in sensitized conditions and $t_{1/2} = 15$ –93 d in unsensitized conditions; stable to acids, but unstable in alkaline media, $t_{1/2} = 85$ d at pH 5, 64–99 h at pH 7, 26 min at pH 9 (Tomlin 1994).

Ground water:

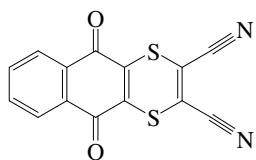
Sediment:

Soil: field $t_{1/2} = 45$ d (Wauchope et al. 1992; Hornsby et al. 1996);

soil photodegradation $t_{1/2} = 30$ d in silt loam, soil metabolism $t_{1/2} = 61$ d under aerobic conditions and $t_{1/2} = 16$ d under anaerobic conditions in silt loam; field dissipation $t_{1/2} = 60$ –100 d (Tomlin 1994).

Biota:

19.1.15 DITHIANON



Common Name: Dithianon

Synonym: Delan, Delan-Col

Chemical Name: 2,3-dicyano-1,4-dithia-anthraquinone; 5,10-dihydro-5,10-dioxonaphtho[2,3-b]-*p*-dithin-2,3-dicarbonylnitrile

CAS Registry No: 3347-22-6

Uses: as fungicide for control of many foliar diseases.

Molecular Formula: $C_{14}H_4N_2O_2S_2$

Molecular Weight: 296.324

Melting Point ($^{\circ}C$):

220 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.580 (Tomlin 1994)

Molar Volume (cm^3/mol):

264.0 (calculated-Le Bas method at normal boiling point)

187.6 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0122 (mp at $220^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.50 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

6.6×10^{-5} (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0391 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.84 (Worthing & Hance 1991)

3.20 (Tomlin 1994)

2.84 (selected, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.96 (calculated-S per Kenaga 1980, this work)

Sorption Partition Coefficient, $\log K_{OC}$:

3.81 (soil, calculated-S per Kenaga 1980, this work)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 19$ h when exposed to artificial sunlight in 0.1 mg/L aqueous solution (Tomlin 1994).

Oxidation:

Hydrolysis: $t_{1/2} = 12.2$ h at pH 7 (Tomlin 1994).

Biodegradation:

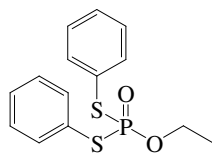
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Surface water: hydrolysis $t_{1/2} = 12.2$ h at pH 7 and photolytic $t_{1/2} = 19$ h when exposed to artificial sunlight in 0.1 mg/L aqueous solutions (Tomlin 1994).

19.1.16 EDIFENPHOS



Common Name: Edifenphos

Synonym: EDDP, Hinosan, edifenfos

Chemical Name: *O*-ethyl *S,S*-diphenyl phosphorodithioate

CAS Registry No: 17109-49-8

Uses: as fungicide for control of blast and blight diseases in rice, etc.

Molecular Formula: $C_{14}H_{15}O_2PS_2$

Molecular Weight: 310.371

Melting Point ($^{\circ}C$):

-25 (Tomlin 1994)

Boiling Point ($^{\circ}C$):

154 (at 0.01 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991)

Density (g/cm^3 at $20^{\circ}C$):

1.230 (Hartley & Kidd 1987; Worthing & Hance 1991)

1.251 (Tomlin 1994)

Molar Volume (cm^3/mol):

250.5 (calculated from density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

56.0 ($20^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

insoluble (Worthing & Hance 1991)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.013 ($20^{\circ}C$, Hartley & Kidd 1987)

0.013 ($20^{\circ}C$, Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

0.0721 ($20^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{OW} :

3.48 (RP-HPLC-RT correlation, Saito et al. 1993)

4.20 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, log BCF:

1.81 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC} :

2.68 (calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: hydrolyzed by strong acids and alkalis, at $25^{\circ}C$, $t_{1/2} = 19$ d at pH 7 and $t_{1/2} = 2$ d at pH 9 (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} = 19$ d at pH 7 and $t_{1/2} = 2$ d at pH 9 (Tomlin 1994).

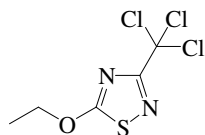
Groundwater:

Sediment:

Soil: half-life in soil in the range of few days to a few weeks (Tomlin 1994).

Biota:

19.1.17 ETRIDIAZOLE



Common Name: Etridiazole

Synonym: Aaterra, Banrot, Dwell, Echlomezol, ETCMTD, Ethazole, ETMT, Koban, MF-344, OM 2425, Pansoil, Terracoat, Terrazole, Truban

Chemical Name: 5-ethoxy-3-(trichloromethyl)-1,2,4-thiadiazole; ethyl 3-trichloromethyl-1,2,4-thiadiazolyl ether

Uses: as fungicide for control of *Phytophthora* and *Pythium* spp. in cotton, ornamentals, vegetables, groundnuts, cucurbits, tomatoes, and other crops; also used as a nitrification inhibitor in maize, cotton and wheat.

CAS Registry No: 2593-15-9

Molecular Formula: $C_5H_5Cl_3N_2OS$

Molecular Weight: 247.530

Melting Point ($^{\circ}C$):

19.9 (Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

95.0 (at 1 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.503 ($25^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994)

Molar Volume (cm^3/mol):

219.0 (calculated-Le Bas method at normal boiling point)

164.7 (calculated-density)

Dissociation Constant pK_a :

2.77 (Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

50.0 (Hartley Kidd 1987; Worthing & Hance 1991; Milne 1995; selected, Lohninger 1994)

50.0 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.013 ($20^{\circ}C$, Hartley & Kidd 1987)

0.013 (rm. temp., Worthing & Hance 1991)

0.013 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

0.0644 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

2.48–2.60 (Worthing & Hance 1991; Milne 1995)

3.36 (Tomlin 1994)

2.55 (selected, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.83 (calculated-S as per Kenaga 1980, this work)

1.22 (calculated- K_{ow} as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{oc} :

0.725 (sandy soil, Worthing & Hance 1991)

0.149 (silt loam, Worthing & Hance 1991)

3.00 (soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
3.00 (selected, Lohninger 1994)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 103$ d at pH 6 (Worthing & Hance 1991);

$t_{1/2} = 12$ d at pH 6, 45°C, $t_{1/2} = 103$ d at pH 6, 25°C (Tomlin 1994).

Biodegradation: soil $t_{1/2} = 9.5$ d under aerobic conditions and $t_{1/2} = 3$ d under anaerobic conditions (Tomlin 1994).

Biotransformation:

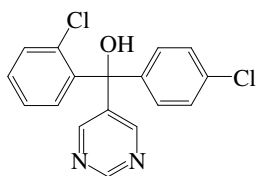
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} = 9.5$ d under aerobic, $t_{1/2} = 3$ d under anaerobic conditions, field dissipation $t_{1/2} = 1$ wk in sandy clay loam (Tomlin 1994);

field $t_{1/2} = 103$ d (20–25°C, selected, Hornsby et al. 1996).

19.1.18 FENARIMOL



Common Name: Fenarimol

Synonym: Bloc, EL-222, Rimidin, Rubigan

Chemical Name: (±)-2,4'-dichloro- α -(pyrimidin-5-yl)benzhydryl alcohol; α -(2-chlorophenyl)- α -(4-chlorophenyl)-5-pyrimidinemethanol

CAS Registry No: 60168-88-9

Uses: as fungicide for control of powdery mildews in pome fruit, strawberries, vines, cucurbits, roses, and beet; also for control of scab on pome fruit, brown patch and snow mold of turf.

Molecular Formula: $C_{17}H_{12}Cl_2N_2O$

Molecular Weight: 331.195

Melting Point ($^{\circ}C$):

118 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

338.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

2.58 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.122 (mp at $118^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

13.7 (Martin & Worthing 1977)

13.7 (at pH 7, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

14.0 (20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

14.0 (selected, Lohninger 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

$< 1.3 \times 10^{-5}$ (Hartley & Kidd 1987)

1.30×10^{-5} (Worthing & Hance 1991)

2.93×10^{-5} (20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

6.5×10^{-5} (vapor pressure balance, Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$ or as indicated):

6.93×10^{-4} (20– $25^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

0.67 (shake flask, at pH 5.3, Martin & Edgington 1981)

–1.59 (shake flask-UV at pH 5, Barak et al. 1983)

3.70 (Stevens et al. 1988)

3.60 (shake flask-HPLC, Bateman et al. 1990)

3.69 (pH 7, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

3.60 (selected, Hansch et al. 1995)

3.61 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

2.16 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

3.01 (calculated-S, Kenaga 1980)

2.78 (soil, 20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.176–1.08 (soil, Tomlin 1994)

2.78 (estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: decomposed readily by sunlight (Tomlin 1994).

Oxidation:

Hydrolysis: $t_{1/2} = 28$ d at 52°C and pH 3, 6 and 9 (Tomlin 1994).

Biodegradation: $t_{1/2} > 365$ d under aerobic conditions in soil, and microbial degradation is accelerated by light (Tomlin 1994).

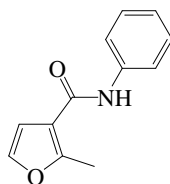
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} > 365$ d under aerobic conditions in soil (28% sand, 14.7% clay, 57.3% silt and pH 6 (Tomlin 1994)
field $t_{1/2} = 360$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.19 FENFURAM



Common Name: Fenfuram

Synonym: Panoram

Chemical Name: 2-methylfuran-3-carboxanilide; 2-methyl-3-furanilide; 2-methyl-N-phenyl-3-furancarboxamide

CAS Registry No: 24691-80-3

Uses: as fungicide for control of bunts and smuts (*Tilletia* and *Ustilago* spp.) in cereals, when applied as a seed treatment.

Molecular Formula: $C_{12}H_{11}NO_2$

Molecular Weight: 201.221

Melting Point ($^{\circ}C$):

109–110 (Worthing & Hance 1991)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.36 (Worthing & Hance 1991)

Molar Volume (cm^3/mol):

217.1 (calculated-Le Bas method at normal boiling point)

148.0 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

100 (Martin & Worthing 1977; Kenaga 1980)

100 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

100 (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

2.0×10^{-5} ($20^{\circ}C$, Hartley & Kidd 1987)

2.0×10^{-5} (extrapolated to $20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

2.0×10^{-5} (20 – $25^{\circ}C$, selected, Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Bioconcentration Factor, $\log BCF$:

1.66 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{OC}$:

2.54 (calculated-S, Kenaga 1980)

2.48 (20 – $25^{\circ}C$, estimated, Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

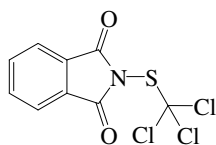
Hydrolysis: stable in neutral media, but hydrolyzed by strong acids and alkalis (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} \sim 42$ d (Hartley & Kidd 1987; Tomlin 1994);

field $t_{1/2} = 42$ d (20 – $25^{\circ}C$, selected, Hornsby et al. 1996).

19.1.20 FOLPET



Common Name: Folpet

Synonym: ENT-26539, Faltan, Folpan, Fospel, Ftalan, Fungitrol, Orthophaltan, Phaltan, Spolacid, Thiophal, Vinicoll

Chemical Name: *N*-(trichloromethylthio)phthalimide; 2-[(trichloromethylthio)-1*H*-isoindole-1,3(2*H*)-dione

CAS Registry No: 133-07-3

Uses: fungicide for control of downy/powdery mildews, leaf spot diseases, etc.

Molecular Formula: $C_9H_4Cl_3NO_2S$

Molecular Weight: 296.558

Melting Point ($^{\circ}C$):

177 (Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

246.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.50 (DSC method, Plato 1972)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0323 (mp at $177^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1.0 (Martin & Worthing 1977)

1.0 (rm. temp., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

< 0.0013 ($20^{\circ}C$, Hartley & Kidd 1987)

0.0013 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.63 (shake flask-UV, Briggs 1981)

2.85 (selected, Yoshioka et al. 1986)

2.85 (shake flask, $\log P$ database, Hansch & Leo 1987)

2.85 (recommended, Sangster 1993)

3.11 (Tomlin 1994)

2.85 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.91 (calculated-S, Kenaga 1980)

3.32 (earthworms, Lord et al. 1980)

Sorption Partition Coefficient, $\log K_{OC}$:

1.78 (calculated-S, Kenaga 1980)

3.03 (reported as $\log K_{OM}$, Briggs 1981)

3.27, 2.16 (soil, quoted exptl., calculated-fragment contribution method, Meylan et al. 1992)

3.27 (soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: $t_{1/2} = 101$ min in isopropanol, $t_{1/2} = 144$ min in cyclohexene and $t_{1/2} = 1620$ min in cyclohexane by UV-irradiation ($\lambda > 280$ nm): (Schwack & Flöber-Müller 1990).

Oxidation:

Hydrolysis: hydrolyze at pH 7 with rates similar to captan, i.e., first-order rate constant $k = 6.5 \times 10^{-5} \text{ s}^{-1}$ with $t_{1/2} = 2.96$ h in a phosphate buffer solution at pH 7.07 and 28°C (Wolfe et al. 1976).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 4.3$ d (Tomlin 1994).

Groundwater:

Sediment:

Soil: $t_{1/2} = 4.3$ d (Tomlin 1994).

Biota:

19.1.21 FORMALDEHYDE



Common Name: Formaldehyde

Synonym: formalin, methanal, oxomethane

Chemical Name: formaldehyde

Uses: fungicide/bactericide; used as soil sterilant in mushroom houses and other areas; also used as a silage preservative.

CAS Registry No: 50-00-0

Molecular Formula: HCHO

Molecular Weight: 30.026

Melting Point (°C):

−92 (Weast 1982–83; Dean 1985; Lide 2003)

Boiling Point (°C):

−19.1 (Lide 2003)

Density (g/cm³):

0.815 (Weast 1982–83)

0.815 (−20°C, Verschueren 1983; Dean 1985)

Acid Dissociation Constant, pK_a:

Molar Volume (cm³/mol):

29.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

1,220,000 (Dean 1985)

very soluble, up to 55% (Howard 1989)

Vapor Pressure (Pa at 25°C or as indicated):

1333 (−88°C, Verschueren 1983)

451030 (> 1 atmospheric pressure, Howard 1989)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.0331 (Dong et al. 1986)

0.0169 (Gaffney et al. 1987)

0.0298 (gas stripping-HPLC, Zhou & Mopper 1990)

Octanol/Water Partition Coefficient, log K_{ow}:

−0.75 (calculated-f const. per Rekker 1977, Deneer et al. 1988)

0.00 (calculated, Verschueren 1983)

0.35 (Howard 1989)

0.35 (recommended, Sangster 1989, 1993)

Bioconcentration Factor, log BCF:

no bioconcentration in fish and shrimp observed (Howard 1989)

Sorption Partition Coefficient, log K_{oc}:

0.365 (estimated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatilization:

Photolysis: sunlight photolysis t_{1/2} = 1.25–6.0 h, based on measured gas-phase photolysis by simulated sunlight (Calvert et al. 1972; Su et al. 1979; quoted, Howard et al. 1991).

Oxidation: rate constant $k = 3.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with NO_3 radicals in the atmosphere at $(298 \pm 1) \text{ K}$ (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986);
rate constant $k = 4.50 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with HO_2 radicals in the atmosphere at 298 K (Baulch et al. 1984; quoted, Carlier et al. 1986);
rate constant $k = 111.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with OH radicals in the atmosphere at 298 K (Baulch et al. 1984; quoted, Carlier et al. 1986);
atmospheric photooxidation $t_{1/2} = 7.13\text{--}71.3 \text{ h}$, based on measured rate constant for the vapor-phase reaction with OH radicals in air (Atkinson 1985; quoted, Howard et al. 1991);
aqueous photooxidation $t_{1/2} = 4,813\text{--}190,000 \text{ h}$, based on measured rate constant for the reaction with OH radicals in water (Dorfman & Adams 1973; quoted, Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aqueous aerobic biodegradation screening test data (Gellman & Heukelekian 1950; Heukelekian & Rand 1955; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: photooxidation $t_{1/2} = 7.13\text{--}71.3 \text{ h}$, based on measured rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1985; quoted, Howard et al. 1991);
 $t_{1/2} = 1.26\text{--}6.0 \text{ h}$, based on photolysis half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

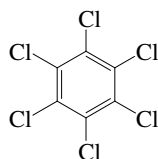
Sediment:

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

19.1.22 HEXACHLOROBENZENE

(See also [Chapter 6](#). Chlorobenzenes and other Halogenated Mononuclear Aromatics)



Common Name: Hexachlorobenzene

Synonym: HCB, perchlorobenzene, anticarie, Bunt-cure, Bunt-no-more, Julin's carbon chloride

Chemical Name: hexachlorobenzene

Uses: as fungicide for seed treatment to control common bunt and dwarf bunt of wheat.

CAS Registry No: 118-74-1

Molecular Formula: C_6Cl_6

Molecular Weight: 284.782

Melting Point ($^{\circ}C$):

230.0 (Weast 1982–83)

228.83 (Lide 2003)

Boiling Point ($^{\circ}C$):

322 (sublime, Weast 1982–83)

325 (Lide 2003)

Density (g/cm^3):

1.5691 (23.6 $^{\circ}C$, Weast 1982–83; Horvath 1982)

Molar Volume (cm^3/mol):

181.5 (23.6 $^{\circ}C$, calculated-density, Weast 1972–73; Horvath 1982)

221.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

28.744 (Tsonopoulos & Prausnitz 1971)

22.40 (Miller et al. 1984)

Entropy of Fusion, ΔS_{fus} (J/mol K):

57.32 (Tsonopoulos & Prausnitz 1971)

44.77 (Miller et al. 1984)

Fugacity Ratio (assuming $\Delta S_{fusion} = 56$ J/mol K), F: 0.010 (mp at 228.83 $^{\circ}C$)

0.0090 (25 $^{\circ}C$, Miller et al. 1985)

0.0075, 0.0094 (20 $^{\circ}C$, 25 $^{\circ}C$, Suntio et al. 1988)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

0.005 (generator column-GC/ECD, Weil et al. 1974)

0.006 (shake flask-LSC/ ^{14}C , Lu & Metcalf 1975)

0.110 (shake flask-nephelometry, Hollifield 1979)

0.005 (shake flask-UV, Yalkowsky et al. 1979)

0.0034 (calculated- K_{ow} , Yalkowsky et al. 1979; Yalkowsky & Valvani 1980)

0.0035 (selected, Neely 1980)

0.036 (selected, Briggs 1981)

0.0039 (shake flask-GC, Könemann 1981)

0.0054 (generator column-GC/ECD, Hashimoto et al. 1982)

0.0012–0.014 (shake flask-GC/ECD, Hashimoto et al. 1982)

0.005 (recommended, Horvath 1982)

0.0051 (Deutsche Forschungsgemeinschaft 1983; Fischer et al. 1991)

0.0066 (selected, Yoshida et al. 1983b)

0.047 (generator column-GC/ECD, Miller et al. 1984; 1985)

0.0162 (calculated-UNIFAC activity coeff., Banerjee 1985)

0.005 (recommended, IUPAC 1985)

- 0.0146 (calculated- K_{ow} and HPLC-RT, Chin et al. 1986)
 0.006–0.2 (calculated- K_{ow} , Anliker & Moser 1987)
 0.00537 (calculated-UNIFAC activity coeff., Banerjee et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated):

- 0.00028 (Sears & Hopke 1949)
 0.0015 (Callahan et al. 1979)
 0.0026 (selected, OECD 1979)
 0.00145 (20°C, Kiltzer et al. 1979)
 0.0023 (gas saturation-GC, Farmer et al. 1980)
 0.0013 (selected, Neely 1980; Suntio et al. 1988; Nash 1989)
 0.000453; 0.000167 (Klein et al. 1981)
 0.00046 (evaporation rate, Dobbs & Cull 1982)
 0.00121 (extrapolated, Antoine eq., Gückel et al. 1982)
 0.0006 (20°C, evaporation rate & gravimetric, Gückel et al. 1982)
 0.0024 (20°C, Deutsche Forschungsgemeinschaft 1983; Fischer et al. 1991)
 0.00147 (selected, Yoshida et al. 1983b)
 0.303; 0.159; 0.121 (supercooled liquid P_L , selected; GC-RT, Bidleman 1984)
 0.0031 (selected, Mackay et al. 1985)
 0.00147, 0.187 (20°C, selected, solid, supercooled liquid, Bidleman & Foreman 1987)
 0.245 (selected, Suntio et al. 1988; quoted, Ballschmiter & Wittlinger 1991)
 0.303, 0.127 (supercooled liquid, selected, Hinckley et al. 1990)
 0.0023 (selected from Mackay et al. 1992, Mortimer & Connell 1995)
 0.034; 0.141 (liquid P_L , GC-RT correlation; quoted lit., Donovan 1996)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

- 68.2 (20°C, Callahan et al. 1979)
 5.07 (calculated-P/C, Mackay & Shiu 1981)
 131.3 (batch stripping, Atlas et al. 1982)
 68.9 (20°C, calculated, Mabey et al. 1982)
 12.16 (calculated-P/C, Calamari et al. 1983)
 62.0 (calculated-P/C, Yoshida et al. 1983b)
 139 (calculated-P/C, Bobra et al. 1985)
 48.6 (20°C, batch stripping, Oliver 1985)
 133, 115.9 (observed, calculated-QSAR, Nirmalakhandan & Speece 1988)
 7.12 (20°C, calculated-P/C, Suntio et al. 1988)
 11.0 (calculated, Nash 1989)
 139.0 (calculated-P/C, Fischer et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow} :

- 6.18 (Neely et al. 1974; selected, McKim et al. 1985)
 4.13 (radioisotope tracer-¹⁴C, Lu & Metcalf 1975)
 6.51 (calculated-f const., Rekker 1977; quoted, Harnish et al. 1983)
 6.18 (selected, Callahan et al. 1979; Neuhauser et al. 1985)
 4.13 (Hansch & Leo 1979)
 5.0, 6.27 (shake flask-GC, HPLC- k' correlation, Könemann et al. 1979; selected, Figueroa & Simmons 1991)
 6.44 (calculated-f constant, Könemann et al. 1979; Könemann 1981; selected, Opperhuizen 1986)
 5.23 (HPLC-RT correlation, Veith et al. 1979a; selected, Mackay 1982; Freitag et al. 1985)
 6.18 (HPLC-RT, Veith et al. 1979b; quoted, Veith & Kosian 1982; Ryan et al. 1988; Saito et al. 1992)
 6.53 (calculated-f const., Yalkowsky et al. 1979, 1983; Yalkowsky & Valvani 1980; Valvani & Yalkowsky 1980; selected, Miller et al. 1984)
 5.23 (selected, Kenaga & Goring 1980; selected, Yoshida et al. 1983b)
 5.44 (selected, Briggs 1981)
 6.22 (HPLC-RT correlation, McDuffie 1981)

- 5.50 (shake flask-GC, Chiou et al. 1982; Chiou 1985; selected, Oliver & Niimi 1983; Oliver & Charlton 1984; Bobra et al. 1985; Hawker & Connell 1985; Oliver 1987a,b & c; Geyer et al. 1987; Suntio et al. 1988; Connell & Hawker 1988; Thomann 1989; Hawker 1990; Ballschmiter & Wittlinger 1991; Fischer et al. 1991)
- 5.66 (HPLC-RT correlation, Hammers et al. 1982)
- 5.40 (shake flask-GC, Watarai et al. 1982; quoted, Suntio et al. 1988)
- 6.13–6.27, 5.66 (range, mean, shake flask method, Eadsforth & Moser 1983)
- 6.27–6.48, 6.38 (range, mean, HPLC method, Eadsforth & Moser 1983)
- 5.0, 5.19 (selected, calculated, Kaiser 1983; Kaiser et al. 1984)
- 5.89 (selected, Calamari et al. 1983)
- 6.42 (calculated-f const., Veith et al. 1983)
- 5.23, 4.61 (selected, calculated-molar refraction, Yoshida et al. 1983)
- 5.47 (generator column-GC/ECD, Miller et al. 1984, 1985; Kerler & Schönherr 1988; Mackay & Paterson 1991)
- 5.75; 5.70–5.79 (quoted lit.; HPLC-RV correlation, Garst & Wilson 1984; Garst 1984)
- 5.20, 5.23, 5.44, 5.50, 5.55 (reported lit. values, Geyer et al. 1984)
- 5.47 (Sarna et al. 1984)
- 5.47, 6.86, 6.42 (selected, HPLC/MS, calculated- π const., Burkhard et al. 1985)
- 5.61 (selected, Mackay et al. 1985)
- 5.75 (selected OECD value, Brooke et al. 1986)
- 5.6, 5.9 (HPLC-RV correlation, Brooke et al. 1986)
- 6.51, 6.18 (selected, calculated- K_{OW} & HPLC-RT, Chin et al. 1986)
- 6.92 (HPLC- k' correlation, De Kock & Lord 1987)
- 5.64 (HPLC- k' correlation, Mailhot 1987)
- 5.45 (selected, Gobas et al. 1987, 1989; Travis & Arms 1988)
- 5.66 (correlated, Isnard & Lambert 1988, 1989)
- 5.47; 6.42, 6.55, 6.22, 5.34, 4.86, 4.75 (selected exptl.; calculated- π const., f const., HPLC-RT correlation, MW, MCI χ , TSA, Doucette & Andren 1988)
- 5.47; 5.37 (selected; calculated- V_1 and solvatochromic parameters, Kamlet et al. 1988)
- 5.50 (shake flask-GC, Pereira et al. 1988)
- 5.31, 6.58 (selected, calculated-UNIFAC activity coeff., Banerjee & Howard 1988)
- 6.68 (calculated-f const., De Bruijn et al. 1989)
- 5.73 (shake flask/slow stirring-GC, De Bruijn et al. 1989; De Bruijn & Hermens 1990; quoted, Bintein & Devillers 1994; Sijm et al. 1995)
- 5.44 (recommended, Sangster 1993)
- 5.73 (recommended, Hansch et al. 1995)
- 6.42 (quoted Pomona-database, Müller & Kördel 1996)

Bioconcentration Factor, log BCF:

- 3.89 (rainbow trout, calculated- k_1/k_2 , Neely et al. 1974)
- 3.09 (fish, Körte et al. 1978)
- 4.27, 3.73, 4.34 (fathead minnow, rainbow trout, green sunfish, Veith et al. 1979)
- 5.46 (guppy, lipid basis, Könnemann & van Leeuwen 1980; selected, Chiou 1985)
- 4.27 (fish, Giam et al. 1980)
- 1.20 (rats, adipose tissue, Geyer et al. 1980)
- 3.93, 2.46 (fish, flowing water, static water, Kenaga & Goring 1980; Kenaga 1980a)
- 3.61, 2.45 (calculated from water solubility, K_{OC} , Kenaga 1980a)
- 4.39, 4.20 (algae, calculated, Geyer et al. 1981)
- 3.91 (fish, correlated, Mackay 1982)
- 4.27, 3.89 (fathead minnow, rainbow trout, selected, Bysshe 1982)
- 4.60 (guppy, calculated-MCI χ , Koch 1983)
- 4.08–4.30 (rainbow trout, Oliver & Niimi 1983)
- 5.16–5.37 (rainbow trout, lipid basis, Oliver & Niimi 1983; selected, Chiou 1985)
- 4.31 (calculated- K_{OW} , Calamari et al. 1983)
- 3.93 (calculated- K_{OW} , Yoshida et al. 1983b)

- 4.39, 3.36, 4.54 (algae, fish, activated sludge, Klein et al. 1984)
 4.39, 3.83 (algae: exptl., calculated, Geyer et al. 1984; quoted, Wang et al. 1996)
 4.27 (fathead minnow, 25°C, calculated, Davies & Dobbs 1984; Anliker & Moser 1987)
 4.34, 3.74 (green sunfish, rainbow trout, 15°C, calculated, Davies & Dobbs 1984)
 4.39, 3.36, 4.54 (algae, fish, sludge, Klein et al. 1984)
 4.54 (activated sludge, Freitag et al. 1984; Halfon & Reggiani 1986)
 4.39, 3.41, 4.54 (algae, fish, activated sludge, Freitag et al. 1985)
 3.05 (fish, selected, Hawker & Connell 1986)
 2.62–2.97 (human fat, lipid basis, Geyer et al. 1987)
 2.44–2.79 (human fat, wet weight, Geyer et al. 1987)
 4.41 (algae, Mailhot 1987)
 4.34 (fathead minnow, Carlson & Kosian 1987)
 4.38, 4.30 (worms, fish, Oliver 1987a)
 3.48 (fish-normalized, Tadokoro & Tomita 1987)
 4.19 (guppy, calculated, Gobas et al. 1987)
 5.46 (guppy-lipid phase, calculated- K_{OW} , Gobas et al. 1987, 1989)
 6.42, 6.71, 5.96, 5.98 (field data-lipid base: Atlantic croakers, blue crabs, spotted sea trout, blue catfish, Pereira et al. 1988)
 –1.35 (beef, reported as biotransfer factor $\log B_b$, Travis & Arms 1988)
 –2.07 (milk, reported as biotransfer factor $\log B_m$, Travis & Arms 1988)
 –0.32 (vegetable, reported as biotransfer factor $\log B_v$, Travis & Arms 1988)
 5.30 (guppy-lipid phase, calculated- K_{OW} , Gobas et al. 1989)
 3.90, 4.19 (fish, selected, Connell & Hawker 1988; Hawker 1990)
 5.30 (guppy, correlated, Gobas et al. 1989)
 3.53 (picea omorika, Reischl et al. 1989)
 3.57 (fish, calculated, Figueroa & Simmons 1991)
 4.37, 4.16 (rainbow trout, guppy, Saito et al. 1992)
 4.27, 4.37 (fathead minnows, Saito et al. 1992)
 4.25 (*Chlorella pyrenoidosa*, Sijm et al. 1995)
 4.39, 3.18 (*Chlorella fusca*, *Myriophyllum spicatum*, Wang et al. 1996)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.59 (Kenaga & Goring 1980; Kenaga 1980a; selected, Lyman 1982; Yoshida 1983b; Nash 1989)
 4.45 (Kenaga 1980a)
 4.44, 4.21, 3.59 (estimated-S, K_{OW} , BCF, Lyman 1982)
 6.08 (calculated, Mabey et al. 1982)
 3.59 (selected, Bysshe 1982; Lyman et al. 1982)
 2.56 (shake flask-GC/ECD, Speyer soil, Freundlich isotherm, Rippen et al. 1982)
 2.70 (shake flask-GC/ECD, Alfisol, Freundlich isotherm, Rippen et al. 1982)
 4.58 (calculated- K_{OW} , Calamari et al. 1983)
 5.90 (field data, Oliver & Charlton 1984)
 4.90 (bottom sediment, Karickhoff & Morris 1985a)
 5.10 (calculated- K_{OW} , Oliver & Charlton 1984)
 5.2–6.7, 6.1 (suspended sediment, average, Oliver 1987c)
 5.80 (algae > 50 μm , Oliver 1987c)
 6.0–6.5, 6.3; 5.1 (Niagara River plume, range, mean; calculated- K_{OW} , Oliver 1987b)
 4.77 (HPLC- k' , Hodson & Williams 1988)
 4.70; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

Sorption Partition Coefficient, $\log K_{OM}$:

- 4.25 (shake flask-GC, soil-organic matter, Briggs 1981)
 5.50 (Niagara River-organic matter, Oliver & Charlton 1984)

Sorption Partition Coefficient, log K_p :

- 3.04–4.51 (sediment suspensions, Karickhoff & Morris 1985b; selected, Brusseau & Rao 1989)
 5.11 (simulation of Oliver 1985, Brusseau & Rao 1989)

Half-Lives in the Environment:

- Air: degradation rate constant of 0.0144 h^{-1} (Mackay et al. 1985; quoted, Mackay & Paterson 1991); 3753–37530 h, based on estimated photooxidation half-life (Atkinson 1987); 17000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).
 Surface Water: 23256–50136 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974); 1.4–50 d estimated, 0.3–3 d for river water and 30–300 d for lakes, estimated from persistence (Zoeteman et al. 1980); 55000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).
 Ground Water: 46512–100272 h, based on unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974); 30–300 d, estimated from persistence (Zoeteman et al. 1980).
 Soil: 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen, 1974); > 50 d (Ryan et al. 1988).
 Sediment: 55000 h (selected from Mackay et al. 1992, Mortimer & Connell 1995).
 Biota: half-life in rainbow trout, > 224 d (Niimi & Cho 1980); in subadult rainbow trout-calculated to be 210 d at 4°C , 80 d at 12°C and 70 d at 18°C (Niimi & Palazzo 1985); in worms at 8°C , 27 d (Oliver 1987a); picea omorika, 30 d (Reischl et al. 1989); 163 h, clearance from fish (Neely 1980).

Environmental Fate Rate Constants, k , or Half Lives, $t_{1/2}$:

Volatilization/Evaporation: $3.45 \times 10^{-10} \text{ mol/m}^2\text{-h}$ (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant in air, $1.44 \times 10^{-2} \text{ h}^{-1}$ (Brown et al. 1975; selected, Mackay et al. 1985); photooxidation half-life in air: 3753–37530 h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Atkinson 1987).

Hydrolysis: not expected to be important, based on $k_h = 0$, observed after 13 d at pH 3, 7, 11 and 85°C (Ellington et al. 1987).

Biodegradation: aqueous aerobic biodegradation half-life: 23256–50136 h, based on unacclimated aerobic soil grab sample data (Beck & Hansen 1974); anaerobic aqueous biodegradation half-life: 93024–200544 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Beck & Hansen 1974) and degradation rate constant in soil, $1.9 \times 10^{-5} \text{ h}^{-1}$ (Beck & Hansen 1974; selected, Mackay et al. 1985; Mackay & Paterson 1991); not significant in an aerobic environment, and no significant degradation rate (Tabak et al. 1981; Mills et al. 1982).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

- k_1 : 18.76 h^{-1} (trout muscle, Neely et al. 1974)
 k_2 : 0.00238 h^{-1} (trout muscle, Neely et al. 1974)
 k_1 : 10000 d^{-1} (guppy, Könnemann & van Leeuwen 1980)
 k_1 : 22.5 h^{-1} (guppy, selected, Hawker & Connell 1985)
 k_1 : 18.8 h^{-1} (trout, selected, Hawker & Connell 1985)
 k_1 : 540.0 d^{-1} (fish, selected, Opperhuizen 1986)
 k_2 : $0.00510, 0.00818, 0.00640, 0.0047 \text{ d}^{-1}$ (rainbow trout, calculated-fish mean body weight, Barber et al. 1988)
 $1/k_2$: 420 h (trout, selected, Hawker & Connell 1985)
 $\log k_1$: 2.73 d^{-1} (fish, selected, Connell & Hawker 1988)
 $\log k_1$: 2.65 d^{-1} (fish, selected, Connell & Hawker 1988)
 $\log 1/k_2$: 1.24 d^{-1} (fish, selected, Connell & Hawker 1988)
 $\log k_2$: -1.24 d^{-1} (fish, calculated- K_{ow} , Thomann 1989)
 k_1 : 0.049 h^{-1} (uptake of mayfly-sediment model II, Gobas et al. 1989b)
 k_2 : 0.023 h^{-1} (depuration of mayfly-sediment model II, Gobas et al. 1989b)
 k_1 : 10489 h^{-1} (*Chlorella fusca*, Wang et al. 1996)
 k_2 : 0.424 h^{-1} (*Chlorella fusca*, Wang et al. 1996)

k_1 : 6.558 h^{-1} (*Myriophyllum spicatum*, Wang et al. 1996)

k_2 : 0.00429 h^{-1} (*Myriophyllum spicatum*, Wang et al. 1996)

Sediment Exchange Rate Constant:

$0.026\text{--}1.2 \text{ d}^{-1}$ (natural sediment, Karickhoff & Morris 1985).

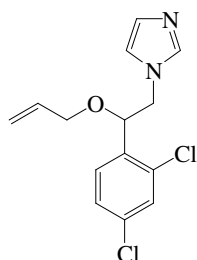
Sediment Burial Rate Constant:

$4.6 \times 10^{-6} \text{ h}^{-1}$ (Di Toro et al. 1981; selected, Mackay et al. 1985)

Stratospheric Diffusion Rate Constant:

$1.7 \times 10^{-6} \text{ h}^{-1}$ (Mackay et al. 1985)

19.1.23 IMAZALIL



Common Name: Imazalil

Synonym: Bromazil, Deccoil, Enilconazole, Fecundal, Freshgard, Fungaflor, Fungazil, R 23979

Chemical Name: 1-(β -allyloxy-2,4-dichlorophenylethyl)imidazole; 1-[2-(2,4-dichlorophenyl)-2-(2-propenyloxy)ethyl]-1*H*-imidazole

CAS Registry No: 35554-44-0

Uses: as fungicide for control of a wide range of fungal diseases on fruit, vegetables, and ornamentals; also used as a seed dressing, for control of diseases of cereal and cotton, etc.

Molecular Formula: $C_{14}H_{14}Cl_2N_2O$

Molecular Weight: 297.129

Melting Point ($^{\circ}C$):

50.0 (Hartley & Kidd 1987; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

> 340 (Worthing & Hance 1991; Tomlin 1994)

dec (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.243 ($23^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

1.348 ($26^{\circ}C$, Tomlin 1994)

Molar Volume (cm^3/mol):

318.8 (calculated-Le Bas method at normal boiling point)

239.1 (calculated-density)

Dissociation Constant pK_a :

6.53 (Worthing & Hance 1991)

7.47 (pK_b , Tomlin 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

96.53 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

29.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

90 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.568 (mp at $50^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1400 ($20^{\circ}C$, Hartley & Kidd 1987; Milne 1995)

180 (pH 7.6, Worthing & Hance 1991; Tomlin 1994)

1400 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations.):

9.30×10^{-6} ($20^{\circ}C$, Hartley & Kidd 1987)

1.60×10^{-4} , 8.0×10^{-3} , 0.230, 4.20, 53.0 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 18.21 - 6562.5/(T/K)$; measured range 53 – $129^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 13.52 - 5042.4/(T/K)$; measured range 53.6 – $129^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

1.60×10^{-4} ($20^{\circ}C$, Worthing & Hance 1991)

1.58×10^{-4} ($20^{\circ}C$, Tomlin 1994)

9.30×10^{-6} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

1.97×10^{-6} (20– 25°C , calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.82 (Worthing & Hance 1991; Milne 1995)

3.82 (pH 9.2, Tomlin 1994)

3.82 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

4.57 (calculated-S as per Kenaga 1980, this work)

2.70 (calculated- K_{OW} as per Kenaga 1980, this work)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

2.26 (clay loam, Worthing & Hance 1991; Tomlin 1994)

2.32 (sandy loam, Worthing & Hance 1991; Tomlin 1994)

1.83 (sandy soil, Worthing & Hance 1991; Tomlin 1994)

3.60 (soil, 20– 25°C , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

3.73 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

3.73; 3.52 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: stable to light under normal storage conditions (Tomlin 1994).

Oxidation:

Hydrolysis: very stable to hydrolysis in dilute acids and alkalis at room temperature (Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Soil: $t_{1/2} = 30\text{--}170$ d (Tomlin 1994);

field $t_{1/2} = 150$ d (20– 25°C , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.24 MANCOZEB

Common Name: Mancozeb

Synonym: dithane ultra, Dithane M45, Dithane SPC, Fore, Manzate, Manseb, Maezin, Nemispor, Penncozeb, Vondozeb, Zimanat, zine manganese ethylenebis[dithiocarbamate]

Chemical Name: manganese ethylenebis(dithiocarbamate) (polymeric) complex with zinc salt

CAS Registry No: 8018-01-7

Uses: fungicide

Molecular Formula: $(C_4H_6MnN_2S_4)_x(Zn)_y$

Molecular Weight:

Melting Point ($^{\circ}C$):

192–194 (dec., Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

192–204 (dec., Tomlin 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

insoluble (Spencer 1982; Hartley & Kidd 1987; Milne 1995)

6–20 (Montgomery 1993)

6–20 (Tomlin 1994)

6.0 (20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$):

negligible (Hartley & Kidd 1987; Tomlin 1994)

0 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, log K_{ow} :

3.12–3.70 (Montgomery 1993)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

2.93–3.21 (soil, calculated, Montgomery 1993)

> 3.30 (soil, Wauchope et al. 1992; Hornsby et al. 1996)

> 3.30 (soil, Tomlin 1994)

Environmental Fate Rate Constants, or Half-Lives:

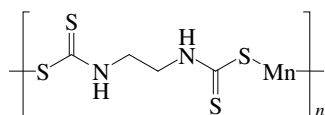
Hydrolysis: unstable in acidic media (Hartley & Kidd 1987); $t_{1/2} = 20$ d at pH 5, $t_{1/2} = 17$ h at pH 7, $t_{1/2} = 34$ h at pH 9 (Montgomery 1993; Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2} = 70$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} \sim 6$ –15 d (Tomlin 1994).

19.1.25 MANEB



Common Name: Maneb

Synonym: MEB, Dithane, Bravo

Chemical Name: manganese ethylenebis(dithiocarbamate)

CAS Registry No: 12427-38-2

Uses: fungicide

Molecular Formula: $(\text{C}_4\text{H}_6\text{MnN}_2\text{S}_4)_x$

Molecular Weight: $(265.302)_x$

Melting Point ($^{\circ}\text{C}$):

200 (dec, Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

Density (g/cm^3 at 20°C):

1.92 (Spencer 1982; Worthing & Walker 1983; Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F:

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

slightly soluble (Spencer 1982)

insoluble (Worthing & Walker 1983; Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

slight, 200, 6 (quoted, Wauchope et al. 1992)

6.0 (20– 25°C , estimated and selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

negligible (20°C , Worthing 1983; Hartley & Kidd 1987; Tomlin 1994)

0 (selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

2.40 (activated sludge, Freitag et al. 1983)

2.40, 2.26, < 1.0 (activated sludge, algae, *Golden ide*, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

> 3.30 (soil, estimated, Wauchope et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: rapidly hydrolyzed in acidic media (Hartley & Kidd 198);

$t_{1/2} < 24 \text{ h}$ at pH 5.7 or 9 (Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 7\text{--}14$ d, green house experiment in microagroecosystem chamber (Nash & Beall 1980).

Surface water: rapidly hydrolyzed in acidic media (Hartley & Kidd 1987).

Groundwater:

Sediment:

Soil: $t_{1/2} = 36$ d in soil (sandy loam with pH 6.7),

green house experiment in microagroecosystem chamber (Nash & Beall 1980);

$t_{1/2} \sim 25$ d in loamy sand in dark, aerobic conditions (Tomlin 1994);

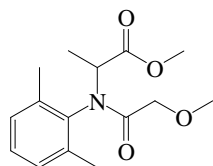
field $t_{1/2} \sim 70$ d (estimated, Wauchope et al. 1992; Hornsby et al. 1996).

Biota: $t_{1/2} = 6.4$ d for beans, $t_{1/2} = 7.4$ d for tomatoes (Nash & Beall 1980);

$t_{1/2} = 14$ d on tomato leaves, green house experiment in microagroecosystem chamber (Nash & Beall 1980);

$t_{1/2} = 10$ d for tomato fruit, $t_{1/2} = 4.5$ d for tomato leaves in the field, $t_{1/2} = 3$ d for tomatoes and soybean leaves in microagroecosystem (Nash 1983).

19.1.26 METALAXYL



Common Name: Metalaxyl

Synonym: Apron, CGA 48988, Ridomil, Subdue

Chemical Name: methyl *N*-(2-methoxyacetyl)-*N*-(2,6-xylyl)-DL-alaninate; methyl-*N*-(2,6-dimethylphenyl)-*N*-(methoxyacetyl)-DL-alaninate

CAS Registry No: 57837-19-1

Uses: fungicide to control of foliar and soil-borne diseases caused by *Peronosporates* on a wide range of crops; also used to treat seeds, etc.

Molecular Formula: C₁₅H₂₁NO₄

Molecular Weight: 279.333

Melting Point (°C):

71 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.21 (Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

Molar Volume (cm³/mol):

328.2 (calculated-Le Bas method at normal boiling point)

230.9 (calculated-density)

Dissociation Constant pK_a: << 0 (Tomlin 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

89.73 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.4 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

79 (Rordorf 1989)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.354 (mp at 71°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

7100 (quoted, Burkhard & Guth 1981)

7000 (shake flask-HPLC, Ellgehausen et al. 1981)

7100 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Montgomery 1993)

7000 (quoted-Yalkowsky & Dannenfelser 1994, Pinsuwan et al. 1995)

8400 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

8400 (selected, Lohninger 1994)

8400 (22°C, Tomlin 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

2.93×10^{-4} (20°C, volatilization rate, Burkhard & Guth 1981)

2.93×10^{-4} (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)

7.50×10^{-4} , 2.90×10^{-2} , 0.67, 10.0, 110 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log(P_s/\text{Pa}) = 17.423 - 4687.6/(T/\text{K})$; measured range 32.7–69.7°C (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/\text{Pa}) = 13.243 - 4687.6/(T/\text{K})$; measured range 72.3–130°C (liquid, gas saturation-GC, Rordorf 1989)

7.5×10^{-4} (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

2.93×10^{-4} (20°C, Montgomery 1993)

7.5×10^{-4} (Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

1.155 (20°C, evaporation rate, Burkhard & Guth 1981)

2.48×10^{-5} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

1.65	(shake flask, Ellgehausen et al. 1980, 1981)
1.53	(shake flask, log P Database, Hansch & Leo 1987)
1.60	(shake flask at pH 7, Stevens et al. 1988)
1.70	(shake flask at pH 7, Baker et al. 1992)
1.59	(recommended value, Sangster 1993)
1.75	(Tomlin 1994)
1.693	(calculated-f const., Pinsuwan et al. 1995)
1.65	(recommended, Hansch et al. 1995)
1.40	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

0.03	(<i>Daphnia magna</i> , wet wt. basis, Ellgehausen et al. 1980)
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Sorption Partition Coefficient, log K_{oc} :

1.59	(av. of 3 soils, Sharom & Edgington 1982)
2.26	(av. of 7 soils, Carris 1983)
3.22	(av. of 12 soils, calculated-linearized Freundlich Isotherm, Sukop & Cogger 1992)
1.70	(soil, 20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.53–1.84	(soil, Montgomery 1993)
1.70	(estimated-chemical structure, Lohninger 1994)
1.57	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.57; 2.05	(soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $k(\text{calc}) = 0.71 \text{ ng cm}^{-2} \text{ h}^{-1}$ and $k(\text{measured}) = 0.35 \text{ ng cm}^{-2} \text{ h}^{-1}$ from moist soils at 20°C (Burkhard & Guth 1981).

Photolysis: irradiated by UV at 290 nm in the presence of hydrogen peroxide and titanium dioxide, respectively, in aqueous solution resulted in 29% and 84% transformation in 2.5 h (Moza et al. 1994).

Oxidation:

Hydrolysis: stable in neutral and acidic media at room temp., calculated $t_{1/2} > 200 \text{ d}$ at 20°C and pH 1, $t_{1/2} = 115 \text{ d}$ at pH 9 and $t_{1/2} = 12 \text{ d}$ at pH 10 (Worthing & Hance 1991; Montgomery 1993; Tomlin 1994).

Biodegradation: overall degradation rate constant $k = 0.0081 \text{ h}^{-1}$ with $t_{1/2} = 85.5 \text{ h}$ in sewage sludge and $k = 0.0217 \text{ d}^{-1}$ with $t_{1/2} = 31.9 \text{ d}$ in garden soil (Müller & Buser 1995);

rate constant $k = 0.060 \text{ d}^{-1}$ for *R*-metalaxyl (fungicidally active) in soil expt incubated with *rac*-metalaxyl, $k = 0.080 \text{ d}^{-1}$ in soil expt incubated with *R*-metalaxyl; rate constant $k = 0.015 \text{ d}^{-1}$ for *S*-metalaxyl (fungicidally inactive) in soil expt incubated with *rac*-metalaxyl, $k = 0.010/0.12 \text{ d}^{-1}$ for in soil expt incubated with *S*-metalaxyl (Buser et al. 2002);

degradation rate constants for formulated racemic metalaxyl were found to be 0.039 d^{-1} with $t_{1/2} = 18 \text{ d}$ for German soil, $k = 0.018 \text{ d}^{-1}$ with $t_{1/2} = 38 \text{ d}$ for Cameroonian soil; for unformulated racemic metalaxyl rate constants were: $k = 0.039 \text{ d}^{-1}$ with $t_{1/2} = 18 \text{ d}$ for German soil, $k = 0.019 \text{ d}^{-1}$ with $t_{1/2} = 17 \text{ d}$ from Cameroonian soil; and for formulated *R*-metalaxyl rate constants were: $k = 0.041 \text{ d}^{-1}$ with $t_{1/2} = 17 \text{ d}$ for German soil, $k = 0.018 \text{ d}^{-1}$ with $t_{1/2} = 38 \text{ d}$ from Cameroonian soil. For soil incubated with metalaxyl enantiomers, *R*-metalaxyl degraded faster ($k = 0.064 \text{ d}^{-1}$) than *S*-metalaxyl ($k = 0.033 \text{ d}^{-1}$) in German soil when spiked with formulated racemic metalaxyl, while *S*-metalaxyl degraded faster ($k = 0.026 \text{ d}^{-1}$) than *R*-metalaxyl ($k = 0.014 \text{ d}^{-1}$) in Cameroonian soil when spiked with formulated racemic metalaxyl (Monkiedje et al. 2003).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

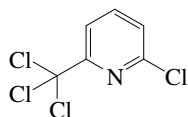
Soil: degradation $t_{1/2} = 39.5 \text{ d}$ in garden soil (Müller & Buser 1995);

field $t_{1/2} = 70 \text{ d}$ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

residual activity in soil is about 70–90 d (Tomlin 1994);

degradation $t_{1/2} = 17–38 \text{ d}$ of the racemic mixture and enantiomers of metalaxyl in controlled incubation experiments in typical soils from Germany and Cameroon. (Monkiedje et al. 2003).

19.1.27 NITRAPYRIN



Common Name: Nitrapyrin

Synonym: N-Serve

Chemical Name: 2-chloro-6-(trichloromethyl)pyridine

CAS Registry No: 1929-82-4

Uses: bactericide

Molecular Formula: $C_6H_3Cl_4N$

Molecular Weight: 230.907

Melting Point ($^{\circ}C$):

63 (Lide 2003)

Boiling Point ($^{\circ}C$):

136–137.5/11 mmHg (Tomlin 1994)

Density (g/cm^3 at $25^{\circ}C$):

1.744 (Montgomery 1993)

1.579 (Tomlin 1994)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.424 (mp at $63^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

40 (quoted, Briggs 1981)

40 ($22^{\circ}C$, Spencer 1982; Worthing & Walker 1983, 1987; Montgomery 1993; Tomlin 1994)

92; 54 (generator column-RI; HPLC-RT correlation, Swann et al. 1983)

40 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.37 ($23^{\circ}C$, Spencer 1982; Worthing & Walker 1983, 1987)

0.373 ($20^{\circ}C$, Montgomery 1993)

0.373 (20 – $25^{\circ}C$, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant (Pa· m^3/mol at $25^{\circ}C$):

216 (calculated-P/C, Montgomery 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.02 (shake flask-UV, Briggs 1981)

3.02–3.41 (Montgomery 1993)

3.325 (Tomlin 1994)

3.41 (recommended, Hansch et al. 1995)

3.41 (LOGPSTAR or CLOGP data, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.87, 1.36 (calcd-solubility, K_{ow} , Kenaga 1980b)

Sorption Partition Coefficient, $\log K_{OC}$:

1.93–2.42; 2.19 (quoted: 10 soils range; mean, Briggs 1981)

2.0 (Cottenham soil, shake flask-GC, $20^{\circ}C$, Briggs 1981)

- 2.76 (calculated, Kenaga 1980b)
 2.66 (average of 3 soils, HPLC-RT correlation, McCall et al. 1980)
 2.64, 2.68, 2.66; 2.66 (Commeree soil, Tracy soil, Catlin soil; mean, HPLC-RT, Swann et al. 1981; quoted, McCall et al. 1981)
 2.24–2.76 (quoted literature range, Wauchope et al. 1992)
 2.76 (soil, Wauchope et al. 1992; Hornsby et al. 1996)
 2.62–2.68 (soil, Montgomery 1993)
 2.40–3.96 (soil, Tomlin 1994)
 2.62 (soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: water photolysis $t_{1/2} = 2$ h (Tomlin 1994).

Oxidation:

Hydrolysis: hydrolysis $t_{1/2} = 2$ d at pH 7 (Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} = 2$ d at pH 7, water photolysis $t_{1/2} = 2$ h (Tomlin 1994).

Groundwater:

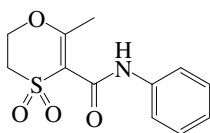
Sediment:

Soil: field $t_{1/2} = 10$ d (Wauchope et al. 1992; Hornsby et al. 1992);

aerobic soil metabolism $t_{1/2} = 6.42$ d, anaerobic metabolism $t_{1/2} \sim 2.5$ h (Tomlin 1994).

Biota:

19.1.28 OXYCARBOXIN



Common Name: Oxycarboxin

Synonym: DCMOD, Oxycarboxine

Chemical Name: 5,6-dihydro-2-methyl-1,4-oxathi-ine-3-carboxanilide 4,4-dioxide; 5,6-dihydro-2-methyl-*N*-phenyl-1,4-oxathin-3-carboxamide 4,4-dioxide

CAS Registry No: 5259-88-1

Uses: as fungicide for control of rust diseases on ornamentals, cereals, and nursery trees, etc.

Molecular Formula: $C_{12}H_{13}NO_4S$

Molecular Weight: 267.301

Melting Point ($^{\circ}C$):

129 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.14 (Tomlin 1994)

Molar Volume (cm^3/mol):

261.4 (calculated-Le Bas method at normal boiling point)

234.5 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.054 (mp at $129^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1000 (Martin & Worthing 1977; quoted, Kenaga 1980)

1000 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

1000 (20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

1000 (selected, Lohninger 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.0010 ($20^{\circ}C$, Hartley & Kidd 1987)

< 133 ($20^{\circ}C$, Worthing & Hance 1991)

5.60×10^{-6} (Tomlin 1994)

1.33×10^{-3} (20– $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

3.56×10^{-4} (20– $25^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.74 (shake flask-UV, Mathre 1971)

0.74 (recommended, Sangster 1993)

0.772 (Tomlin 1994)

0.740 (selected, Hansch et al. 1995)

1.13 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log BCF$:

1.11 (calculated-S, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

1.99 (calculated-S, Kenaga 1980)

- 1.98 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
1.98 (selected, Lohninger 1994)

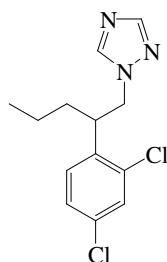
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} = 44$ d at pH 6, 25°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} = 2.5\text{--}8$ wk in sandy loam by aerobic soil metabolism (Tomlin 1994);
field $t_{1/2} = 20$ d (Wauchope et al. 1992; Hornsby et al. 1996).

19.1.29 PENCONAZOLE



Common Name: Penconazole

Synonym: Award, CGA 71818, Topas, Topaz, Topaze

Chemical Name: 1-(2,4-dichloro- β -propylphenylethyl)-1*H*-1,2,4-triazole; 1-[2-(2,4-dichlorophenyl)pentyl]-1*H*-1,2,4-triazole

CAS Registry No: 66246-88-6

Uses: as fungicide for control of pathogenic *Ascomycetes*, *Basidiomycetes* and *Deuteromycetes* (especially powdery mildews) on vines, cucurbits, pome fruit, ornamentals and vegetables.

Molecular Formula: $C_{13}H_{15}Cl_2N_3$

Molecular Weight: 284.184

Melting Point ($^{\circ}C$):

60.0 (Hartley & Kidd 1987; Worthing & Hance 1991)

62.1 (Rordorf 1989)

57.6–60.3 (Tomlin 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.30 (Tomlin 1994)

Molar Volume (cm^3/mol):

312.3 (calculated-Le Bas method at normal boiling point)

218.6 (calculated-density)

Dissociation Constant pK_a :

1.51 (Tomlin 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.45 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.1 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

81 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.454 (mp at $60^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

70 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991)

73 ($20^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.00021 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994)

3.70×10^{-4} , 1.30×10^{-2} , 0.28, 4.0, 41.0 (25 , 50 , 70 , 100 , $125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 16.671 - 5995.1/(T/K)$; measured range 36.6 – $58.3^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 13.088 - 4777.0/(T/K)$; measured range 60.9 – $129^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.00082 ($20^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.40 (shake flask-HPLC, Bateman et al. 1990)

3.20 (shake flask-HPLC, Chamberlain et al. 1991)

3.72 (pH 5.7, Tomlin 1994)
3.40, 3.20 (Sangster 1993)
3.40, 3.50 (Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.75 (20°C, calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, log K_{OC} :

2.62 (20°C, calculated-S as per Kenaga 1980, this work)

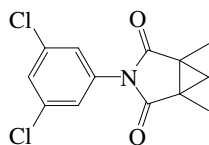
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: stable to hydrolysis pH 1–13, and to temperature up to 350°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: half-life is several months (Tomlin 1994).

19.1.30 PROCYMIDONE



Common Name: Procymidone

Synonym: S-7131, Sialex, Sumiboto, Sumilex, Sumisclex

Chemical Name: *N*-(3,5-dichlorophenyl)-1,2-dimethylcyclopropane-1,2-dicarboximide; 3-(3,5-dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3,1,0]hexane-2,4-dione

CAS Registry No: 32809-16-8

Uses: as fungicide for control of *Botrytis*, *Sclerotinia*, *Monilia*, and *Helminthosporium* spp. on fruit, vines, vegetables, cereals and ornamentals, etc.

Molecular Formula: $C_{13}H_{11}Cl_2NO_2$

Molecular Weight: 284.138

Melting Point ($^{\circ}C$):

166 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

1.452 ($25^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

225.9 (calculated-Le Bas method at normal boiling point)

195.7 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0414 (mp at $166^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4.50 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

4.50 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.018 (Hartley & Kidd 1987)

0.011 ($20^{\circ}C$, Worthing & Hance 1991)

0.018, 0.0105 (20 , $25^{\circ}C$, Tomlin 1994)

0.0187 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

1.181 (20 – $25^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.14 ($26^{\circ}C$, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

3.0 (selected, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.42 (calculated-S as per Kenaga 1980, this work)

Sorption Partition Coefficient, $\log K_{OC}$:

3.18 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

3.28 (soil, calculated-S as per Kenaga 1980, this work)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Photolysis: when irradiation with UV light, $\lambda \geq 290$ nm, for procymidone solution (2 ppm): 9% and 11% photo-degraded in 1 h, in the presence of 1 ppm humic acid and 1 ppm fulvic acid, respectively; rapid degradation with $t_{1/2} = 3$ min in the presence of TiO_2 (20 ppm), but degraded slowly as 9% transformation in 2 h with Fe_2O_3 (100 ppm). (Hustert & Moza 1997)

Half-Lives in the Environment:

Air:

Surface water: photodegradation of procymidone solution (2 ppm), $t_{1/2} = 3$ min in the presence of TiO_2 (20 ppm) when irradiated with UV light (Hustert & Moza 1997)

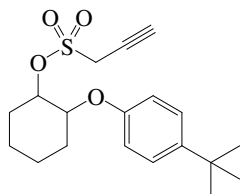
Groundwater:

Sediment:

Soil: persists for ca. 4–12 weeks (Hartley & Kidd 1987; Tomlin 1994);
field $t_{1/2} = 7$ d (Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.31 PROPARGITE



Common Name: Propargite

Synonym: Comite, Omite

Chemical Name: 2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl sulfite

CAS Registry No: 2312-35-8

Uses: acaricide

Molecular Formula: $C_{16}H_{26}O_4S$

Molecular Weight: 360.472

Melting Point ($^{\circ}C$):

dark brown liquid (Hartley & Kidd 1987)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $25^{\circ}C$):

1.085–1.115 (Hartley & Kidd 1987; Worthing & Walker 1983, 1987)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

practically insoluble in water (Worthing & Walker 1983, 1987)

0.5 ($20^{\circ}C$, Hartley & Kidd 1987)

0.50 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.5 (20 – $25^{\circ}C$, Majewski & Capel 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

400 ($20^{\circ}C$, Worthing & Walker 1983, 1987; Hartley & Kidd 1987)

0.4 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.4 (20 – $25^{\circ}C$, quoted, Majewski & Capel 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated)

280 (20 – $25^{\circ}C$, Majewski & Capel 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

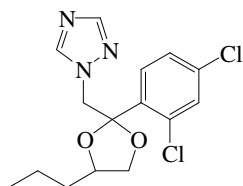
3.60 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Soil: field $t_{1/2} = 40$ and 56 d, the recommended $t_{1/2} = 56$ d (Wauchope et al. 1992; Hornsby et al. 1996).

19.1.32 PROPICONAZOLE



Common Name: Propiconazole

Synonym: Alamo, Banner, CGA 64250, Desmel, Orbit, Practis, Radar, Spire, Tilt

Chemical Name: (±)-1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-ylmethyl]-1H-1,2,4-triazole; 1-[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxalan-2-ylmethyl]-1H-1,2,4-triazole

CAS Registry No: 60207-90-1

Uses: as fungicide for control of mildews, rusts on cereals, ornamentals, fruits and other crops; and also used for other diseases of turf and grass seed crops, etc.

Molecular Formula: $C_{15}H_{17}Cl_2N_3O_2$

Molecular Weight: 342.221

Melting Point (°C): liquid

Boiling Point (°C):

180 (at 0.1 mmHg, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Density (g/cm³ at 20°C):

1.27 (Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

1.29 (20°C, Tomlin 1994)

Molar Volume (cm³/mol):

358.6 (calculated-Le Bas method at normal boiling point)

267.3 (calculated-density)

Dissociation Constant pK_a :

1.09 (Tomlin 1994)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

106.8 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

110 (20°C, Hartley & Kidd; Worthing & Hance 1991; Milne 1995)

100 (20°C, Tomlin 1994)

110 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

110 (selected, Lohninger 1994)

110 (20°C, quoted, Siebers et al. 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

0.00013 (20°C, Hartley & Kidd 1987)

5.60×10^{-5} , 1.60×10^{-3} , 0.027, 0.32, 28.0 (25, 50, 70, 100, 125°C, gas saturation-GC, Rordorf 1989)

$\log(P_L/\text{Pa}) = 14.468 - 5581.2/(T/K)$; measured range 32.5–124°C (liquid, gas saturation-GC, Rordorf 1989)

0.000133 (20°C, Worthing & Hance 1991)

5.6×10^{-5} (20–25°C, Wauchope et al. 1992; Hornsby et al. 1996)

5.6×10^{-5} (Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C or as indicated):

4.0×10^{-4} (20°C, calculated-P/C, Siebers et al. 1994)

0.00017 (20–25°C, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.50	(Bateman et al. 1990; quoted, Sangster 1993)
3.72	(Siebers et al. 1994)
3.72	(pH 6.6, Tomlin 1994)
3.50	(selected, Hansch et al. 1995)
3.50	(LOGPSTAR or CLOGP data, Sabljic et al. 1995)
3.33	(RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log BCF$:Sorption Partition Coefficient, $\log K_{oc}$:

2.81	(soil, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.52	(soil, calculated-S as per Kenaga 1980, this work)
2.81	(selected, Lohninger 1994)
3.39	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
3.39; 3.62	(soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: no significant hydrolysis (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 25\text{--}85$ d in aerobic aquatic systems at 25°C (Tomlin 1994).

Groundwater:

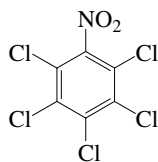
Sediment:

Soil: field $t_{1/2} = 110$ d (Wauchope et al. 1992; Hornsby et al. 1996);

$t_{1/2} = 40\text{--}70$ d in aerobic soils at 25°C (Tomlin 1994).

Biota:

19.1.33 QUINTOZENE



Common Name: Quintozene

Synonym: Avicol, Batrilex, Brassicol, Chinozan, earthcide, Fartox, Folosan, Fomac 2, Fungiclor, Kobutol, KOBU, KP 2, Marisan forte, Olpisan, PCNB, Pentagen, Phomasan, PKhNB, Quinosan, Quinocene, saniclor 30, Terraclor, Terrafun

Chemical Name: pentachloronitrobenzene

CAS Registry No: 82-68-8

Uses: as fungicide for seed and soil treatment, for control of *Botrytis*, *Rhizoctonia*, and *Sclerotinia* spp. on brassicas, vegetables, ornamentals and other crops, and *Telletia caries* of wheat.

Molecular Formula: $C_6Cl_5NO_2$

Molecular Weight: 295.335

Melting Point ($^{\circ}C$):

144 (Lide 2003)

Boiling Point ($^{\circ}C$):

328 (dec, Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.718 ($25^{\circ}C$, Spencer 1982; Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

1.907 ($21^{\circ}C$, Tomlin 1994)

Molar Volume (cm^3/mol):

207.3 (calculated-Le Bas method at normal boiling point)

154.9 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.3 (Rordorf 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18 (Rordorf 1989)

Entropy of Fusion, ΔS_{fus} (J/mol K):

43 (Rordorf 1989)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0680 (mp at $144^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

practically insoluble (Spencer 1982; Worthing & Hance 1991; Milne 1995)

0.55 ($20-25^{\circ}C$, shake flask-GC, Kanazawa 1981)

0.44 ($20^{\circ}C$, Hartley & Kidd 1987; Pait et al. 1992; Milne 1995)

0.40 (Davies & Lee 1987)

0.44 ($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.10 (selected, Lohninger 1994)

0.10 ($20^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0151 (Spencer 1982)

6.60×10^{-3} ($20^{\circ}C$, Hartley & Kidd 1987)

8.40×10^{-3} , 0.16, 1.90, 17.0, 110 ($25, 50, 70, 100, 125^{\circ}C$, gas saturation-GC, Rordorf 1989)

$\log(P_s/Pa) = 14.34 - 4893.9/(T/K)$; measured range $49.9-140^{\circ}C$ (solid, gas saturation-GC, Rordorf 1989)

$\log(P_L/Pa) = 12.234 - 4037.9/(T/K)$; measured range $150-196^{\circ}C$ (liquid, gas saturation-GC, Rordorf 1989)

1.80 (Worthing & Hance 1991)

0.0147 ($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.0127 (Tomlin 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 0.3718 (known LWAPC of Kawamoto & Urano 1989, Meylan & Howard 1991)
 0.4812 (calculated-bond contribution method LWAPC, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

- 4.22 (20°C , shake flask-GC, Kanazawa 1981)
 5.21 (HPLC-RT correlation, McDuffie 1981)
 5.00 (HPLC-RT correlation, Ohori & Ihashi 1987)
 5.18 (HPLC-RT correlation, Kawamoto & Urano 1989)
 4.77; 5.40 (shake flask-GC; calculated-fragment const., Niimi et al. 1989)
 5.02 (RP-HPLC-RT correlation, Saito et al. 1993)
 4.64 (recommended, Sangster 1993)
 5.0–6.0 (Tomlin 1994)
 4.22 (selected, Hansch et al. 1995)
 4.89 (Pomona-database, Müller & Kördel 1996)
 5.01 (RP-HPLC-RT correlation, Nakamura et al. 2001)
 5.30 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$:

- 2.38 (topmouth gudgeon, Kanazawa 1981)
 3.49, 3.65, 3.06 (algae, activated sludge, fish, Freitag et al. 1985)
 2.23 (rainbow trout, Niimi et al. 1989)
 2.91 (quoted, Pait et al. 1992)

Sorption Partition Coefficient, $\log K_{\text{oc}}$:

- 4.30 (correlated-Freundlich Isotherm, Kawamoto & Urano 1989)
 4.30, 3.38 (soil, quoted exptl., calculated-MCI χ and fragments contribution, Meylan et al. 1992)
 3.70 (soil, estimated, Wauchope et al. 1992; Hornsby et al. 1996)
 4.34 (soil, HPLC-screening method, mean value of different stationary and mobile phases, Kördel et al. 1993, 1995)
 3.78, 3.47 (for adsorption: silt loam, sand, Tomlin 1994)
 3.98, 3.52 (for desorption: silt loam, sand, Tomlin 1994)
 4.30 (estimated-chemical structure, Lohninger 1994)
 4.34; 3.38 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

- Biodegradation: rate constant $k(\text{aerobic}) = 0.16 \text{ d}^{-1}$ with $t_{1/2} = 4.3 \text{ d}$ at 20°C by aerobic activated sludge and $k(\text{anaerobic}) = 0.16 \text{ d}^{-1}$ with $t_{1/2} = 4.3 \text{ d}$ at 20°C by anaerobic microorganisms cultivated an artificial sewage (Kawamoto & Urano 1990)
 rate constant $k = 6.5 \text{ d}^{-1}$ with $t_{1/2} = 0.11 \text{ d}$ (Corrigendum, Kawamoto & Urano 1991).

Half-Lives in the Environment:

Air:

Surface water: biodegradation $t_{1/2} = 4.3 \text{ d}$ at 20°C by aerobic activated sludge or anaerobic microorganisms cultivated by an artificial sewage (Kawamoto & Urano 1990)

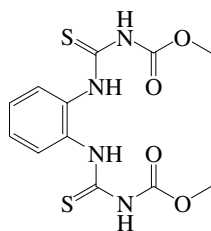
Groundwater:

Sediment:

Soil: $t_{1/2} \sim 4\text{--}10$ months (Hartley & Kidd 1987; Tomlin 1994),
 $t_{1/2} = 4 \text{ d}$ (Pait et al. 1992);
 field $t_{1/2} = 21 \text{ d}$ (Wauchope et al. 1992; Hornsby et al. 1996).

Biota:

19.1.34 THIOPHANATE-METHYL



Common Name: Thiophanate-methyl

Synonym: Cerobin, Enovit, Fumidor, Fungitox, Fungo, Fungus Fighter, Labilite, Mildothane, Neotosin, NF-44, Pelt 44, Seal 7 Heal, Sigma, Sipcaplant, Sipcasan, Topsin M, Trevin

Chemical Name: dimethyl 4,4'-(*o*-phenylene)bis(3-thioallophanate; dimethyl [1,2-phenylene-bis(monocarbonothioyl)]-biscarbamate

Uses: fungicide/wound protectant

CAS Registry No: 23564-05-8

Molecular Formula: $C_{12}H_{14}N_4O_4S_2$

Molecular Weight: 342.394

Melting Point (C):

172 (dec., Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

344.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

7.28 (Worthing & Hance 1991; Tomlin 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0361 (mp at 172°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

3.50 (20°C, Hartley & Kidd 1987)

26.6 (Worthing & Hance 1991)

3.50 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

3.50 (selected, Lohninger 1994)

26.6 (20°C, Milne 1995)

Vapor Pressure (Pa at 25°C or as indicated):

$< 1.0 \times 10^{-5}$ (20°C, Hartley & Kidd 1987)

$< 1.33 \times 10^{-5}$ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

9.50×10^{-6} (Tomlin 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.0013 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, log K_{ow} :

1.40 (Worthing & Hance 1991; Milne 1995)

1.50 (Tomlin 1994)

1.40 (selected, Hansch et al. 1995)

1.86 (RP-HPLC-RT correlation, pH 3.5, Hu et al. 1997)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

0.079 (Worthing & Hance 1991)

3.26 (20–25°C, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

3.26 (selected, Lohninger 1994)

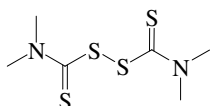
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Hydrolysis: stable neutral, aqueous solution, $t_{1/2} = 24.5$ h at pH 9, 22°C (Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2} = 10$ d (Wauchope et al. 1992; Hornsby et al. 1996);
persistence ca. 3–4 weeks (Tomlin 1994).

19.1.35 THIRAM



Common Name: Thiram

Synonym: Aapirol, Aatiram, Accel TMT, Accelerator T, Aceto TETD, Arasan, Atiram, Cyuram, Delsan, Ekagom TB, ENT-987, Falitiram, Fermide, Fernacol, Fernasan, Fernide, Thiuram, TMTD

Chemical Name: tetramethylthiuram disulphide; bis(dimethylthiocarbomoyl) disulfide

CAS Registry No: 137-26-8

Uses: fungicide and also as seed disinfectant.

Molecular Formula: $C_6H_{12}N_2S_4$

Molecular Weight: 240.432

Melting Point ($^{\circ}C$):

155.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

129 (20 mmHg, Howard 1991)

310–315 (15 mmHg, Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

1.29 (Spencer 1982; Worthing & Hance 1991; Montgomery 1993; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

256.6 (calculated-Le Bas method at normal boiling point)

186.4 (calculated-density,)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0523 (mp at $155.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

17.4 ($22^{\circ}C$, Spencer 1973, 1982)

30 (Martin & Worthing 1977; Worthing & Walker 1987, Worthing & Hance 1991)

30 (Hartley & Kidd 1987; Montgomery 1993; Milne 1995)

30 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

18 (room temp., Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

negligible (Hartley & Kidd 1987; Worthing & Hance 1991)

0.00133 (Halfon et al. 1996)

< 0.00133 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

0.307 (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

< 0.008 (calculated-P/C, Lyman et al. 1982)

0.0107 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.73 (Tomlin 1994)

Bioconcentration Factor, $\log BCF$:

1.96 (calculated-S, Kenaga 1980)

1.96 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.83 (calculated-S, Kenaga 1980)
- 2.83 (calculated-S, Lyman et al. 1982; quoted, Howard 1991)
- 2.83 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
- 2.82–3.39 (soil, Montgomery 1993)
- 2.83 (estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: assuming an ambient hydroxyl radical concn. of 8.0×10^5 mol/cm³, the photooxidation reaction $t_{1/2} \sim 26.6$ d at 25°C (estimated, GEMS 1986; quoted, Howard 1991).

Hydrolysis: $t_{1/2} = 5.3$ d was estimated based on exptl. rate $k = 5.0 \times 10^{-3}$ h⁻¹ (Ellington et al. 1988; quoted, Howard 1991; Montgomery 1993);

$t_{1/2} = 128$ d at pH 4, $t_{1/2} = 18$ d at pH 7 and $t_{1/2} = 9$ h at pH 9 (Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: assuming an ambient hydroxyl radical concn. of 8.0×10^5 mol/cm³, the photooxidation reaction $t_{1/2} \sim 26.6$ d at 25°C (estimated, GEMS 1986; quoted, Howard 1991).

Surface water: calculated hydrolysis $t_{1/2} = 5.3$ d at pH 7 (Ellington et al. 1988);

hydrolysis $t_{1/2} = 128$ d, $t_{1/2} = 18$ d and $t_{1/2} = 9$ h at pH 4, 7 and 9 (Tomlin 1994).

Groundwater:

Sediment:

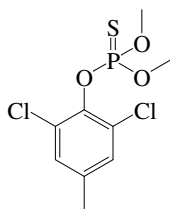
Soil: $t_{1/2} = 15$ d in soil (Halfon et al. 1996);

field $t_{1/2} = 15$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996);

degradation $t_{1/2} = 0.5$ d in sandy soil at pH 6.7 (Tomlin 1994).

Biota:

19.1.36 TOLCLOFOS-METHYL



Common Name: Tolclofos-methyl

Synonym: Risolex, Rizolex, S-3349

Chemical Name: *O*-2,6-dichloro-*p*-tolyl *O*,*O*-dimethyl phosphorothioate; *O*-(2,6-dichloro-4-methylphenyl) *O*,*O*-dimethyl phosphorothioate

CAS Registry No: 57018-04-9

Uses: as fungicide for control of soil-borne diseases caused by *Rhizoctonia*, *Sclerotium* and *Typhula* spp.; also used as a seed, bulb or tuber treatment, soil drench, foliar spray, or by soil incorporation.

Molecular Formula: $C_9H_{11}Cl_2O_3PS$

Molecular Weight: 301.127

Melting Point ($^{\circ}C$):

78–80 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

0.3–0.4 (23 $^{\circ}C$, Hartley & Kidd 1987)

0.3–0.4 (23 $^{\circ}C$, Worthing & Hance 1991)

1.10 (Tomlin 1994)

0.30 (20–25 $^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

0.057 (20 $^{\circ}C$, Hartley & Kidd 1987)

0.057 (20 $^{\circ}C$, Worthing & Hance 1991; Tomlin 1995)

0.0573 (20–25 $^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

5.25×10^{-3} ; 6.61×10^{-3} ; 0.0234 (gradient GC method; estimation using modified Watson method: Sugden's parachor, McGowan's parachor, Tsuzuki 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

57.5 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.56 (Worthing & Hance 1991; Tomlin 1994)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

3.30 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Photolysis: photodegradable with 8 h of sunlight: $t_{1/2} = 44$ d in water, $t_{1/2} = 15\text{--}28$ d in lake and river water, and $t_{1/2} < 2$ d on soil surface (Hartley & Kidd 1987; Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: photodegradable with 8 hours of sunlight in water with $t_{1/2} = 44$ d, $t_{1/2} = 15\text{--}28$ d in lake and river water, and $t_{1/2} < 2$ d on soil surface (Hartley & Kidd 1987);

Photodegradation $t_{1/2} = 44$ d in water, $t_{1/2} = 15\text{--}28$ d in lake (Tomlin 1994).

Groundwater:

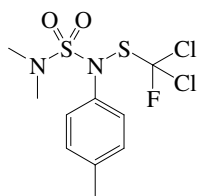
Sediment:

Soil: $t_{1/2} < 2$ d from soil surface by photodegradation (Tomlin 1994);

field $t_{1/2} = 30$ d (20–25°C, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Biota:

19.1.37 TOLYLFLUANID



Common Name: Tolyfluanid

Synonym: Tolyfluanide

Chemical Name: *N*-dichlorofluoromethylthio-*N,N'*-dimethyl-*N*-*p*-tolylsulphamide; 1,1-dichloro-*N*-[(dimethylamino)-sulfonyl]-1-fluoro-*N*-(4-methylphenyl)methane-sulfenamide

Uses: fungicide/acaricide; to control scab on apples and pears; *Botrytis* on strawberries, raspberries, blackberries, currants, grapes, ornamentals, etc.

CAS Registry No: 731-27-1

Molecular Formula: $C_{10}H_{13}Cl_2FN_2O_2S_2$

Molecular Weight: 347.257

Melting Point ($^{\circ}C$):

95–97 (Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

96 (Tomlin 1994)

Boiling Point ($^{\circ}C$): dec. on distillation (Tomlin 1994)

Density (g/cm^3 at $20^{\circ}C$): 1.52 (Tomlin 1994)

Molar Volume (cm^3/mol):

326.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.201 (mp at $96^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

4000 (Martin & Worthing 1977; quoted, Kenaga 1980)

4000 (room temp., Hartley & Kidd 1987; Worthing & Hance 1991)

0.90 (room temp., Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

< 0.001 ($20^{\circ}C$, Hartley & Kidd 1987)

1.3×10^{-5} ($45^{\circ}C$, Worthing & Hance 1991)

1.6×10^{-5} ($20^{\circ}C$, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.95 ($20^{\circ}C$, Worthing & Hance 1991)

3.90 (Tomlin 1994)

3.95 (selected, Hansch et al. 1995)

4.36 (RP-HPLC-RT correlation, Nakamura et al. 2001)

Bioconcentration Factor, $\log BCF$:

0.778 (calculated, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

1.66 (soil, calculated-S, Kenaga 1980)

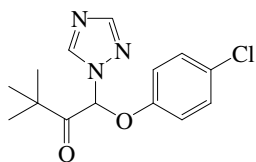
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} = 12$ d at 22°C and pH 4, $t_{1/2} = 29$ h at pH 7 and $t_{1/2} < 10$ min at pH 9 (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: half-life of a few days (Tomlin 1994).

19.1.38 TRIADIMEFON



Common Name: Triadimefon

Synonym: Amiral, Bayleton, MEB 6447, Triadimefone

Chemical Name: 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)butanone; 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1*H*-1,2,4-triazol-1-yl)-2-butanone

CAS Registry No: 43121-43-3

Uses: as fungicide for control of powdery mildews, rusts in cereals and *Rhynchosporium* in cereals and control of bunt, smuts, *Typhula* spp., seedling blight, leaf stripe, net blotch, and other cereal diseases when used for seed treatment, etc.

Molecular Formula: C₁₄H₁₆ClN₃O₂

Molecular Weight: 293.749

Melting Point (°C):

82 (Lide 2003)

Boiling Point (°C):

Density (g/cm³ at 20°C):

1.22 (Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm³/mol):

321 (calculated-Le Bas method at normal boiling point)

240.8 (calculated-density)

Dissociation Constant pK_a:

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.276 (mp at 82°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):

260 (Martin & Worthing 1977)

260 (20°C, Hartley & Kidd 1987; Worthing & Hance 1991; Milne 1995)

71.5 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

71.5 (selected, Lohninger 1994)

64 (20°C, Tomlin 1994)

69; 72 (calculated-group contribution fragmentation method; quoted exptl., Kühne et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated):

< 1.0 × 10⁻⁴ (20°C, Hartley & Kidd 1987; Worthing & Hance 1991)

2.00 × 10⁻⁶ (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)

2.00 × 10⁻⁵, 6.0 × 10⁻⁵ (20, 25°C, Tomlin 1994)

Henry's Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{ow}:

1.80 (shake flask-UV at pH 5, Barak et al. 1983)

3.26 (shake flask, Hansch & Leo 1987)

2.77 (shake flask-LC, Patil et al. 1988)

3.18 (Worthing & Hance 1991; Milne 1995)

2.90 (shake flask at pH 7, Baker et al. 1992)

3.26 (recommended, Sangster 1993)

2.77 (recommended, Hansch et al. 1995)

- 3.03 (Pomona-database, Müller & Kördel 1996)
3.12 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, log BCF:

- 1.43 (calculated, Kenaga 1980)

Sorption Partition Coefficient, log K_{OC} :

- 2.41 (soil, calculated-S, Kenaga 1980)
2.48 (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996)
2.57 (HPLC-screening method, Kördel et al. 1993)
2.48 (estimated-chemical structure, Lohninger 1994)
2.48 (soil, Tomlin 1994)
2.71 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
2.57; 3.72 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1996)
3.19, 2.277, 2.536, 2.39, 2.96 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
2.826, 2.56, 2.512, 2.381, 3.046 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV Gawlik et al. 1999)
2.826, 2.560, 2.512, 2.381, 3.046 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
2.71; 2.43 (soil, quoted obs.; estimated-general model using molecular descriptors, Gramatica et al. 2000)

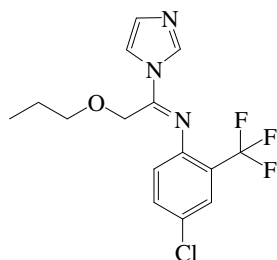
Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: $t_{1/2} > 1$ yr at 22°C and pH 3, 6, and 9 (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: field $t_{1/2} = 26$ d (20–25°C, selected, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.39 TRIFLUMIZOLE



Common Name: Triflumizole

Synonym: NF-114, Triflumizol, Trifmine

Chemical Name: (*E*)-4-chloro- α,α,α -trifluoro-*N*-(1-imidazol-1-yl-2-propoxyethylidene)-*o*-toluidine; 1-[1-[[4-chloro-2-(trifluoromethyl)phenyl]imino]-2-propoxyethyl]-1*H*-imidazole

CAS Registry No: 68694-11-1

Uses: as fungicide for control of powdery mildews in fruit, vines, and vegetables; scab and rust in apples and pears; also used as seed treatment for barley, etc.

Molecular Formula: $C_{15}H_{15}ClF_3N_3O$

Molecular Weight: 345.574

Melting Point ($^{\circ}C$):

63.5 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

359.5 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

3.70 (Augustijn-Beckers et al. 1994; Tomlin 1994; Hornsby et al. 1996)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.419 (mp at $63.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

12500 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995)

12500 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.40×10^{-6} (Worthing & Hance 1991)

1.47×10^{-6} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1992; Hornsby et al. 1996)

1.86×10^{-4} (Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

4.07×10^{-8} (20 – $25^{\circ}C$, calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.40 (Worthing & Hance 1991; Milne 1995; Tomlin 1994)

1.40 (selected, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

3.03–3.22 (Tomlin 1994)

1.60 (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

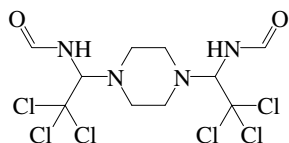
Photolysis: aqueous solutions degraded by sunlight with $t_{1/2} = 29$ h (Worthing & Hance 1991; Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} = 14$ d on clay (Worthing & Hance 1991);

field $t_{1/2} = 14$ d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

19.1.40 TRIFORINE



Common Name: Triforine

Synonym: Biformychloazin, Cela W524, Compound W, Denarin, FMC, Funginex, Saprol, W 524

Chemical Name: 1,1'-piperazine-1,4-diyl-di-[N-(2,2,2-trichloroethyl)formamide]; 1,4-bis(2,2,2-trichloro-1-formamidoethyl)piperazine; *N,N'*-[1,4-piperazinediylbis(2,2,2-trichloro-ethylidene)]bisformamide

Uses: systemic fungicide to control powdery mildews on cereals, fruit, vines, hops, cucurbits, vegetables, and ornamentals, etc.; also used to suppress spider mite activity.

CAS Registry No: 26644-46-2

Molecular Formula: $C_{10}H_{14}Cl_6N_4O_2$

Molecular Weight: 434.962

Melting Point ($^{\circ}C$):

155 (dec., Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$): 1.554 (Tomlin 1994)

Molar Volume (cm^3/mol):

389.2 (calculated-Le Bas method at normal boiling point)

279.9 (calculated-density)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.053 (mp at $155^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

30 (rm. temp., Hartley & Kidd 1987; Worthing & Hance 1991)

6.0 (rm. temp., Worthing & Hance 1991; Milne 1995)

30 ($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

30 (selected, Lohninger 1994)

9.0 ($20^{\circ}C$, Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

2.6×10^{-5} (Hartley & Kidd 1987)

2.7×10^{-5} (Worthing & Hance 1991; Tomlin 1994)

2.7×10^{-5} ($20-25^{\circ}C$, selected, Wauchope et al. 1992; Hornsby et al. 1996)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.20 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

2.73 ($20-25^{\circ}C$, estimated, Wauchope et al. 1992; Hornsby et al. 1996)

2.30 (estimated-chemical structure, Lohninger 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

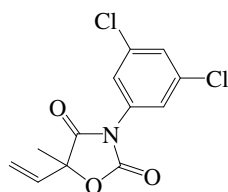
Hydrolysis: $t_{1/2} = 3.5$ d at pH 5, $25^{\circ}C$ in aqueous solutions (Tomlin 1994).

Half-Lives in the Environment:

Soil: $t_{1/2} \sim 3$ wk in soil (Hartley & Kidd 1987; Tomlin 1994);

field $t_{1/2} = 21$ d ($20-25^{\circ}C$, estimated, Wauchope et al. 1992; Hornsby et al. 1996).

19.1.41 VINCLOZOLIN



Common Name: Vinclozolin

Synonym: BAS 352F, Ronilan, Vorlan

Chemical Name: (*RS*)-3-(3,5-dichlorophenyl)-5-vinyl-1,3-oxazolidine-2,4-dione; 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione

CAS Registry No: 50471-44-8

Uses: fungicide to control *Botrytis/Sclerotinia* spp. in vines, oilseed rape, vegetables, fruit, and ornamentals, etc.

Molecular Formula: $C_{12}H_9Cl_2NO_3$

Molecular Weight: 286.110

Melting Point ($^{\circ}C$):

108 (Hartley & Kidd 1987; Worthing & Hance 1991; Tomlin 1994; Milne 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

131 (at 0.05 mmHg, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Density (g/cm^3 at $20^{\circ}C$):

1.51 (Worthing & Hance 1991; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

266.3 (calculated-Le Bas method at normal boiling point, this work)

189.5 (calculated-density, this work)

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.153 (mp at $108^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

1000 (Martin & Worthing 1977)

1000 ($20^{\circ}C$, Hartley & Kidd 1987)

3.40 ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

1000 (20 – $25^{\circ}C$, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

< 0.010 ($20^{\circ}C$, Hartley & Kidd 1987)

1.6×10^{-5} ($20^{\circ}C$, Worthing & Hance 1991; Tomlin 1994)

1.6×10^{-5} (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

1.3×10^{-4} ($20^{\circ}C$, Siebers et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated):

0.011 ($20^{\circ}C$, quoted, Siebers et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.00 (Stevens et al. 1988)

3.00 (pH 7, Worthing & Hance 1991; Tomlin 1994; Milne 1995)

2.47 (shake flask-HPLC at pH 6, Nielsen et al. 1992)

3.00, 2.47 (Sangster 1993)

3.10 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.26 (calculated, Kenaga 1980)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.99 (soil, calculated-S, Kenaga 1980)
- 2.0–2.87 (soil, Tomlin 1994)
- 2.0 (soil, 20–25°C, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: when irradiation with UV light, $\lambda \geq 290$ nm, for vinclozolin aqueous solution (1 ppm): 10% and 11% photodegraded in 1 h, in the presence of 1 ppm humic acid and 1 ppm fulvic acid, respectively; irradiation of vinclozolin (2 ppm) in water with $t_{1/2} = 7$ min and 92 min in the presence of TiO_2 (20 ppm), and Fe_2O_3 (100 ppm), respectively. (Hustert & Moza 1997)

Oxidation:

Hydrolysis: stable in neutral and weakly acidic media, in 0.1 N NaOH, 50% hydrolysis occurs in 3.8 h (Hartley & Kidd 1987; Tomlin 1994).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: photodegradation of vinclozolin aqueous solution (2 ppm), $t_{1/2} = 7$ min and 92 min in the presence of TiO_2 (20 ppm), and Fe_2O_3 (100 ppm), respectively, when irradiated with UV light (Hustert & Moza 1997)

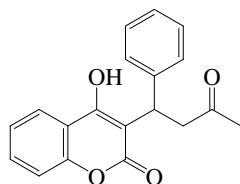
Groundwater:

Sediment:

Soil: field $t_{1/2} = 20$ d (20–25°C, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota:

19.1.42 WARFARIN



Common Name: Warfarin

Synonym: Coumafen, Zoocoumarin

Chemical Name: 3-(α -acetonylbenzyl)-4-hydroxycoumarin

CAS Registry No: 81-81-2

Use: rodenticide

Molecular Formula: $C_{19}H_{16}O_4$

Molecular Weight: 308.328

Melting Point ($^{\circ}C$):

161 (Lide 2003)

Boiling Point ($^{\circ}C$): dec. (Montgomery 1993)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.0463 (mp at $161^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

40 (shake flask, Coon et al. 1954)

17 ($20^{\circ}C$, Hartley & Kidd 1987; Worthing & Walker 1987)

17 ($20^{\circ}C$, Montgomery 1993; Tomlin 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

1.55×10^{-4} ($21.5^{\circ}C$, Hartley & Kidd 1987)

9.0 ($21.5^{\circ}C$, Worthing & Walker 1987; Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.86×10^{-4} (calculated-P/C, Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.52 (at pH 3, Howard 1991)

3.20 (calculated, Montgomery 1993)

3.12 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.68 (calculated, Howard 1991)

Sorption Partition Coefficient, $\log K_{oc}$:

2.75 (estimated, Howard 1991)

2.96 (calculated, Montgomery 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: Photooxidation $t_{1/2} = 0.254\text{--}1.87$ h was estimated based on rate constants for reaction with hydroxyl radicals and ozone in air (Howard et al. 1991).

Hydrolysis: very slow with a $t_{1/2} = 16$ yr at pH 7; the chemical hydrolysis rate constants, $k = 1.4 \times 10^{-4} \text{ M}^{-1} \text{ h}^{-1}$ for acid, neutral- $k = 4.9 \times 10^{-6} \text{ M}^{-1} \text{ h}^{-1}$ and $k = 0.026 \text{ M}^{-1} \text{ h}^{-1}$ for base (Ellington et al. 1988; quoted, Howard 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 168\text{--}672$ h, anaerobic $t_{1/2} = 672\text{--}2688$ h were estimated based on aqueous aerobic biodegradation (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 11.6$ min due to reaction with photochemically produced hydroxyl radicals and ozone in the vapor phase (Howard 1991);

$t_{1/2} = 0.254\text{--}1.87$ h based on estimated photooxidation in air (Howard et al. 1991).

Surface water: $t_{1/2} = 168\text{--}672$ h based on estimated unacclimated aqueous aerobic biodegradation (Howard et al. 1991);

slow hydrolysis $t_{1/2} = 15$ yr at pH 7 (Howard 1991).

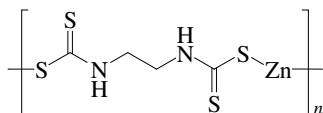
Groundwater: $t_{1/2} = 336\text{--}1344$ h based on estimated aqueous aerobic biodegradation (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672$ h based on estimated unacclimated aqueous aerobic biodegradation (Howard et al. 1991).

Biota:

19.1.43 ZINEB



Common Name: Zineb

Synonym: Dithane Z-78, Parzate Zineb, Lonaol, Aspor

Chemical Name: zinc ethylene-1,2-bisdithiocarbamate

CAS Registry No: 12122-67-7

Uses: fungicide

Molecular Formula: $(\text{C}_4\text{H}_6\text{N}_2\text{S}_4\text{Zn})_x$

Molecular Weight: $(275.773)_x$

Melting Point ($^{\circ}\text{C}$):

decomposes without melting (Worthing & Walker 1983)

157 (dec., Tomlin 1994; Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

Density (g/cm^3 at 20°C):

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 0.0507 (mp at 157°C)

Water Solubility (g/m^3 or mg/L at 25°C or as indicated):

1 (Melnikov 1971)

10 (Spencer 1982)

≈ 10 (Worthing & Walker 1983, 1987; quoted, Howard 1991)

10 (room temp., Tomlin 1994)

10 (20 – 25°C , selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated):

negligible at rm. temp. (Worthing & Walker 1983)

1.07×10^{-5} (20°C , quoted, Howard 1991)

$< 1 \times 10^{-5}$ (20°C , Hartley & Kidd 1987; Tomlin 1994)

1.0×10^{-5} (10 – 25°C , estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

≤ 1.30 (Tomlin 1994)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

2.11, 2.23, < 1.0 , (activated sludge, algae, Golden ide, Freitag et al. 1985)

2.28 (calculated-S, Kenaga 1980b; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.08 (soil, calculated-S, Kenaga 1980b; quoted, Howard 1991)

3.0 (soil, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Photolysis: unstable to light, moisture and heat on prolonged storage (Tomlin 1994).

Half-Lives in the Environment:

Air: $t_{1/2}$ = 11–14 d in greenhouse experiment, microagroecosystem chambers (Nash & Beall 1980);
 $t_{1/2}$ = 11–14 d by gravitational settling and degradation (Howard 1991).

Surface water:

Groundwater:

Sediment:

Soil: $t_{1/2}$ = 23 d in 1-cm surface soil (sandy loam with pH 6.7), greenhouse experiment in microagroecosystem chambers (Nash & Beall 1980);

$t_{1/2}$ = 16–23 d upper layer of soil (Howard 1991);

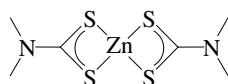
field $t_{1/2}$ ~ 30 d (estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996).

Biota: $t_{1/2}$ = 14 d on tomato leaves, green house experiment, microagroecosystem chambers (Nash & Beall 1980);

$t_{1/2}$ = 7 d for tomato fruit in the field, $t_{1/2}$ = 3.4 d for soybean leaves and $t_{1/2}$ = 9 d for tomatoes (Nash 1983);

$t_{1/2}$ = 14 d for tomato leaves, $t_{1/2}$ = 7 d for tomatoes, $t_{1/2}$ = 11 d for lettuce and $t_{1/2}$ = 35 d for grapes (Howard 1991).

19.1.44 ZIRAM



Common Name: Ziram

Synonym: Aaprotect, Fuklasin, Zerlate, zirmane

Chemical Name: zinc bis(dimethyldithiocarbamate)

CAS Registry No: 137-30-4

Uses: fungicide, bird and rodent repellent

Molecular Formula: $C_6H_{12}N_2S_4Zn$

Molecular Weight: 305.841

Melting Point ($^{\circ}C$):

250 (Howard 1991; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

2.00 (Spencer 1982)

1.66 ($25^{\circ}C$, Hartley & Kidd 1987; Tomlin 1994; Milne 1995)

Molar Volume (cm^3/mol):

Dissociation Constant pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0062 (mp at $250^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

65 (Melnikov 1971)

65 (Martin & Worthing 1977; Worthing & Walker 1983, 1987)

4.0 ($20^{\circ}C$, Spencer 1982)

65 (Hartley & Kidd 1987)

0.03 ($20^{\circ}C$, Tomlin 1994)

65 (20 – $25^{\circ}C$, selected, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

65 (Milne 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

negligible (Worthing & Walker 1983, 1987; quoted, Howard 1991)

1.33×10^{-5} (20 – $25^{\circ}C$, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

$< 1 \times 10^{-6}$ (extrapolated, Tomlin 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.086 (Tomlin 1994)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.77 (calculated-S, Kenaga 1980b; quoted, Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

2.64 (soil, calculated-solubility, Kenaga 1980b; quoted, Howard 1991)

2.60 (soil, estimated, Augustijn-Beckers et al. 1994; Hornsby et al. 1996)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Hydrolysis: decomposed in acidic media (Tomlin 1994).

Half-Lives in the Environment:

Air:

Surface water: decomposed in acidic media, and by UV irradiation (Tomlin 1994).

Groundwater:

Sediment:

Soil: field $t_{1/2} \sim 30$ d (estimated, Augustijn-Beckers et al. 1992; Hornsby et al. 1996).

Biota: for orally administered to rate was mostly eliminated within 1–2 d (Tomlin 1994).

19.2 SUMMARY TABLES

TABLE 19.2.1

Common names, chemical names and physical properties of fungicides

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK _a
Anilazine [101-05-3]	Botrysan, Direz, Dyren	2-chloro- <i>N</i> -(4,6-dichloro-1,3,5-triazin-2-yl)aniline	C ₉ H ₅ Cl ₃ N ₄	275.522	160	0.0474	
Benalaxyl [71626-11-4]	Galben	methyl <i>N</i> -phenylacetyl- <i>N</i> -2,6-xylyl- <i>DL</i> -alaninate	C ₂₀ H ₂₃ NO ₃	325.402	79	0.295	
Benodanil [15310-01-8]	Calirux	2-iodo- <i>N</i> -phenylbenzamide	C ₁₃ H ₁₀ INO	323.129	137	0.0796	
Benomyl [17804-35-2]	Benlate	methyl 1-(butylcarbamoyl)benzimidazol-2-ylcarbamate	C ₁₄ H ₁₈ N ₄ O ₃	290.318	140	0.0744	
Bitertanol [70585-36-3]	Baycor, Baymat, Biloxa, Siibutol	1-(biphenyl-4-yloxy)-3,3-dimethyl-1- <i>H</i> -1,2,4-triazol-1-yl)butan-2-ol	C ₂₀ H ₂₃ N ₃ O ₂	337.415	118 eutectic	0.122	
diastereoisomer A [70585-38-5]			337.415	136.7	0.0802		
diastereoisomer B [55179-31-2]			337.415	145.2	0.0662		
Bupirimate [41483-43-6]	Nimrod, Nimrod T	5-butyl-2-ethylamino-6-methyl-pyrimidinyl dimethylsulfamate	C ₁₃ H ₂₄ N ₄ O ₃ S	316.419	50–51	0.562	
Captan [133-06-2]	Aacaptan, Amercide, Captab, orthocide	<i>N</i> -trichloromethylthio-4-cyclohexene-1,2-dicarboximide	C ₉ H ₈ Cl ₃ NO ₂ S	300.590	172.5	0.0357	
Carbendazim [10605-21-7]	Bavistin, BCM, Carbendazol	carbamic acid, methyl-1 <i>H</i> -benzimidazol-2-yl	C ₉ H ₉ N ₃ O ₂	191.186	300 dec	0.0020	4.48 4.2
Carboxin [5234-68-4]	Vitavax, carbathiin	5,6-dihydro-2-methy-1,4-oxathi-ine-3-carboxanilide	C ₁₂ H ₁₃ NO ₂ S	235.302	94	0.210	
Chloroneb [2675-77-6]	Tersan SP	1,4-dichloro-2,5-dimethoxybenzene	C ₈ H ₈ Cl ₂ O ₂	207.055	134	0.0852	
Chloropicrin [76-06-2]	Nitrochloroform	trichloronitromethane	CCl ₃ NO ₂	164.376	–64	1	
Chlorothalonil [1897-45-6]	Bravo, Daconil	2,4,6-tetrachloro-1,3-benzene-dicarbonitrile	C ₈ Cl ₄ N ₂	265.911	250	0.0062	
Dazomet (Fum.) [533-74-4]	Salvo, Mylone, Basamid	3,5-dimethyl-1,3,5-thiadiazinane-2-thione	C ₅ H ₁₀ N ₂ S ₂	162.276	106	0.16	
Dichlofluanid [1085-98-9]	Euaren, Elvaron	<i>N</i> -dichlorofluoromethylthio- <i>N,N'</i> -dimethyl- <i>N</i> -phenylsuphamide	C ₉ H ₁₁ Cl ₂ FN ₂ O ₂ S ₂	333.229	105.3	0.163	
Dichlone [117-80-6]	Phygon	2,3-dichloro-1,4-naphthoquinone	C ₁₀ H ₄ Cl ₂ O ₂	227.044	195	0.0215	
Dicofol [115-32-2]	Kelthan	2,2,2-trichloro-1,1-bis(4-chlorophenyl)ethanol	C ₁₄ H ₉ Cl ₅ O	370.485	77.5	0.305	
Dithianon [3347-22-6]	Delan	5,10-dihydro-5,10-dioxonaphtho[2,3- <i>b</i>]-1,4-dithi-in-2,3-dicarbonitrile	C ₁₃ H ₄ N ₂ O ₂ S ₂	296.324	220	0.0122	

Edifenphos [17109-49-8]	EDDP, Hinosan	<i>O</i> -ethyl <i>S,S</i> -diphenyl-phosphoradithioate	C ₁₄ H ₁₅ O ₂ PS ₂	310.371	–25	1	
Ethirimol [23947-60-6]		5-butyl-2-ethylamino-6-methyl-pyrimidin-4-ol	C ₁₁ H ₁₉ N ₃ O	209.288	160	0.0474	
Etridiazole [2593-15-9]	ethazol, ethazole, Terazole	ethyl 3-trichloromethyl-1,2,4-thiadiazolyl ether	C ₅ H ₅ Cl ₃ N ₂ OS	247.530	19.9	1	2.27
Fenarimol [60168-88-9]	Bloc, Rimidin, Rubigan	(±)-2,4-dichloro- α -(pyrimidin-5-yl) benzhydryl alcohol	C ₁₇ H ₁₂ Cl ₂ N ₂ O	331.195	118	0.122	
Fenfuram [24691-80-3]	fenfurame	2-methyl-3-fruanilide	C ₁₂ H ₁₁ NO ₂	201.221	109–110	0.148	
Fenpropimorph [67564-91-4]	Corbel, Mistral	(±)- <i>cis</i> -4-[3-(4- <i>tert</i> -butylphenyl)-2-methylpropyl]-2,6-dimethylmorpholine	C ₂₀ H ₃₃ NO	303.482	oil	1	6.98
Folpet [133-07-3]	Foltan, Folpan, Felpel, Spolacid	<i>N</i> -(trichloromethylthio)phthalimide	C ₉ H ₄ Cl ₃ NO ₂ S	296.558	177	0.0323	
Formaldehyde [50–00–0]	Formalin, methanal	formaldehyde	HCHO	30.026	–92	1	
Furalaxyl [57646-30-7]	Fongarid	methyl <i>N</i> -(2-furoyl)- <i>N</i> -(2,6-xylyl)- <i>DL</i> -alaninate	C ₁₇ H ₁₉ NO ₄	301.337	70	0.362	
Hexachlorobenzene [118–74–1]	HCB	hexachlorobenzene	C ₆ Cl ₆	284.782	228.83	0.010	
Imazalil [35554-44-0]	Bromazil, Deccozil	(±)-1-(β -allyloxy-2,4-dichlorophenyl-ethyl)imidazole	C ₁₄ H ₁₄ Cl ₂ N ₂ O	297.179	50	0.568	
Iprobenfos [26087-47-8]	Kitazin	<i>S</i> -benzy <i>O,O</i> -di-isopropyl phosphoro-thioate	C ₁₃ H ₂₁ O ₃ PS	288.342	oil	1	
Mancozeb [8018–01–7]	Dithane ultra, Dithane M45				192–194 dec		
Maneb [12427–38–2]	MEB, Dithane, Bravo	manganese ethylenebis(dithiocarbamate)	(C ₄ H ₆ MnN ₂ S ₄) _x	(265.302) _x	dec 200		
Metalaxyl [57837-19-1]	Ridomil, Apron Fubol	methyl <i>N</i> -(2-methoxyacetyl)-2,6-xylyl)- <i>DL</i> -alaninate	C ₁₅ H ₂₁ NO ₄	279.333	71	0.354	<< 0
Metiram [9006-42-4]	Carbatene, Polyram	zinc ammoniate ethylenebis(dithio-carbamate-poly(ethylenethiurmdisulfide)					
Nitrapyrin [1929–82–4]	N-Serve	2-chloro-6-(trichloromethyl)pyridine	C ₆ H ₃ Cl ₃ N	230.907	63	0.424	
Oxycarboxin [5259-88-1]	Plantvax	5,6-dihydro-2-methyl-1,4-oxathi-ine-3- carboxanilide 4,4-dioxide	C ₁₂ H ₁₃ NO ₄ S	267.301	129	0.0954	
Penconazole [66246-88-6]	Topas, Topaz, Topaze	1-(2,4-dichloro- β -propylphenyl-ethyl)-1 <i>H</i> -1,2,4-triazole	C ₁₃ H ₁₅ Cl ₂ N ₃	284.184	60	0.454	1.51
Procymidone [32809-16-8]	Sumisclex, Sumilex	<i>N</i> -(3,5-dichlorophenyl)-1,2-dimethyl-cyclopropane-1,2-dicarboximide	C ₁₃ H ₁₁ Cl ₂ NO ₂	284.138	166	0.0414	
Propargite [2312–35–8]	Comite, Omite	2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl sulfite	C ₁₆ H ₂₆ O ₄ S	360.472	liquid	1	
Propiconazole [60207-90-1]		(±)-1-[2,4-(dichlorophenyl)-4-propyl-1,3-dioxolan-2-methyl]-	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	342.221	liquid	1	1.09

(Continued)

TABLE 19.2.1 (Continued)

Name	Synonym	Chemical name	Molecular formula	Molecular weight, MW g/mol	m.p. °C	Fugacity ratio, F at 25°C*	pK _a
Quintozene [82-68-8]	Tritisan, Botrilex, Terrachlor	pentachloronitrobenzene	C ₆ Cl ₅ NO ₂	295.335	144	0.0680	
Tecnazene [117-18-0]	Folosan, Fusarex	1,2,4,5-tetrachloro-3-nitrobenzene	C ₆ HCl ₄ NO ₂	260.890	99.5	0.186	
Thiabendazole [148-79-8]	Mertect, Storite	2-(thiazol-4-yl)benzimidazole	C ₁₀ H ₇ N ₃ S	201.248	304–305	0.00181	
Thiophanate-methyl [23564-05-8]	Topsin M, Mildothane	dimethyl 4,4'-(<i>o</i> -phenylene)bis(3-thioallphanate)	C ₁₂ H ₁₄ N ₄ O ₄ S ₂	342.394	172 dec	0.0361	7.28
Thiram [137-26-8]	Arasan, Tersan, Fernasan	tetramethylthiuram disulphide	C ₆ H ₁₂ N ₂ S ₄	240.432	155.6	0.0523	
Tolclofos-methyl [57018-04-9]	Rizolex	<i>O</i> -2,6-dichloro- <i>p</i> -tolyl <i>O,O</i> -dimethyl phosphorothioate	C ₉ H ₁₁ Cl ₂ O ₃ PS	301.127	78-80	0.295	
Tolylfluanid [731-27-1]	Euparen M	<i>N</i> -dichlorofluoromethylthio- <i>N,N'</i> -dimethyl- <i>N-p</i> -tolysulphamide	C ₁₀ H ₁₃ Cl ₂ FN ₂ O ₂ S ₂	347.257	96	0.201	
Triadimefon [43121-43-3]	Amiral, Bayeton	1-(<i>o</i> -chlorophenoxy)-3,3-dimethyl-1- <i>H</i> -1,2,4-triazol-1-yl)butanone	C ₁₄ H ₁₆ ClN ₃ O ₂	293.749	82	0.276	
Triadimenol [55219-65-3]	Baytan	1-(4-chlorophenoxy)-3,3-dimethyl-1-(1- <i>H</i> -1,2,4-triazol-1-yl)butan-2-ol	C ₁₄ H ₁₈ ClN ₃ O ₂	295.764	121–127		
Tricyclazole [41814-78-2]	Beam, Bim, Blascide	5-methyl-1,2,4-triazolo[3,4- <i>b</i>]-benzothiazole	C ₉ H ₇ N ₃ S	189.237	187	0.0257	
Triflumizole [99387–89–0]	Trifmine	(<i>E</i>)-4-chloro- α,α,α -trifluoro- <i>N</i> -(1-imidazol-1-yl-propoxyethylidene)- <i>o</i> -toluidine	C ₁₅ H ₁₅ ClF ₃ N ₃ O	345.747	63.5	0.419	3.70
Triforine [26644-46-2]		1,4-bis(2,2,2-trichloro-1-formamido-ethyl) piperazine	C ₁₀ H ₁₄ Cl ₆ N ₄ O ₂	434.962	155 dec	0.0530	
Vinclozolin [50471-44-8]	Ronilan	(<i>RS</i>)-3-(3,5-dichlorophenyl)-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione	C ₁₂ H ₉ Cl ₂ NO ₃	286.110	108	0.153	
Warfarin (R.) [81-81-2]	Coumarin Dethmor	4-hydroxy-3-(3- <i>oxo</i> -1-phenylbutyl)-2 <i>H</i> -1-benzopyran-2-one	C ₁₉ H ₁₆ O ₄	308.328	161	0.0463	
Zineb [12122-67-7]	Zinebe	zine ethylenebis(dithiocarbamate)	C ₄ H ₆ N ₂ S ₄ Zn	275.773	157 dec	0.0507	
Ziram [137-30-4]	Zirame	zinc bis(dimethyldithiocarbamate)	C ₆ H ₁₂ N ₂ S ₄ Zn	305.841	250	0.0062	

Note: Fum.—fumigant, I—insecticide, R.—rodenticide

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$

TABLE 19.2.2
Summary of selected physical-chemical properties of fungicides at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol) calcd P/C	log K _{OC} reported
	Vapor pressure		Solubility			log K _{OW}		
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)			
Anilazine	8.20 × 10 ⁻⁷	1.77 × 10 ⁻⁵	8	0.0290	0.628	3.80	2.82 × 10 ⁻⁵	3.0
Benalaxyl	0.00133	4.65 × 10 ⁻³	37	0.1137	0.398	3.40	0.012	3.44–3.86
Benodanil	1.00 × 10 ⁻⁸	1.28 × 10 ⁻⁷	2	0.0062	0.0793		1.62 × 10 ⁻⁶	2.85
Benomyl	1.33 × 10 ^{-8*}	1.82 × 10 ⁻⁷	2.0*	0.0069	0.0945	2.30	1.93 × 10 ⁻⁶	3.28
Bitertanol	1.00 × 10 ⁻⁶	8.31 × 10 ⁻⁶	5	0.0118	0.0984		8.45 × 10 ⁻⁵	
diastereoisomer A	2.20 × 10 ⁻⁹	2.80 × 10 ⁻⁸	2.9	0.0069	0.0874	4.10	3.20 × 10 ⁻⁷	
diastereoisomer B	2.50 × 10 ⁻⁹	3.86 × 10 ⁻⁸	1.6	0.0038	0.0585	4.40	6.60 × 10 ⁻⁷	
Buprimate	0.00067	1.21 × 10 ⁻³	22	0.0695	0.126	3.90	9.64 × 10 ⁻³	2.9
Captan	1.10 × 10 ⁻⁵	4.23 × 10 ⁻⁴	5.1	0.0170	0.653	2.30	6.48 × 10 ⁻⁴	2.29
Carbendazim	6.50 × 10 ⁻⁸	3.82 × 10 ⁻⁵	8	0.0418	24.60	1.52	1.55 × 10 ⁻⁶	2.35
Carboxin	1.30 × 10 ⁻⁵	5.98 × 10 ⁻⁵	195	0.829	3.811	2.17	1.57 × 10 ⁻⁵	2.41
Chloroneb	0.40	4.788	8	0.0386	0.462		173.8	3.06
Chloropicrin (I,Fum.)	2400	2400	2270	13.81	13.81	2.07	197.3	1.79
Chlorothalonil	0.133*	22.86	0.6	0.0023	0.388	2.64	58.94	3.2
Dazomet (Fum.)	4.0 × 10 ⁻⁴	2.47 × 10 ⁻³	3000	18.48	114.3	0.15	2.16 × 10 ⁻⁵	0.48
Dichlofluanid	2.10 × 10 ⁻⁵	1.32 × 10 ⁻⁴	1.3	0.0039	0.0245	3.70	5.38 × 10 ⁻³	
Dithianon	6.60 × 10 ⁻⁵	6.28 × 10 ⁻⁴	0.5	0.0017	0.1605	3.20	0.0391	
Edifenphos	0.013	0.013	56	0.180	0.180	3.48	0.072	
Ethirimol	2.67 × 10 ⁻⁴	5.78 × 10 ⁻³	200	0.956	20.68	2.3	2.79 × 10 ⁻⁴	
Etridiazole	0.013	0.013	50	0.202	0.202	3.37	0.0644	
Fenarimol	2.93 × 10 ⁻⁵	2.44 × 10 ⁻⁴	14	0.0423	0.351	3.69	6.93 × 10 ⁻⁴	2.78
Fenfuram	2.0 × 10 ⁻⁵	1.39 × 10 ⁻⁴	100	0.497	3.444		4.02 × 10 ⁻⁵	2.48
Fenpropimorph	0.0023	2.30 × 10 ⁻³	4.3	0.0142	0.014		0.162	2.94–3.65
Folpet	0.0013	0.0414	1	0.0034	0.107	3.63	0.386	3.27
Formaldehyde	> 1 atm		miscible			0.35		
Furalaxyl			230	0.763	2.127	2.61		
Imazalil	9.30 × 10 ⁻⁶	1.75 × 10 ⁻⁵	1400	4.71	8.853	3.82	1.97 × 10 ⁻⁶	3.60
Metalaxyl	7.47 × 10 ⁻⁴	2.18 × 10 ⁻³	8400	30.08	87.71	1.75	2.48 × 10 ⁻⁵	1.7
Metiram	< 0.00001		0.1			0.30		5.7
Oxycarboxin	0.00133	0.0139	1000	3.741	39.06	0.74	3.56 × 10 ⁻⁴	1.98
Penconazole	0.00021	4.66 × 10 ⁻⁴	73	0.257	0.570	3.72	8.18 × 10 ⁻⁴	2.62

(Continued)

TABLE 19.2.2 (Continued)

Compound	Selected properties						Henry's law constant H/(Pa·m ³ /mol) calcd P/C	log K _{OC} reported
	Vapor pressure		Solubility			log K _{OW}		
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)			
Procymidone	0.0187	0.4534	4.5	0.0158	0.384	3.14	1.181	3.18
Propiconazole	5.60 × 10 ⁻⁵	5.60 × 10 ⁻⁵	110	0.321	0.321	3.72	1.74 × 10 ⁻⁴	2.82
Quintozene	0.0066	0.104	0.44	0.0015	0.023	4.64	4.430	4.3, 3.38
Tecnazene			0.44	0.0017	0.0091			
Thiabendazole	5.33 × 10 ⁻⁷	3.13 × 10 ⁻⁴	50	0.249	146.1	2.69	2.14 × 10 ⁻⁶	3.4
Thiophanate-methyl	1.30 × 10 ⁻⁵	3.70 × 10 ⁻⁴	3.5	0.0102	0.291	1.50	1.27 × 10 ⁻³	3.26
Thiram	0.00133	0.0209	30	0.125	1.963	1.73	0.0107	2.83
Tolclofos-methyl	0.0573	0.196	0.3	0.001	0.0034	4.56	57.51	3.3
Tolylfluanid	1.6 × 10 ⁻⁵	8.06 × 10 ⁻⁵	0.9	0.0026	0.0131	3.90	6.17 × 10 ⁻³	1.66
Triadimefon	2.0 × 10 ⁻⁶	7.37 × 10 ⁻⁶	71.5	0.243	0.897	3.26	8.22 × 10 ⁻⁶	
Triadimenol	4.13 × 10 ⁻⁸	4.03 × 10 ⁻⁷	47	0.159	1.549	3.08	2.60 × 10 ⁻⁷	3.00
diastereoisomer A	< 0.001		62	0.210	2.761	3.08		
diastereoisomer B	4.10 × 10 ⁻⁸	4.85 × 10 ⁻⁷	32	0.108	1.280	3.28		
Tricyclazole	2.67 × 10 ⁻⁵	1.09 × 10 ⁻³	1600	8.46	346.2	1.40	3.16 × 10 ⁻⁶	3.00
Triflumizole	1.47 × 10 ⁻⁶	3.53 × 10 ⁻⁶	12500	36.16	86.90		4.07 × 10 ⁻⁸	
Triforine	2.67 × 10 ⁻⁵	5.16 × 10 ⁻⁴	30	0.069	1.332	2.20	3.87 × 10 ⁻⁴	2.3
Vinclozolin	1.33 × 10 ⁻⁵	8.81 × 10 ⁻⁵	1000	3.495	23.14	3.00	3.81 × 10 ⁻⁶	2.6
Warfarin (R.)	1.55 × 10 ⁻⁴	3.43 × 10 ⁻³	17	0.0551	1.221	3.20	2.81 × 10 ⁻³	2.96
Zineb	1.33 × 10 ⁻⁵		10	0.0363		1.30	3.67 × 10 ⁻⁴	3.00
Ziram	1.0 × 10 ⁻⁶	1.53 × 10 ⁻⁴	65	0.213	32.61	1.086	4.70 × 10 ⁻⁶	2.60

Note: * The reported values for this quantity vary considerably, whereas this selected value represents the best judgment of the authors. The reader is cautioned that it may be subject to a large error.

TABLE 19.2.3**Suggested half-life classes of fungicides in various environmental compartments at 25°C**

Compound	Air class	Water class	Soil class	Sediment class
Benomyl	1	4	6	7
Captan	2	2	5	5
Chloropicrin	4	3	3	4
Chlorothalonil	4	4	5	6
Thiram	4	4	5	6

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	55000 (~ 6 years)	> 30,000

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Appendix 1

1.1 LIST OF SYMBOLS AND ABBREVIATIONS

A_i	area of phase i, m ²
ALPM	automated log-P measurement
AS	absorption spectrophotometry
BCF	bioconcentration factor
bp	boiling point, °C
C	molar concentration, mol/L or mmol/m ³
C ^S	saturated aqueous concentration, mol/L or mmol/m ³
C _L	liquid or supercooled liquid concentration, mol/L or mmol/m ³
C _S	solid molar concentration, mol/L or mmol/m ³
C _A	concentration in air phase, mol/L or mmol/m ³
C _W	concentration in water phase, mol/L or mmol/m ³
¹⁴ C	radioactive labelled carbon-14 compound
CC	countercurrent chromatography
COD	chemical oxygen demand
CPC	centrifugal partition chromatography
D	D values, mol/Pa·h
D _A	D values for advection, mol/Pa·h
D _{Ai}	D values for advective loss in phase i, mol/Pa·h
D _R	D value for reaction, mol/Pa·h
D _{Ri}	D value for reaction loss in phase i, mol/Pa·h
D _{ij}	intermedia D values, mol/Pa·h
D _{VW}	intermedia D value for air-water diffusion (absorption), mol/Pa·h
D _{RW}	intermedia D value for air-water dissolution, mol/Pa·h
D _{QW}	D value for total particle transport (dry and wet), mol/Pa·h
D _{RS}	D value for rain dissolution (air-soil), mol/Pa·h
D _{QS}	D value for wet and dry deposition (air-soil), mol/Pa·h
D _{VS}	D value for total soil-air transport, mol/Pa·h
D _S	D value for air-soil boundary layer diffusion, mol/Pa·h
D _{SW}	D value for water transport in soil, mol/Pa·h
D _{SA}	D value for air transport in soil, mol/Pa·h
D _{Ti}	total transport D value in bulk phase i, mol/Pa·h
DOC	dissolved organic carbon
DOM	dissolved organic matter
DSC	differential scanning calorimetry
DTA	differential thermal analyzer
E	emission rate, mol/h or kg/h
EPICS	equilibrium partitioning in closed system
F	fugacity ratio
f	fugacity, Pa
f _i	fugacity in pure phase i, Pa
f-const.	fragmental constants

fluor.	fluorescence method
G	advective inflow, m ³ /h
G _B	advective inflow to bottom sediment m ³ /h
ΔG _v	Gibbs's free energy of vaporization kJ/mol or kcal/mol
GC	gas chromatography
GC/FID	GC analysis with flame ionization detector
GC/ECD	GC analysis with electron capture detector
GC-RT	GC retention time
gen. col.	generator-column
H, HLC	Henry's law constant, Pa·m ³ /mol, or atm m ³ /mol
ΔH _{fus}	enthalpy of fusion, kJ/mol
ΔH _{subl}	enthalpy of sublimation, kJ/mol
ΔH _v	enthalpy of vaporization, kJ/mol or kcal/mol
HPLC	high pressure liquid chromatography
HPLC/MS	HPLC analysis with mass spectrometer detector
HPLC/UV	HPLC analysis with UV detector
HPLC/fluor.	HPLC analysis with fluorescence detector
HPLC-k'	HPLC-capacity factor correlation
HPLC-RI	HPLC-retention index correlation
HPLC-RT	HPLC-retention time correlation
HPLC-RV	HPLC-retention volume correlation
IP	ionization potential
IR	infrared absorption
J	intermediate quantities for fugacity calculation
K	Kjeldahl method
k	reaction rate constant
k _i	first-order rate constant in phase i, h ⁻¹
k _A	air/water mass transfer coefficient, air-side, m/h
k _W	air/water mass transfer coefficient, water-side, m/h
K _{AR/W}	aerosol/water partition coefficient
K _{AW}	dimensionless air/water partition coefficient
k _H	Henry's law constant with units of vapor pressure
K _B	bioconcentration factor
K _h	association coefficient
K _{OC}	organic-carbon sorption partition coefficient
K _{OM}	organic-matter sorption partition coefficient
K _{OA}	octanol/air partition coefficient
K _{OW}	octanol/water partition coefficient
K _{SD/W}	sediment-water partition coefficient
K _{SSD/W}	suspended sediment/water partition coefficient
K _{SW}	soil/water partition coefficient
K _p or K _d	sorption coefficient
k ₁	uptake/accumulation rate constant, d ⁻¹ (day ⁻¹)
k ₂	elimination/clearance/depuration rate constant, d ⁻¹
k _b	biodegradation rate constant, d ⁻¹
k _h	hydrolysis rate constant, d ⁻¹
k _p	photolysis rate constant, d ⁻¹
k _{OH}	photooxidation rate constant for hydroxyl radical
k _{NO3}	photooxidation rate constant for NO ₃ radical
k _{O3}	photooxidation rate constant for ozone
L	lipid content of fish
LSC	liquid scintillation counting
LSS	liquid scintillation spectrometry
m _i	amount of chemical in phase i, mol or kg
M	total amount of chemical, mol or kg

MCI	molecular connectivity indices
MO	molecular orbital calculation
mp.	melting point, °C
MR	molar refraction
MS	mass spectrometry
MW	molecular weight, g/mol
n_C	number of carbon atoms
n_{Cl}	number of chlorine atoms
P	vapor pressure, Pa (Pascal)
P_L	liquid or supercooled liquid vapor pressure, Pa
P_S	solid vapor pressure, Pa
Q	scavenging ratio
QSAR	quantitative structure-activity relationship
QSPR	quantitative structure-property relationship
RC	Radiochemical method
RP-HPLC	reversed phase high pressure liquid chromatography
RP-TLC	reversed phase thin layer chromatography
S	water solubility, mg/L or g/m ³
ΔS_{fus}	entropy of fusion, J/mol·K or cal/mol·K (e.u.)
$S_{octanol}$	solubility in octanol
SD	standard deviation
SPARC	a computational expert system that predicts chemical reactivity
$t/^{\circ}C$	temperature in degree centigrade
t	residence time, h (hour)
t_o	overall residence time, h
t_A	advection persistence time, h
t_B	sediment burial residence time, h
t_R	reaction persistence time, h
$t_{1/2}$	half-life, s, h, min, d, month or yr
T_{ij}	intermedia transport rate, mol/h or kg/h
T	system temperature, K
T_B	boiling point, K
T_M	melting point, K
TLC	thin-layer chromatography
TMV	total molecular volume per molecule, Å ³ (Angstrom ³)
TN	titration method
TSA	total surface area per molecule, Å ²
U_1	air side, air-water MTC (same as k_A), m/h
U_2	water side, air-water MTC (same as k_W), m/h
U_3	rain rate (same as U_R), m/h
U_4	aerosol deposition rate, m/h
U_5	soil-air phase diffusion MTC, m/h
U_6	soil-water phase diffusion MTC, m/h
U_7	soil-air boundary layer MTC, m/h
U_8	sediment-water MTC, m/h
U_9	sediment deposition rate, m/h
U_{10}	sediment resuspension rate, m/h
U_{11}	soil-water run-off rate, m/h
U_{12}	soil-solids run-off rate, m/h
U_R	rain rate, m/h
U_Q	dry deposition velocity, m/h
U_B	sediment burial rate, m/h
UV	UV spectrometry
UNIFAC	UNIQUAC functional group activity coefficients
V_i	volume of pure phase i, m ³

V_S	volume of bottom sediment, m ³
V_{Bi}	volume of bulk phase i, m ³
V_I	intrinsic molar volume, cm ³ /mol
V_M	molar volume, cm ³ /mol
v_i	volume fraction of phase i
v_Q	volume fraction of aerosol
VOC	volatile organic chemicals
W	molecular mass, g/mol
Z_i	fugacity capacity of phase i, mol/m ³ Pa
Z_{Bi}	fugacity capacity of bulk phase i, mol/m ³ Pa

1.2 GREEK CHARACTERS

π -const.	substituent constants for K_{OW} estimation
γ	solute activity coefficient
γ_o	solute activity coefficient in octanol phase
γ_w	solute activity coefficient in water phase
ρ_i	density of pure phase i, kg/m ³
ρ_{Bi}	density of bulk phase i, kg/m ³
χ	molecular connectivity indices
ϕ_{OC} or f_{OC}	organic carbon fraction
ϕ_i	organic carbon fraction in phase i

Appendix 2

2.1 ALPHABETICAL INDEX

Acenaphthene	691
Acenaphthylene	688
Acephate	3715
Acetaldehyde (Ethanal)	2589
Acetamide	3328
Acetic acid	2692
Acetone	2619
Acetonitrile	3197
Acetophenone	2664
Acridine	3380
Acrolein (2-Propenal)	2605
Acrylamide	3330
Acrylic acid (2-Propenoic acid)	2718
Acrylonitrile (2-Propenenitrile)	3210
Alachlor	3461
Aldicarb	3717
Aldrin	3721
Allyl alcohol	2557
Ametryn	3466
Aminocarb	3728
Amitrole	3469
Anilazine	4027
Aniline	3243
Anisole (Methoxybenzene)	2329
Anthracene	725
Aroclor 1016	2015
Aroclor 1221	2017
Aroclor 1232	2019
Aroclor 1242	2021
Aroclor 1248	2024
Aroclor 1254	2026
Aroclor 1260	2030
Atrazine	3471
Azinphos-methyl	3729
Barban	3480
Benalaxyl	4029
Bendiocarb	3732
Benefin	3482
Benomyl	4031
Benzaldehyde	2613
Benzamide	3331

Benz[<i>a</i>]anthracene	788
Benzene	407
Benzenethiol	3412
Benzidine	3283
Benzo[<i>c</i> g]carbazole	3378
Benzo[<i>b</i>]fluoranthene	796
Benzo[<i>j</i>]fluoranthene	799
Benzo[<i>k</i>]fluoranthene	800
Benzo[<i>a</i>]fluorene	767
Benzo[<i>b</i>]fluorene	769
Benzoic acid	2728
Benzonitrile	3214
Benzo[<i>ghi</i>]perylene	823
Benzophenone	2670
Benzo[<i>a</i>]pyrene	804
Benzo[<i>e</i>]pyrene	811
Benzo[<i>f</i>]quinoline	3372
Benzo[<i>b</i>]thiophene	3419
Benzyl alcohol	2565
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Bis(2-chloroethyl)ether	2319
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3-Bromochlorobenzene	1448
4-Bromochlorobenzene	1450
Bromochloromethane	1186
Bromocyclohexane	1166
1-Bromodecane	1164
Bromodichloromethane	1188
2-Bromodiphenyl ether (PBDE-1)	2401
3-Bromodiphenyl ether (PBDE-2)	2402
4-Bromodiphenyl ether (PBDE-3)	2403
1-Bromododecane	1165
Bromoethane (Ethyl bromide)	1139
1-Bromoheptane	1161
1-Bromohexane	1160
4-Bromiodobenzene	1453
Bromomethane (Methyl bromide)	1123
1-Bromonaphthalene	875
2-Bromonaphthalene	879
1-Bromooctane	1162
1-Bromopentane (<i>n</i> -Amyl bromide)	1158

4-Bromophenyl phenyl ether	2403
Bromophos	3734
Bromophos-ethyl	3736
1-Bromopropane (<i>n</i> -Propyl bromide)	1148
2-Bromopropane (<i>i</i> -Propyl bromide)	1152
2-Bromotoluene	1431
3-Bromotoluene	1433
4-Bromotoluene	1435
Bromoxynil	3489
<i>sec</i> -Bumeton	3491
Bupirimate	4035
Butachlor	3493
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<i>n</i> -Butane	70
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1-Butanol (<i>n</i> -Butanol)	2497
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<i>sec</i> -Butyl alcohol	2511
<i>tert</i> -Butyl alcohol	2518
<i>n</i> -Butyl amine	3234
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<i>n</i> -Butylbenzene	520
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<i>tert</i> -Butylbenzene	532
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Carbaryl	3738
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Carbendazim	4040
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Chlorazine	3501
Chlorbromuron	3502
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Chlorfenvinphos	3758
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4-Chloroaniline.....	3257
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3-Chlorobenzoic acid.....	2753
4-Chlorobenzoic acid.....	2755
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3-Chlorobiphenyl (PCB-2)	1497
4-Chlorobiphenyl (PCB-3)	1501
1-Chlorobutane (<i>n</i> -Butyl chloride)	1041
2-Chlorobutane (<i>i</i> -Butyl chloride).....	1045
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4-Chloriodobenzene	1456
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1-Chlorooctane	1056
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3-Chlorophenol (<i>m</i> -Chlorophenol).....	2882
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2-Chlorotoluene	1352
3-Chlorotoluene	1355
4-Chlorotoluene	1357
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Chlorotrifluoroethene	1209
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Cyclohexanone	2660
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Decachlorodiphenyl ether (PCDE-209)	2400
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<i>n</i> -Decane	159
Decanol	2549
1-Decene	314
Decylbenzene	564
Deltamethrin	3798
Diallyl phthalate (DAP)	3090
Demeton	3800
Dialifor	3802
Diallate	3527
Diazinon	3804
Dibenz[<i>a,c</i>]anthracene	828
Dibenz[<i>a,h</i>]anthracene	830
Dibenz[<i>a,i</i>]anthracene	834
Dibenzo- <i>p</i> -dioxin	2064
Dibenzofuran	2168
Dibenzothiophene	3421
1,2-Dibromobenzene	1416
1,3-Dibromobenzene	1418
1,4-Dibromobenzene	1420
4,4'-Dibromobiphenyl	885
2,4-Dibromodiphenyl ether (PBDE-7)	2405
2,4'-Dibromodiphenyl ether (PBDE-9)	2406
2,6-Dibromodiphenyl ether (PBDE-10)	2407
3,4-Dibromodiphenyl ether (PBDE-12)	2408
3,4'-Dibromodiphenyl ether (PBDE-13)	2409
4,4'-Dibromodiphenyl ether (PBDE-15)	2410
Dibromochloromethane	1190
1,2-Dibromoethane	1143
Dibromomethane	1128
1,4-Dibromonaphthalene	882
2,3-Dibromonaphthalene	883
1,2-Dibromopropane	1154
Di- <i>n</i> -butyl ether	2289
Dibutyl phenyl phosphate (DBPP)	3159
Di- <i>n</i> -butyl phthalate (DBP)	3095
Dicamba	3530
Dichlobenil	3534
Dichlone	4052
Dichloroacetic acid	2723
3,4-Dichloroaniline	3261
2,3-Dichloroanisole	2337
2,6-Dichloroanisole	2338
1,2-Dichlorobenzene (<i>o</i> -Dichlorobenzene)	1268
1,3-Dichlorobenzene (<i>m</i> -Dichlorobenzene)	1278
1,4-Dichlorobenzene (<i>p</i> -Dichlorobenzene)	1287
3,3'-Dichlorobenzidine	3285
2,2'-Dichlorobiphenyl (PCB-4)	1508
2,3-Dichlorobiphenyl (PCB-5)	1511
2,3'-Dichlorobiphenyl (PCB-6)	1514
2,4-Dichlorobiphenyl (PCB-7)	1516
2,4'-Dichlorobiphenyl (PCB-8)	1519
2,5-Dichlorobiphenyl (PCB-9)	1522

2,6-Dichlorobiphenyl (PCB-10)	1525
3,3'-Dichlorobiphenyl (PCB-11)	1528
3,4-Dichlorobiphenyl (PCB-12)	1530
3,4'-Dichlorobiphenyl (PCB-13)	1533
3,5-Dichlorobiphenyl (PCB-14)	1535
4,4'-Dichlorobiphenyl (PCB-15)	1537
Dichlorobiphenyls (isomer group)	2001
3,5-Dichlorocatechol	2956
4,5-Dichlorocatechol	2957
2,3-Dichlorodibenzo- <i>p</i> -dioxin	2073
2,7-Dichlorodibenzo- <i>p</i> -dioxin	2076
2,8-Dichlorodibenzo- <i>p</i> -dioxin	2080
2,3-Dichlorodibenzofuran	2177
2,7-Dichlorodibenzofuran	2179
2,8-Dichlorodibenzofuran	2181
3,6-Dichlorodibenzofuran	2184
1,2-Dichloro-1,1-difluoroethane	1209
1,1-Dichloro-2,2-difluoroethene	1209
1,2-Dichloro-1,2-difluoroethene	1209
Dichlorodifluoromethane	1196
2,4-Dichlorodiphenyl ether (PCDE-8)	2362
2,6-Dichlorodiphenyl ether (PCDE-10)	2363
1,1-Dichloroethane	966
1,2-Dichloroethane	975
1,1-Dichloroethene	1070
<i>cis</i> -1,2-Dichloroethene	1077
<i>trans</i> -1,2-Dichloroethene	1084
1,1-Dichloro-1-fluoroethane	1209
Dichlorofluoromethane	1209
4,5-Dichloroguaiacol	2975
Dichloromethane	930
1,2-Dichloronaphthalene	848
1,4-Dichloronaphthalene	849
1,8-Dichloronaphthalene	851
2,3-Dichloronaphthalene	852
2,7-Dichloronaphthalene	853
2,4-Dichlorophenol	2892
2,6-Dichlorophenol	2898
3,4-Dichlorophneol	2901
2,4-Dichlorophenoxyacetic acid (2,4-D)	2761, 3517
1,2-Dichloropropane	1031
1,3-Dichloropropene	1115
3,5-Dichlorosyringol	2991
2,6-Dichlorosyringolaldehyde	2994
1,1-Dichloro-1,2,2,2-tetrafluoroethane	1209
1,2-Dichloro-1,1,2,2-tetrafluoroethane	1209
2,4-Dichlorotoluene	1360
2,6-Dichlorotoluene	1362
3,4-Dichlorotoluene	1364
1,1-Dichlorotrifluoroethane	1209
4,5-Dichloroveratrole	2345
5,6-Dichlorovanillin	2988
Dichlorprop	3537
Dichlorvos	3811
Diclofop-methyl	3539

Dicofol	4054
Dicrotophos	3816
Dieldrin	3819
Diethanolamine	3239
Diethylamine	3228
Diethyl ether (ethyl ether)	2266
Diethyl phthalate (DEP)	3084
Diflubenzuron	3827
1,2-Difluorobenzene	1384
1,3-Difluorobenzene	1386
1,4-Difluorobenzene	1388
1,1-Difluoroethane	1209
1,2-Difluoroethane	1209
1,1-Difluoroethene	1209
Difluoromethane	1209
1,1-Difluorotetrachloroethane	1209
Di- <i>n</i> -hexyl phthalate (DHP)	3108
1,2-Diiodobenzene	1441
1,3-Diiodobenzene	1442
1,4-Diiodobenzene	1443
Di-isobutyl phthalate (DIBP)	3104
Di-isodecyl phthalate (DIDP)	3129
Di-isononyl phthalate (DINP)	3127
Di-isooctyl phthalate (DIOP)	3116
Di-isopropyl phthalate (DIPP)	3094
Di-isopropyl ether	2280
Dimethoate	3829
Dimethylamine	3218
<i>N,N'</i> -Dimethylaniline	3274
9,10-Dimethylantracene	745
7,12-Dimethylbenz[<i>a</i>]anthracene	818
9,10-Dimethylbenz[<i>a</i>]anthracene	820
4,4'-Dimethylbiphenyl	678
2,3-Dimethyl-1,3-butadiene	328
2,2-Dimethylbutane	77
2,3-Dimethylbutane	79
1,2- <i>cis</i> -Dimethylcyclohexane	240
1,4- <i>trans</i> -Dimethylcyclohexane	245
Dimethyl disulfide	3391
Dimethyl ether (methyl ether)	2262
1,3-Dimethylnaphthalene	651
1,4-Dimethylnaphthalene	653
1,5-Dimethylnaphthalene	655
2,3-Dimethylnaphthalene	657
2,6-Dimethylnaphthalene	659
2,2-Dimethylpentane	101
2,4-Dimethylpentane	103
3,3-Dimethylpentane	105
2,2-Dimethylpropane (Neopentane)	67
2,3-Dimethylphenol	2821
2,4-Dimethylphenol	2825
2,5-Dimethylphenol	2831
2,6-Dimethylphenol	2834
3,4-Dimethylphenol	2838
3,5-Dimethylphenol	2842

Dimethyl phthalate (DMP)	3079
2,3-Dimethylpyridine	3362
Dimethyl sulfate	3397
Dimethyl sulfide	3386
Dimethylsulfoxide (DMSO)	3394
Dinitramine	3542
4,6-Dinitro- <i>o</i> -cresol	2950
2,4-Dinitrophenol	2945
2,4-Dinitrotoluene (DNT)	3313
2,6-Dinitrotoluene	3317
Dinoseb	3544
Di-isononyl phthalate (DINP)	3127
Di- <i>n</i> -octyl phthalate (DOP)	3113
1,4-Dioxane	2309
Dipentyl phthalate (DPP)	3106
Diphenamid	3547
Diphenylamine	3279
Diphenyl ether	2355
4-Diphenylmethane	679
Diphenyl nitrosamine	3340
Di- <i>i</i> -propyl ether	2280
Di- <i>n</i> -propyl ether	2276
Di- <i>n</i> -propyl phthalate (DnPP)	3092
Diquat	3549
Disulfoton	3832
Dithianon	4056
Di-tridecyl phthalate (DTPP)	3133
Di-undecyl phthalate (DUP)	3131
Diuron	3551
<i>n</i> -Dodecane	167
Dodecylbenzene	569
Edifenphos	4058
Eicosane	194
Endosulfan	3835
Endrin	3840
Epichlorohydrin	2313
EPTC	3555
Ethalfuralin	3558
Ethanal (Acetaldehyde)	2589
Ethanethiol	3402
Ethanol	2480
Ethanolamine	3236
Ethiofencarb	3845
Ethion	3847
Ethoprop	3849
Ethoprophos	3849
Ethyl acetate	3041
Ethylamine	3225
Ethyl acrylate	3062
Ethylbenzene	439
Ethyl benzoate	3072
Ethylcyclohexane	249
Ethyl formate	3028
Ethylene Glycol	2553
2-Ethylhexyl diphenyl phosphate (EHPP)	3161

1-Ethyl-2-methylbenzene	505
1-Ethyl-3-methylbenzene	508
1-Ethyl-4-methylbenzene	512
1-Ethynaphthalene	661
2-Ethynaphthalene	665
2-Ethylphenol (<i>o</i> -Ethylphenol)	2850
4-Ethylphenol (<i>p</i> -Ethylphenol)	2853
Etridiazole	4060
Fenarimol	4062
Fenfuram	4064
Fenitrothion	3851
Fenoprop	3560
Fenoxycarb	3854
Fenpropathrin	3855
Fensulfothion	3857
Fenthion	3859
Fenuron	3562
Fenvalerate	3862
Fluchloralin	3564
Flucythrinate	3865
Fluometuron	3566
Fluoranthene	759
Fluorene	699
Fluorobenzene	1380
Fluorodifen	3568
Fluoroethane	1209
Fluoroethene	1209
Fluoromethane	1209
2-Fluoropropane	1209
3-Fluoropropene	1209
Fluridone	3569
Folpet	4065
Fonofos	3867
Formaldehyde	2584, 4067
Formic acid	2688
Furan	2297
Furfural (2-Furaldehyde)	2609
Glyphosate	3572
Guaiacol	2968
α -HCH	3869
β -HCH	3876
δ -HCH	3881
2,2',3,4,5,5',6-Heptabromodiphenyl ether (PBDE-183)	2450
2',3,3',4,4',5,6-Heptabromodiphenyl ether (PBDE-190)	2452
Heptachlor	3885
Heptachlor epoxide	3890
2,2',3,3',4,4',5-Heptachlorobiphenyl (PCB-170)	1911
2,2',3,3',4,4',6-Heptachlorobiphenyl (PCB-171)	1913
2,2',3,3',4,5,5'-Heptachlorobiphenyl (PCB-172)	1915
2,2',3,3',4,5,6-Heptachlorobiphenyl (PCB-173)	1917
2,2',3,3',4,5,6'-Heptachlorobiphenyl (PCB-174)	1919
2,2',3,3',4,5',6-Heptachlorobiphenyl (PCB-175)	1921
2,2',3,3',4,6,6'-Heptachlorobiphenyl (PCB-176)	1923
2,2',3,3',4,5',6'-Heptachlorobiphenyl (PCB-177)	1925
2,2',3,3',5,5',6-Heptachlorobiphenyl (PCB-178)	1927

2,2',3,3',5,6,6'-Heptachlorobiphenyl (PCB-179).....	1929
2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB-180).....	1931
2,2',3,4,4',5,6-Heptachlorobiphenyl (PCB-181).....	1935
2,2',3,4,4',5,6'-Heptachlorobiphenyl (PCB-182).....	1937
2,2',3,4,4',5',6-Heptachlorobiphenyl (PCB-183).....	1939
2,2',3,4,4',6,6'-Heptachlorobiphenyl (PCB-184).....	1941
2,2',3,4,5,5',6-Heptachlorobiphenyl (PCB-185).....	1943
2,2',3,4,5,6,6'-Heptachlorobiphenyl (PCB-186).....	1945
2,2',3,4',5,5',6-Heptachlorobiphenyl (PCB-187).....	1947
2,2',3,4',5,6,6'-Heptachlorobiphenyl (PCB-188).....	1950
2,3,3',4,4',5,5'-Heptachlorobiphenyl (PCB-189).....	1952
2,3,3',4,4',5,6-Heptachlorobiphenyl (PCB-190).....	1954
2,3,3',4,4',5',6-Heptachlorobiphenyl (PCB-191).....	1956
2,3,3',4,5,5',6-Heptachlorobiphenyl (PCB-192).....	1958
2,3,3',4',5,5',6-Heptachlorobiphenyl (PCB-193).....	1960
1,2,3,4,6,7,8-Heptachlorodibenzo- <i>p</i> -dioxin	2141
1,2,3,4,7,8,9-Heptachlorodibenzo- <i>p</i> -dioxin	2146
1,2,3,4,6,7,8-Heptachlorodibenzofuran	2234
1,2,3,4,6,8,9-Heptachlorodibenzofuran	2237
1,2,3,4,7,8,9-Heptachlorodibenzofuran	2239
Heptachlorobiphenyls (isomer group)	2011
2,2',3,4,4',5,5'-Heptachlorodiphenyl ether (PCDE-180)	2392
2,2',3,4,4',5,6'-Heptachlorodiphenyl ether (PCDE-182)	2394
2,2',3,4,4',6,6'-Heptachlorodiphenyl ether (PCDE-184)	2395
1,2,3,4,5,6,7-Heptachloronaphthalene.....	871
1,2,3,4,5,6,8-Heptachloronaphthalene.....	872
<i>n</i> -Heptadecane	187
1,6-Heptadiene.....	337
1,1,1,2,3,3,3-Heptafluoropropane.....	1209
<i>n</i> -Heptane	129
1-Heptanol	2535
2-Heptanone	2655
1-Heptene	304
1-Heptylbenzene.....	557
1-Heptyne	344
Hexabromobenzene	1429
2,2',4,4',6,6'-Hexabromobiphenyl	889
2,2',3,4,4',5-Hexabromodiphenyl ether (PBDE-138).....	2442
2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE-153).....	2443
2,2',4,4',5,6'-Hexabromodiphenyl ether (PBDE-154).....	2446
2,3,3',4,4',5,-Hexabromodiphenyl ether (PBDE-156).....	2448
Hexachlorobenzene	1343, 4069
2,2',3,3',4,4'-Hexachlorobiphenyl (PCB-128).....	1813
2,2',3,3',4,5-Hexachlorobiphenyl (PCB-129).....	1816
2,2',3,3',4,5'-Hexachlorobiphenyl (PCB-130).....	1818
2,2',3,3',4,6-Hexachlorobiphenyl (PCB-131).....	1820
2,2',3,3',4,6'-Hexachlorobiphenyl (PCB-132).....	1822
2,2',3,3',5,5'-Hexachlorobiphenyl (PCB-133).....	1824
2,2',3,3',5,6-Hexachlorobiphenyl (PCB-134).....	1826
2,2',3,3',5,6'-Hexachlorobiphenyl (PCB-135).....	1828
2,2',3,3',6,6'-Hexachlorobiphenyl (PCB-136).....	1830
2,2',3,4,4',5-Hexachlorobiphenyl (PCB-137).....	1833
2,2',3,4,4',5'-Hexachlorobiphenyl (PCB-138).....	1835
2,2',3,4,4',6-Hexachlorobiphenyl (PCB-139).....	1840
2,2',3,4,4',6'-Hexachlorobiphenyl (PCB-140).....	1842

2,2',3,4,5,5'-Hexachlorobiphenyl (PCB-141).....	1844
2,2',3,4,5,6-Hexachlorobiphenyl (PCB-142).....	1847
2,2',3,4,5,6'-Hexachlorobiphenyl (PCB-143).....	1849
2,2',3,4,5',6-Hexachlorobiphenyl (PCB-144).....	1851
2,2',3,4,6,6'-Hexachlorobiphenyl (PCB-145).....	1853
2,2',3,4',5,5'-Hexachlorobiphenyl (PCB-146).....	1855
2,2',3,4',5,6-Hexachlorobiphenyl (PCB-147).....	1857
2,2',3,4',5,6'-Hexachlorobiphenyl (PCB-148).....	1859
2,2',3,4',5',6-Hexachlorobiphenyl (PCB-149).....	1861
2,2',3,4',6,6'-Hexachlorobiphenyl (PCB-150).....	1863
2,2',3,5,5',6-Hexachlorobiphenyl (PCB-151).....	1865
2,2',3,5,6,6'-Hexachlorobiphenyl (PCB-152).....	1868
2,2',4,4',5,5'-Hexachlorobiphenyl (PCB-153).....	1870
2,2',4,4',5,6'-Hexachlorobiphenyl (PCB-154).....	1877
2,2',4,4',6,6'-Hexachlorobiphenyl (PCB-155).....	1879
2,3,3',4,4',5-Hexachlorobiphenyl (PCB-156).....	1883
2,3,3',4,4',5'-Hexachlorobiphenyl (PCB-157).....	1885
2,3,3',4,4',6-Hexachlorobiphenyl (PCB-158).....	1887
2,3,3',4,5,5'-Hexachlorobiphenyl (PCB-159).....	1889
2,3,3',4,5,6-Hexachlorobiphenyl (PCB-160).....	1891
2,3,3',4,5',6-Hexachlorobiphenyl (PCB-161).....	1893
2,3,3',4',5,5'-Hexachlorobiphenyl (PCB-162).....	1895
2,3,3',4',5,6-Hexachlorobiphenyl (PCB-163).....	1897
2,3,3',4',5',6-Hexachlorobiphenyl (PCB-164).....	1899
2,3,3',5,5',6-Hexachlorobiphenyl (PCB-165).....	1901
2,3,4,4',5,6-Hexachlorobiphenyl (PCB-166).....	1903
2,3',4,4',5,5'-Hexachlorobiphenyl (PCB-167).....	1905
2,3',4,4',5',6-Hexachlorobiphenyl (PCB-168).....	1907
3,3',4,4',5,5'-Hexachlorobiphenyl (PCB-169).....	1909
Hexachlorobiphenyls (isomer group)	2009
Hexachlorobutadiene	1119
Hexachlorocyclopentadiene.....	1121
1,2,3,4,7,8-Hexachlorodibenzo- <i>p</i> -dioxin.....	2128
1,2,3,6,7,8-Hexachlorodibenzo- <i>p</i> -dioxin.....	2133
1,2,3,7,8,9-Hexachlorodibenzo- <i>p</i> -dioxin.....	2136
1,2,4,6,7,9-Hexachlorodibenzo- <i>p</i> -dioxin.....	2139
1,2,3,4,6,8-Hexachlorodibenzofuran	2218
1,2,3,4,7,8-Hexachlorodibenzofuran	2220
1,2,3,6,7,8-Hexachlorodibenzofuran	2223
1,2,3,7,8,9-Hexachlorodibenzofuran	2226
1,2,4,6,7,8-Hexachlorodibenzofuran	2228
1,2,4,6,8,9-Hexachlorodibenzofuran	2230
2,3,4,6,7,8-Hexachlorodibenzofuran	2232
2,2',3,3',4,4'-Hexachlorodiphenyl ether (PCDE-128)	2381
2,2',3,4,4',5-Hexachlorodiphenyl ether (PCDE-137)	2382
2,2',3,4,4',5'-Hexachlorodiphenyl ether (PCDE-138)	2384
2,2',3,4,4',6-Hexachlorodiphenyl ether (PCDE-140)	2385
2,2',4,4',5,5'-Hexachlorodiphenyl ether (PCDE-153)	2386
2,2',4,4',5,6'-Hexachlorodiphenyl ether (PCDE-154)	2388
2,3',4,4',5,5'-Hexachlorodiphenyl ether (PCDE-167)	2390
Hexachloroethane	1021
1,2,3,4,5,7-Hexachloronaphthalene.....	867
1,2,3,4,6,7-Hexachloronaphthalene.....	868
1,2,3,5,6,7-Hexachloronaphthalene.....	869
1,2,3,5,7,8-Hexachloronaphthalene.....	870

Hexacosane	206
Hexadecane	183
1,5-Hexadiene	334
Hexafluorobenzene	1401
Hexafluoroethane	1209
1,1,1,2,3,3-Hexafluoropropane	1209
1,1,1,3,3,3-Hexafluoropropane	1209
Hexafluoropropene	1209
Hexamethylbenzene	550
<i>n</i> -Hexane	114
Hexanoic acid (Caproic acid)	2712
1-Hexanol	2529
2-Hexanone	2650
1-Hexene	299
1-Hexyne	342
<i>n</i> -Hexylbenzene	553
Hydroquinone (1,4-Dihydroxybenzene)	2964
Imazalil	4075
Indan	620
Indeno[1,2,3- <i>cd</i>]pyrene	826
Indole	3346
Iodobenzene	1437
1-Iodobutane (<i>n</i> -Butyl iodide)	1183
Iodoethane (Ethyl iodide)	1174
Iodomethane	1169
1-Iodopentane	1185
1-Iodopropane (<i>n</i> -Propyl iodide)	1178
2-Iodopropane (<i>i</i> -Propyl iodide)	1181
Isobutane (2-Methylpropane)	64
Isobutanol (<i>i</i> -Butyl alcohol)	2507
Isobutylbenzene	525
Isobutyric acid	2705
Isodecyl diphenyl phosphate (IDDP)	3163
Isopentane	73
Isopropalin	3575
Isopropanol (<i>i</i> -Propyl alcohol)	2491
Isopropylbenzene	500
1-Isopropyl-4-methylbenzene	516
Isopropylphenyl diphenyl phosphate (IPDP)	3143
Isoproturon	3577
Isoquinoline	3369
Kepone	3893
lambda-Cyhalothrin	3770
Leptophos	3896
<i>dextro</i> -Limonene [(<i>R</i>)-(+)-limonene]	371
Lindane (γ -HCH)	3898
Linuron	3580
Malathion	3912
Mancozeb	4077
Maneb	4078
MCPA (4-chloro-2-methylphenoxy)acetic acid)	3584
MCPB (4-chloro-2-methylphenoxy)butanoic acid)	3587
Mecoprop	3589
Metalaxyl	4080
Methanal (Formaldehyde)	2584

Methanethiol.....	3399
Methanol.....	2474
Methiocarb.....	3916
Methomyl	3918
Methoxychlor	3920
2-Methoxyphenol (Guaiacol)	2968
3-Methoxyphenol	2971
4-Methoxyphenol	2972
Methyl acetate	3034
Methyl acrylate.....	3060
2-Methylanthracene.....	739
9-Methylanthracene.....	742
Methylbenzene (toluene)	425
Methyl benzoate	3069
2-Methylbenzoic acid (<i>o</i> -Toluic acid)	2735
3-Methylbenzoic acid (<i>m</i> -Toluic acid)	2738
4-Methylbenzoic acid (<i>p</i> -Toluic acid)	2741
4-Methylbiphenyl	677
2-Methyl-1,3-butadiene (isoprene).....	322
2-Methylbutane (isopentane).....	73
2-Methyl-1-butene	276
3-Methyl-1-butene	280
2-Methyl-2-butene	283
Methyl <i>t</i> -butyl ether (MTBE)	2271
Methyl butyl ketone (2-Hexanone).....	2650
Methyl chloride	924
3-Methylcholanthrene.....	821
Methylcyclohexane.....	233
1-Methylcyclohexene	357
Methylcyclopentane.....	217
Methyl ethyl ketone (2-Butanone).....	2626
1-Methylfluorene	708
Methyl formate	3025
2-Methylfuran.....	2301
2-Methylheptane.....	137
3-Methylheptane.....	139
2-Methylhexane (Isoheptane)	123
3-Methylhexane	125
Methyl iodide.....	1169
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Methyl methacrylate.....	3065
1-Methylnaphthalene.....	639
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2-Methylpentane (Isohexane)	93
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4-Methyl-1-pentene	297
1-Methylphenanthrene.....	722
2-Methylpropene	270
2-Methylpyridine	3354
3-Methylpyridine	3358
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β -Methylstyrene	584

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<i>m</i> -Methylstyrene.....	588
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2-Naphthylamine (β -Aminonaphthalene)	3291
1-Naphthol	2865
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2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl (PCB-207)	1991
2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl (PCB-208)	1993
Nonachlorobiphenyls (isomer group).....	2014
2,2',3,3',4,4',5,5',6-Nonachlorodiphenyl ether (PCDE-206).....	2399
<i>n</i> -Nonane	152
1-Nonanol	2546
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Nonylbenzene	562
4-Nonylphenol	2862
Nonylphenyl diphenyl phosphate (NPDPP)	3147
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Norflurazon.....	3614
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2,2',3,3',4,4',5,6-Octachlorobiphenyl (PCB-195).....	1965
2,2',3,3',4,4',5,6'-Octachlorobiphenyl (PCB-196).....	1967
2,2',3,3',4,4',6,6'-Octachlorobiphenyl (PCB-197).....	1969
2,2',3,3',4,5,5',6-Octachlorobiphenyl (PCB-198).....	1971
2,2',3,3',4,5,5',6'-Octachlorobiphenyl (PCB-199).....	1973
2,2',3,3',4,5,6,6'-Octachlorobiphenyl (PCB-200).....	1975

2,2',3,3',4,5',6,6'-Octachlorobiphenyl (PCB-201).....	1977
2,2',3,3',5,5',6,6'-Octachlorobiphenyl (PCB-202).....	1979
2,2',3,4,4',5,5',6-Octachlorobiphenyl (PCB-203).....	1983
2,2',3,3,4',5,6,6'-Octachlorobiphenyl (PCB-204).....	1985
2,3,3',4,4',5,5',6-Octachlorobiphenyl (PCB-205).....	1987
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2,2',3,3',5-Pentachlorobiphenyl (PCB-83).....	1708
2,2',3,3',6-Pentachlorobiphenyl (PCB-84).....	1710
2,2',3,4,4'-Pentachlorobiphenyl (PCB-85).....	1712
2,2',3,4,5-Pentachlorobiphenyl (PCB-86).....	1714
2,2',3,4,5'-Pentachlorobiphenyl (PCB-87).....	1716
2,2',3,4,6-Pentachlorobiphenyl (PCB-88).....	1719
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2,2',3,4',6-Pentachlorobiphenyl (PCB-91).....	1725
2,2',3,5,5'-Pentachlorobiphenyl (PCB-92).....	1727
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2,2',3,5,6'-Pentachlorobiphenyl (PCB-94).....	1731
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2,2',3,4',6'-Pentachlorobiphenyl (PCB-98)	1741
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2,2',4,4',6-Pentachlorobiphenyl (PCB-100)	1746
2,2',4,5,5'-Pentachlorobiphenyl (PCB-101)	1748
2,2',4,5,6'-Pentachlorobiphenyl (PCB-102)	1755
2,2',4,5',6-Pentachlorobiphenyl (PCB-103)	1757
2,2',4,6,6'-Pentachlorobiphenyl (PCB-104)	1759
2,3,3',4,4'-Pentachlorobiphenyl (PCB-105)	1761
2,3,3',4,5-Pentachlorobiphenyl (PCB-106)	1765
2,3,3',4',5-Pentachlorobiphenyl (PCB-107)	1767
2,3,3',4,5'-Pentachlorobiphenyl (PCB-108)	1769
2,3,3',4,6-Pentachlorobiphenyl (PCB-109)	1771
2,3,3',4',6-Pentachlorobiphenyl (PCB-110)	1773
2,3,3',5,5'-Pentachlorobiphenyl (PCB-111)	1776
2,3,3',5,6-Pentachlorobiphenyl (PCB-112)	1778
2,3,3',5',6-Pentachlorobiphenyl (PCB-113)	1780
2,3,4,4',5-Pentachlorobiphenyl (PCB-114)	1782
2,3,4,4',6-Pentachlorobiphenyl (PCB-115)	1784
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2,3',4,4',6-Pentachlorobiphenyl (PCB-119)	1794
2,3',4,5,5'-Pentachlorobiphenyl (PCB-120)	1796
2,3',4,5',6-Pentachlorobiphenyl (PCB-121)	1798
2,3,3',4',5'-Pentachlorobiphenyl (PCB-122)	1800
2,3',4,4',5'-Pentachlorobiphenyl (PCB-123)	1802
2,3',4',5,5'-Pentachlorobiphenyl (PCB-124)	1804
2,3',4',5',6-Pentachlorobiphenyl (PCB-125)	1807
3,3',4,4',5-Pentachlorobiphenyl (PCB-126)	1808
3,3',4,5,5'-Pentachlorobiphenyl (PCB-127)	1811
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1,2,3,7,8-Pentachlorodibenzo- <i>p</i> -dioxin	2123
1,2,4,7,8-Pentachlorodibenzo- <i>p</i> -dioxin	2126
1,2,3,4,7-Pentachlorodibenzofuran.....	2209
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1,2,4,7,8-Pentachlorodibenzofuran.....	2213
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2,3,3',4,4'-Pentachlorodiphenyl ether (PCDE-105).....	2379
3,3',4,4',5-Pentachlorodiphenyl ether (PCDE-126).....	2380
2,3,3',4,4'-Pentachlorodiphenyl ether (PCDE-128).....	2381
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1,2,3,4,6-Pentachloronaphthalene	864
1,2,3,5,7-Pentachloronaphthalene	865
1,2,3,5,8-Pentachloronaphthalene	866
Pentachlorophenol (PCP)	2922, 3947
Pentachlorotoluene	1373
Pentadecane	179
1,4-Pentadiene	330
Pentafluorobenzene	1399

Pentafluoroethane	1209
1,1,1,2,2-Pentafluoropropane	1209
1,1,1,3,3-Pentafluoropropane	1209
1,1,2,2,3-Pentafluoropropane	1209
Pentafluorophenol	1408
Pentafluorotoluene	1404
Pentamethylbenzene	545
<i>n</i> -Pentane	85
1-Pentanol (<i>n</i> -Amyl alcohol)	2523
2-Pentanone	2634
3-Pentanone	2639
1-Pentene	288
<i>cis</i> -2-Pentene	292
Pentyl acetate	3057
Pentylbenzene	547
Pentylcyclopentane	223
1-Pentyne	340
Perfluorobutane	1209
Perfluorocyclobutane	1209
Perfluorocyclohexane	1209
Perfluorocyclopentane	1209
Perfluorohexane	1209
Perfluoro-2-methylcyclopentane	1209
Perfluoro-3-methylcyclopentane	1209
Perfluoropentane	1209
Permethrin	3953
Perylene	814
Phenanthrene	709
Phenetole	2348
Phenol	2781
Phenthoate	3957
Phenylacetic acid	2745
2-Phenylphenol (2-Hydroxybiphenyl)	2872
4-Phenylphenol (4-Hydroxybiphenyl)	2875
Phorate	3959
Phosmet	3962
Phthalic acid	2748
Picloram	3622
α -Pinene	373
β -Pinene	379
Pirimicarb	3964
Procymidone	4088
Profluralin	3626
Prometon	3628
Prometryn	3631
Pronamide	3634
Propachlor	3636
Propanal (Propionaldehyde)	2595
1-Propanethiol	3406
Propanil	3639
Propanol (<i>n</i> -Propyl alcohol)	2486
Propargite	4090
Propazine	3642
2-Propenal (Acrolein)	2605
Propham	3645

Propiconazole	4091
Propionic acid	2697
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Propoxur	3966
Propyl acetate	3047
<i>n</i> -Propylamine	3231
<i>n</i> -Propylbenzene	493
<i>n</i> -Propyl benzoate	3075
<i>n</i> -Propylcyclopentane	221
1,2-Propylene oxide	2293
Propyl formate	3031
4-Propylphenol	2857
Pyrazon	3647
Pyrene	748
Pyridine	3348
Pyrrole	3342
Quinoline	3365
Quintozene	4093
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Ronnel	3969
Salicylic acid	2757
Simazine	3649
Stearic (Octadecanoic) acid	2716
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Styrene	576
Styrene oxide	2353
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Terbacil	3657
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Terbutryn	3659
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<i>m</i> -Terphenyl	781
<i>p</i> -Terphenyl	783
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2,2',5,5'-Tetrabromobiphenyl	887
2,2',4,4'-Tetrabromodiphenyl ether (PBDE-47)	2422
2,3',4,4'-Tetrabromodiphenyl ether (PBDE-66)	2425
2,4,4',6-Tetrabromodiphenyl ether (PBDE-69)	2427
3,3',4,4'-Tetrabromodiphenyl ether (PBDE-77)	2428
2,3,4,5-Tetrachloroanisole	2341
2,3,5,6-Tetrachloroanisole	2342
1,2,3,4-Tetrachlorobenzene	1320
1,2,3,5-Tetrachlorobenzene	1326
1,2,4,5-Tetrachlorobenzene	1330
2,2',3,3'-Tetrachlorobiphenyl (PCB-40)	1601
2,2',3,4-Tetrachlorobiphenyl (PCB-41)	1604
2,2',3,4'-Tetrachlorobiphenyl (PCB-42)	1606
2,2',3,5-Tetrachlorobiphenyl (PCB-43)	1608
2,2',3,5'-Tetrachlorobiphenyl (PCB-44)	1610
2,2',3,6-Tetrachlorobiphenyl (PCB-45)	1613
2,2',3,6'-Tetrachlorobiphenyl (PCB-46)	1615
2,2',4,4'-Tetrachlorobiphenyl (PCB-47)	1617
2,2',4,5-Tetrachlorobiphenyl (PCB-48)	1620
2,2',4,5'-Tetrachlorobiphenyl (PCB-49)	1622

2,2',4,6-Tetrachlorobiphenyl (PCB-50).....	1625
2,2',4,6'-Tetrachlorobiphenyl (PCB-51).....	1627
2,2',5,5'-Tetrachlorobiphenyl (PCB-52).....	1629
2,2',5,6'-Tetrachlorobiphenyl (PCB-53).....	1636
2,2',6,6'-Tetrachlorobiphenyl (PCB-54).....	1639
2,3,3',4-Tetrachlorobiphenyl (PCB-55).....	1641
2,3,3',4'-Tetrachlorobiphenyl (PCB-56).....	1643
2,3,3',5-Tetrachlorobiphenyl (PCB-57).....	1645
2,3,3',5'-Tetrachlorobiphenyl (PCB-58).....	1647
2,3,3',6-Tetrachlorobiphenyl (PCB-59).....	1649
2,3,4,4'-Tetrachlorobiphenyl (PCB-60).....	1651
2,3,4,5-Tetrachlorobiphenyl (PCB-61).....	1654
2,3,4,6-Tetrachlorobiphenyl (PCB-62).....	1658
2,3,4',5-Tetrachlorobiphenyl (PCB-63).....	1660
2,3,4',6-Tetrachlorobiphenyl (PCB-64).....	1662
2,3,5,6-Tetrachlorobiphenyl (PCB-65).....	1664
2,3',4,4'-Tetrachlorobiphenyl (PCB-66).....	1666
2,3',4,5-Tetrachlorobiphenyl (PCB-67).....	1670
2,3',4,5'-Tetrachlorobiphenyl (PCB-68).....	1672
2,3',4,6-Tetrachlorobiphenyl (PCB-69).....	1674
2,3',4',5-Tetrachlorobiphenyl (PCB-70).....	1676
2,3',4',6-Tetrachlorobiphenyl (PCB-71).....	1680
2,4',5,5'-Tetrachlorobiphenyl (PCB-72).....	1682
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3,3',4,5'-Tetrachlorobiphenyl (PCB-79).....	1700
3,3',5,5'-Tetrachlorobiphenyl (PCB-80).....	1702
3,4,4',5-Tetrachlorobiphenyl (PCB-81).....	1704
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1,2,3,4-Tetrachlorodibenzo- <i>p</i> -dioxin	2092
1,2,3,7-Tetrachlorodibenzo- <i>p</i> -dioxin	2096
1,2,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	2100
1,3,6,8-Tetrachlorodibenzo- <i>p</i> -dioxin	2102
1,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	2107
1,3,7,9-Tetrachlorodibenzo- <i>p</i> -dioxin	2109
2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	2111
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1,2,3,7-Tetrachlorodibenzofuran	2195
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1,3,6,8-Tetrachlorodibenzofuran	2199
1,3,7,8-Tetrachlorodibenzofuran	2201
1,3,7,9-Tetrachlorodibenzofuran	2203
2,3,7,8-Tetrachlorodibenzofuran	2205
1,1,2,2-Tetrachloro-1,2-difluoroethane	1207
2,2',4,4'-Tetrachlorodiphenyl ether (PCDE-47)	2368
2,3',4,4'-Tetrachlorodiphenyl ether (PCDE-66)	2369
2,4,4',5-Tetrachlorodiphenyl ether (PCDE-74)	2370
3,3',4,4'-Tetrachlorodiphenyl ether (PCDE-77)	2371
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1,1,2,2-Tetrachloroethane	1009

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3,4,5,6-Tetrachloroguaiacol	2981
Tetrachloromethane	950
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1,2,3,5-Tetrachloronaphthalene	859
1,3,5,7-Tetrachloronaphthalene	860
1,3,5,8-Tetrachloronaphthalene	862
2,3,4,5-Tetrachlorophenol	2916
2,3,4,6-Tetrachlorophenol	2918
2,3,5,6-Tetrachlorophenol	2921
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<i>n</i> -Tetradecane	175
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1,2,3,4-Tetrafluorobenzene.....	1393
1,2,3,5-Tetrafluorobenzene.....	1395
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1,1,1,2-Tetrafluoroethane	1209
1,1,2,2-Tetrafluoroethane	1209
Tetrafluoroethene.....	1209
Tetrafluoromethane.....	1209
Tetrahydrofuran	2303
Tetrahydropyran.....	2307
Tetralin.....	594
1,2,3,4-Tetramethylbenzene	536
1,2,3,5-Tetramethylbenzene	539
1,2,4,5-Tetramethylbenzene	542
Thioacetamide	3425
Thiobencarb.....	3662
Thiodicarb.....	3973
Thiophanate-methyl.....	4095
Thiophene	3415
Thiourea.....	3423
Thiram	4097
Tolclofos-methyl.....	4099
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<i>o</i> -Toluic acid	2735
<i>m</i> -Toluic acid	2738
<i>p</i> -Toluic acid	2741
<i>o</i> -Toluidine (2-Methylbenzeneamine)	3263
<i>m</i> -Toluidine (3-Methylbenzeneamine)	3267
<i>p</i> -Toluidine (4-Methylbenzeneamine)	3270
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Toxaphene.....	3975
Triadimefon	4103
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1,2,4-Tribromobenzene	1424
1,3,5-Tribromobenzene	1425
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2',3,4-Tribromodiphenyl ether (BDE-33).....	2419
3,3',4-Tribromodiphenyl ether (BDE-35).....	2420
3,4,4'-Tribromodiphenyl ether (BDE-37).....	2421
Tribromomethane	1134
Tributyl phosphate (TBP)	3165
Trichlorfon	3980
Trichloroacetic acid	2725
2,3,4-Trichloroanisole	2339
2,4,6-Trichloroanisole	2340
1,2,3-Trichlorobenzene.....	1298
1,2,4-Trichlorobenzene.....	1305
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2,2',3-Trichlorobiphenyl (PCB-16)	1542
2,2',4-Trichlorobiphenyl (PCB-17)	1545
2,2',5-Trichlorobiphenyl (PCB-18)	1547
2,2',6-Trichlorobiphenyl (PCB-19)	1551
2,3,3'-Trichlorobiphenyl (PCB-20)	1553
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2,3,5-Trichlorobiphenyl (PCB-23)	1559
2,3,6-Trichlorobiphenyl (PCB-24)	1561
2,3',4-Trichlorobiphenyl (PCB-25)	1564
2,3',5-Trichlorobiphenyl (PCB-26)	1566
2,3',6-Trichlorobiphenyl (PCB-27)	1568
2,4,4'-Trichlorobiphenyl (PCB-28)	1570
2,4,5-Trichlorobiphenyl (PCB-29)	1574
2,4,6-Trichlorobiphenyl (PCB-30)	1578
2,4',5-Trichlorobiphenyl (PCB-31)	1580
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2,3',4'-Trichlorobiphenyl (PCB-33)	1586
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Appendix 3

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106-43-4	4-Chlorotoluene	1357
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106-46-7	1,4-Dichlorobenzene	1287
106-47-8	4-Chloroaniline	3257
106-48-9	4-Chlorophenol	2886
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115-10-6	Dimethyl ether (Methyl ether)	2262
115-11-7	2-Methylpropene	270
115-25-3	Perfluorocyclobutane	1209
115-29-7	Endosulfan	3835
115-32-2	Dicofol	4054
115-86-6	Triphenyl phosphate	3149
115-90-2	Fensulfathion	3857
115-96-8	Tris(2-chloroethyl) phosphate	3171
116-06-3	Aldicarb	3717
116-14-3	Tetrafluoroethene	1209
116-15-4	Hexafluoropropene	1209
117-80-6	Dichlone	4052
117-81-7	Bis(2-ethylhexyl) phthalate (DEHP)	3118
117-84-0	Di- <i>n</i> -octyl phthalate (DOP)	3113
118-69-4	2,6-Dichlorotoluene	1362
118-74-1	Hexachlorobenzene	1343

118-90-1	2-Methylbenzoic acid (<i>o</i> -Toluic acid)	2735
118-91-2	2-Chlorobenzoic acid	2751
118-96-7	2,4,6-Trinitrotoluene	3320
119-06-2	Di-tridecyl phthalate	3133
119-61-9	Benzophenone	2670
119-64-2	Tetralin	594
119-65-3	Isoquinoline	3369
120-12-7	Anthracene	725
120-36-5	Dichlorprop	3537
120-51-4	Benzyl benzoate	3077
120-72-9	Indole	3346
120-80-9	Catechol (1,2-Dihydroxybenzene)	2952
120-82-1	1,2,4-Trichlorobenzene	1305
120-83-2	2,4-Dichlorophenol	2892
121-14-2	2,4-Dinitrotoluene (DNT)	3313
121-33-5	Vanillin	2983
121-69-7	N,N'-Dimethylaniline	3274
121-75-5	Malathion	3912
122-14-5	Fenitrothion	3851
122-34-9	Simazine	3649
122-39-4	Diphenylamine	3279
122-42-9	Propham	3645
122-66-7	N,N'-Bianiline	3287
123-01-3	Dodecylbenzene	569
123-02-4	Tridecylbenzene	572
123-07-9	<i>p</i> -Ethylphenol	2853
123-31-9	Hydroquinone (1,4-Dihydroxybenzene)	2964
123-38-6	Propanal (Propionaldehyde)	2595
123-72-8	Butanal (<i>n</i> -Butylaldehyde)	2600
123-86-4	Butyl acetate	3052
123-91-1	1,4-Dioxane	2309
124-11-8	1-Nonene	311
124-18-5	<i>n</i> -Decane	159
124-40-3	Dimethylamine	3218
124-48-1	Dibromochloromethane	1190
126-72-7	Tris(2,3-dibromopropyl) phosphate	3175
126-73-8	Tributyl phosphate	3165
126-99-8	Chloroprene	1117
127-18-4	Tetrachloroethylene	1104
129-00-0	Pyrene	748
131-11-3	Dimethyl phthalate (DMP)	3079
131-16-8	Di- <i>n</i> -propyl phthalate	3092
131-17-9	Diallyl phthalate	3090
131-18-0	Di-pentyl phthalate	3106
132-64-9	Dibenzofuran	2168
132-65-0	Dibenzothiophene	3421
133-06-2	Captan	4037
133-07-3	Folpet	4065
133-90-4	Chloramben	3499
134-32-7	α -Naphthylamine (1-Aminonaphthalene)	3289
135-19-3	2-Naphthol	2868
135-48-8	Pentacene	835
135-98-8	<i>sec</i> -Butylbenzene	528
137-26-8	Thiram	4097
137-30-4	Ziram	4114

139-40-2	Propazine	3642
140-88-5	Ethyl acrylate	3062
141-43-5	Ethanolamine	3236
141-66-2	Dicrotophos	3816
141-78-6	Ethyl acetate	3041
142-29-0	Cyclopentene	349
142-62-1	Hexanoic acid (Caproic acid)	2712
142-68-7	Tetrahydropyran	2307
142-82-5	<i>n</i> -Heptane	129
142-96-1	Di- <i>n</i> -butyl ether	2289
143-08-8	1-Nonanol	2546
143-50-0	Kepone	3893
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150-68-5	Monuron	3602
150-76-5	4-Methoxyphenol	2972
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156-60-5	<i>trans</i> -1,2-Dichloroethene	1084
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191-24-2	Benzo[<i>ghi</i>]perylene	823
192-97-2	Benzo[<i>e</i>]pyrene	811
193-39-5	Indeno[1,2,3- <i>cd</i>]pyrene	826
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205-82-3	Benzo[<i>j</i>]fluoranthene	799
205-99-2	Benzo[<i>b</i>]fluoranthene	796
206-44-0	Fluoranthene	759
207-08-9	Benzo[<i>k</i>]fluoranthene	800
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260-94-6	Acridine	3380
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298-01-1	Mevinphos	3925
298-02-2	Phorate	3959
298-04-4	Disulfoton	3832
299-84-3	Ronnel	3969
300-76-5	Naled	3932
306-83-2	1,1-Dichlorotrifluoroethane	1209
309-00-2	Aldrin	3721
311-81-9	1,2-Dichloro-1,2-difluoroethene	1209
314-40-9	Bromacil	3486
319-84-6	α -HCH	3869
319-85-7	β -HCH	3876
319-86-8	δ -HCH	3881
330-54-1	Diuron	3551
330-55-2	Linuron	3580
333-41-5	Diazinon	3804
338-65-8	1-Chloro-2,2-difluoroethane	1209

344-07-0	Chloropentafluorobenzene	1406
353-36-6	Fluoroethane	1209
354-33-6	Pentafluoroethane	1209
354-58-5	1,1,1-Trichloro-2,2,2-trifluoroethane	1209
355-25-9	Perfluorobutane	1209
355-42-0	Perfluorohexane	1209
355-68-0	Perfluorocyclohexane	1209
359-35-3	1,1,2,2-Tetrafluoroethane	1209
367-11-3	1,2-Difluorobenzene	1209
372-18-9	1,3-Difluorobenzene	1386
374-07-2	1,1-Dichloro-1,2,2,2-tetrafluoroethane	1209
376-77-2	Perfluorocyclopentane	1209
392-56-3	Hexafluorobenzene	1401
406-33-7	1-Fluoropropene	1209
420-26-8	2-Fluoropropane	1209
420-45-1	2,2-Difluoropropane	1209
420-46-2	1,1,1-Trifluoroethane	1209
421-04-5	1-Chloro-1,1,2-trifluoroethane	1209
430-53-5	1,1-Dichloro-2-fluoroethane	1209
430-66-0	1,1,2-Trifluoroethane	1209
431-63-0	1,1,1,2,3,3-Hexafluoropropane	1209
431-89-0	1,1,1,2,3,3,3-Heptafluoropropane	1209
460-73-1	1,1,1,3,3-Pentafluoropropane	1209
462-06-6	Fluorobenzene	1380
463-82-1	2,2-Dimethylpropane (Neopentane)	67
464-06-2	2,2,3-Trimethylbutane	83
470-90-6	Chlorfenvinphos	3758
488-23-3	1,2,3,4-Tetramethylbenzene	536
496-11-7	Indan	620
504-84-1	2,2,4-Trimethylpentane (Isooctane)	109
513-35-9	2-Methyl-2-butene	283
513-81-5	2,3-Dimethyl-1,3-butadiene	328
526-73-8	1,2,3-Trimethylbenzene	476
526-75-0	2,3-Dimethylphenol	2821
527-53-7	1,2,3,5-Tetramethylbenzene	539
527-60-6	2,4,6-Trimethylphenol	2848
527-54-8	3,4,5-Trimethylphenol	2849
533-74-4	Dazomet	4051
534-22-5	2-Methylfuran	2301
534-52-1	4,6-Dinitro- <i>o</i> -cresol	2950
535-80-8	3-Chlorobenzoic acid	2753
538-68-1	Pentylbenzene	547
538-93-2	Isobutylbenzene	525
539-30-0	Benzyl ethyl ether	2351
540-36-3	1,4-Difluorobenzene	1388
540-54-5	1-Chloropropane (<i>n</i> -Propyl chloride)	1024
541-73-1	1,3-Dichlorobenzene	1278
542-69-8	1-Iodobutane	1183
542-75-6	1,3-Dichloropropene	1115
542-88-1	Bis(chloromethyl)ether	2317
543-59-9	1-Chloropentane	1047
544-10-5	1-Chlorohexane	1050
544-25-2	Cycloheptatriene	367
554-84-7	3-Nitrophenol	2937
555-37-3	Neburon	3608

562-49-2	3,3-Dimethylpentane	105
563-04-2	Tricresyl phosphate (<i>m</i> -TCP)	3152
563-12-2	Ethion	3847
563-45-1	3-Methyl-1-butene	280
563-46-2	2-Methyl-1-butene	276
565-75-3	2,3,4-Trimethylpentane	112
571-58-4	1,4-Dimethylnaphthalene	653
571-61-9	1,5-Dimethylnaphthalene	655
575-41-7	1,3-Dimethylnaphthalene	651
576-26-1	2,6-Dimethylphenol	2834
580-13-2	2-Bromonaphthalene	879
580-48-3	Chlorazine	3501
581-42-0	2,6-Dimethylnaphthalene	659
581-40-8	2,3-Dimethylnaphthalene	657
583-53-9	1,2-Dibromobenzene	1416
583-61-9	2,3-Dimethylpyridine	3362
589-34-4	3-Methylhexane	125
589-81-1	3-Methylheptane	139
590-35-2	2,2-Dimethylpentane	101
591-17-3	3-Bromotoluene	1433
591-49-1	1-Methylcyclohexene	357
591-50-4	Iodobenzene	1437
591-76-4	2-Methylhexane (Isoheptane)	123
591-78-6	2-Hexanone	2650
591-93-5	1,4-Pentadiene	330
592-27-8	2-Methylheptane	137
592-42-7	1,5-Hexadiene	334
592-76-7	1-Heptene	304
593-53-3	Fluoromethane	1209
593-60-2	Vinyl bromide	1167
593-70-4	Chlorofluoromethane	1209
605-45-8	Di-isopropyl phthalate	3094
606-20-2	2,6-Dinitrotoluene	3317
608-21-9	1,2,3-Tribromobenzene	1423
608-29-7	1,2,3-Triiodobenzene	1444
608-93-5	Pentachlorobenzene	1335
611-14-3	1-Ethyl-2-methylbenzene	505
613-12-7	2-Methylantracene	739
613-33-2	4,4'-Dimethylbiphenyl	678
615-42-9	1,2-Diiodobenzene	1441
615-54-3	1,2,4-Tribromobenzene	1424
615-68-9	1,2,4-Triiodobenzene	1445
620-14-4	1-Ethyl-3-methylbenzene (<i>m</i> -Ethyltoluene)	508
621-64-7	<i>n</i> -Nitrosodipropylamine	3338
622-96-8	1-Ethyl-4-methylbenzene	512
622-97-9	<i>p</i> -Methyl styrenes	591
623-12-1	4-Chloroanisole	2336
624-38-4	1,4-Diiodobenzene	1443
624-72-6	1,2-Difluoroethane	1209
624-92-0	Dimethyl disulfide	3391
626-00-6	1,3-Diiodobenzene	1442
626-39-1	1,3,5-Tribromobenzene	1425
626-44-8	1,3,5-Triiodobenzene	1446
627-19-0	1-Pentyne	340
627-20-3	<i>cis</i> -2-Pentene	292

628-41-1	1,4-Cyclohexadiene	364
628-63-7	Pentyl acetate	3057
628-71-7	1-Heptyne	344
628-81-9	Butyl ethyl ether	2285
628-92-2	Cycloheptene	359
628-17-1	1-Iodopentane	1185
629-04-9	1-Bromoheptane	1161
629-05-0	1-Octyne	346
629-06-1	1-Chloroheptane	1054
630-20-6	1,1,1,2-Tetrachloroethane	1004
634-66-2	1,2,3,4-Tetrachlorobenzene	1320
634-90-2	1,2,3,5-Tetrachlorobenzene	1326
636-28-2	1,2,4,5-Tetrabromobenzene	1427
644-08-6	4-Methylbiphenyl	677
645-56-7	4-Propylphenol	2857
646-04-8	1-Hexene	299
646-31-1	<i>n</i> -Tetracosane	201
678-26-2	Perfluoropentane	1209
679-86-7	1,1,2,2,3-Pentafluoropropane	1209
690-39-1	1,1,1,3,3,3-Hexafluoropropane	1209
691-37-2	4-Methyl-1-pentene	297
693-02-7	1-Hexyne	342
697-82-5	2,3,5-Trimethylphenol	2845
700-12-9	Pentamethylbenzene	545
709-98-8	Propanil	3639
731-27-1	Tolylfluanid	4101
732-11-6	Phosmet	3962
759-94-4	EPTC	3555
762-50-5	1-Chloro-2-fluoroethane	1209
763-29-1	2-Methyl-1-pentene	295
766-51-8	2-Chloroanisole	2334
771-56-2	Pentafluorotoluene	1404
771-61-9	Pentafluorophenol	1408
779-02-2	9-Methylanthracene	742
786-19-6	Carbophenothion	3746
781-43-1	9,10-Dimethylanthracene	745
789-02-6	<i>o,p'</i> -DDT	3785
811-97-2	1,1,1,2-Tetrafluoroethane	1209
818-92-8	3-Fluoropropane	1209
832-69-6	1-Methylphenanthrene	722
834-12-8	Ametryn	3466
872-05-9	1-Decene	314
877-11-2	Pentachlorotoluene	1373
886-50-0	Terbutryn	3659
935-95-5	2,3,5,6-Tetrachlorophenol	2921
938-86-3	2,3,4,5-Tetrachloroanisole	2341
939-27-5	2-Ethylanthracene	665
944-22-9	Fonofos	3867
944-61-6	Tetrachloroveratrole	2347
957-51-7	Diphenamid	3547
959-98-8	Endosulfan I, α -endosulfan	3835
1024-57-3	Heptachlor epoxide	3890
1071-83-6	Glyphosate	3572
1073-67-2	<i>p</i> -Chlorostyrene	1377
1077-16-3	Hexylbenzene	553

1078-71-3	Heptylbenzene	557
1114-71-2	Pebulate	3618
1120-21-4	<i>n</i> -Undecane	164
1127-76-0	1-Ethyl-naphthalene	661
1163-19-5	Decabromodiphenyl ether (PBDE-209)	2453
1194-65-6	Dichlobenil	3534
1198-55-6	Tetrachlorocatechol	2959
1241-94-7	2-Ethylhexyl diphenyl phosphate	3161
1459-10-5	Tetradecylbenzene	574
1563-66-2	Carbofuran	3742
1582-09-8	Trifluralin	3670
1595-06-0	2,3,4-Trichlorophenol	2903
1610-18-0	Prometon	3628
1634-04-4	Methyl <i>t</i> -butyl ether	2271
1649-08-7	1,2-Dichloro-1,1-difluoroethane	1209
1678-91-7	Ethylcyclohexane	249
1689-84-5	Bromoxynil	3489
1698-60-8	Pyrazon	3647
1717-00-6	1,1-Dichloro-1-fluoroethane	1209
1730-37-6	1-Methylfluorene	708
1746-01-6	2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	2111
1746-81-2	Monolinuron	3600
1806-26-4	4-Octylphenol	2861
1825-31-6	1,4-Dichloronaphthalene	849
1836-75-5	Nitrofen	3612
1861-40-1	Benefin	3482
1897-45-6	Chlorothalonil	4049
1912-24-9	Atrazine	3471
1918-00-9	Dicamba	3530
1918-02-1	Picloram	3622
1918-16-7	Propachlor	3636
1929-77-7	Vernolate	3677
1929-82-4	Nitrapyrin	4082
1984-59-4	2,3-Dichloroanisole	2337
1984-65-2	2,6-Dichloroanisole	2338
2008-41-5	Butylate	3497
2032-59-9	Aminocarb	3728
2032-65-7	Methiocarb	3916
2039-85-2	<i>m</i> -Chlorostyrene	1375
2039-87-4	<i>o</i> -Chlorostyrene	1374
2040-96-2	Propylcyclopentane	221
2050-47-7	4,4'-Dibromodiphenyl ether (PBDE-15)	2410
2050-67-1	3,3'-Dichlorobiphenyl (PCB-11)	1528
2050-68-2	4,4'-Dichlorobiphenyl (PCB-15)	1537
2050-69-3	1,2-Dichloronaphthalene	848
2050-74-0	1,8-Dichloronaphthalene	851
2050-75-1	2,3-Dichloronaphthalene	852
2051-24-3	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl (PCB-209)	1995
2051-60-7	2-Chlorobiphenyl (PCB-1)	1492
2051-61-8	3-Chlorobiphenyl (PCB-2)	1497
2051-62-9	4-Chlorobiphenyl (PCB-3)	1501
2077-46-5	2,3,6-Trichlorotoluene	1365
2104-96-3	Bromophos	3734
2131-41-1	1,4,5-Trimethylnaphthalene	668
2136-99-4	2,2',3,3',5,5',6,6'-Octachlorobiphenyl (PCB-202)	1979

2164-17-2	Fluometuron	3566
2198-77-8	2,7-Dichloronaphthalene	853
2207-01-4	1,2- <i>cis</i> -Dimethylcyclohexane	240
2207-04-7	1,4- <i>trans</i> -Dimethylcyclohexane	245
2212-67-1	Molinate	3597
2216-34-4	4-Methyloctane	150
2234-13-1	Octachloronaphthalene	873
2268-46-4	1,1,1,3-Tetrachlorotetrafluoropropane	1209
2303-16-4	Diallate	3527
2303-17-5	Triallate	3664
2312-35-8	Propargite	1490
2315-68-6	Propyl benzoate	3075
2385-85-5	Mirex	3927
2437-79-8	2,2',4,4'-Tetrachlorobiphenyl (PCB-47)	1617
2460-49-3	4,5-Dichloroguaiacol	2975
2473-01-0	1-Chlorononane	1059
2539-17-5	Tetrachloroguaiacol	2981
2539-26-6	Trichlorosyringol	2992
2593-15-9	Etridiazole	4060
2597-03-7	Phenthoate	3957
2668-24-8	4,5,6-Trichloroguaiacol	2979
2675-77-6	Chloroneb	4044
2764-72-9	Diquat	3549
2772-46-5	4,5-Dichloroveratrole	2345
2837-89-0	1-Chloro-1,2,2,2-tetrafluoroethane	1209
2845-89-8	2-Chloroanisole	2335
2921-88-2	Chlorpyrifos	3760
2974-90-5	3,4'-Dichlorobiphenyl (PCB-13)	1533
2974-92-7	3,4-Dichlorobiphenyl (PCB-12)	1530
3070-53-9	1,6-Heptadiene	337
3073-66-3	1,1,3-Trimethylcyclohexane	247
3268-87-9	Octachlorodibenzo- <i>p</i> -dioxin	2148
3347-22-6	Dithianon	4056
3424-82-6	<i>o,p'</i> -DDE	3779
3428-24-8	4,5-Dichlorocatechol	2957
3452-09-3	1-Nonyne	348
3522-94-9	2,2,5-Trimethylhexane	127
3741-00-2	Pentylcyclopentane	223
4516-69-2	1,1,3-Trimethylcyclopentane	219
4726-14-1	Nitralin	3710
4824-78-6	Bromofos-ethyl	3736
4901-51-3	2,3,4,5-Tetrachlorophenol	2916
5234-68-4	Carboxin	4042
5254-12-6	Cresyl diphenyl phosphate (<i>o</i> -CDP)	3141
5259-88-1	Oxycarboxin	4084
5409-83-6	2,8-Dichlorodibenzofuran	2181
5436-43-1	2,2',4,4'-Tetrabromodiphenyl ether (PBDE-47)	2422
5598-13-0	Chlorpyrifos-methyl	3765
5902-51-2	Terbacil	3657
5989-27-5	<i>dextro</i> -Limonene [(<i>R</i>)-(+)-limonene]	371
6639-30-1	2,4,5-Trichlorotoluene	1366
6742-54-7	Undecylbenzene	567
6876-00-2	3-Bromodiphenyl ether (PBDE-2)	2402
6923-22-4	Monocrotophos	3930
6936-40-9	Tetrachloroanisole	2342

7005-72-3	4-Chlorophenyl phenyl ether	2360
7012-37-5	2,4,4'-Trichlorobiphenyl (PCB-28)	1570
7025-06-1	2-Bromodiphenyl ether(PBDE-1)	2401
7085-19-0	Mecoprop	3589
7287-19-6	Prometryn	3631
7700-17-6	Crotoxyphos	3767
8001-35-2	Toxaphene.	3975
8065-48-3	Demeton	3800
10311-84-9	Dialifos	3802
10605-21-7	Carbendazim.	4040
11096-82-5	Aroclor 1260.	2030
11097-69-1	Aroclor 1254.	2026
11104-28-2	Aroclor 1221.	2017
11141-16-5	Aroclor 1232.	2019
12122-67-7	Zineb.	4112
12427-38-2	Maneb.	4078
12672-29-6	Aroclor 1248.	2024
12674-11-2	Aroclor 1016.	2015
13029-08-8	2,2'-Dichlorobiphenyl (PCB-4)	1508
13071-79-9	Terbufos	3971
13194-48-4	Ethoprophos (Ethoprop).	3849
13360-45-7	Chlorbromuron	3502
13654-09-6	Decabromobiphenyl	890
13673-92-2	3,5-Dichlorocatechol	2956
15299-99-7	Napropamide	3606
15457-05-3	Fluorodifen	3568
15545-48-9	Chlortoluron	3510
15862-07-4	2,4,5-Trichlorobiphenyl (PCB-29)	1574
15968-05-5	2,2',6,6'-Tetrachlorobiphenyl (PCB-54).	1639
15972-60-8	Alachlor	3461
16605-91-7	2,3-Dichlorobiphenyl (PCB-5).	1511
16606-02-3	2,4',5-Trichlorobiphenyl (PCB-31)	1580
16752-77-5	Methomyl	3918
16766-29-3	3,4,5-Trichloroveratrole	2346
16766-30-6	4-Chloroguaiacol	2973
17109-49-8	Edifenphos	4058
17804-35-2	Benomyl	4031
18113-22-9	3-Chlorosyringol.	2990
18259-05-7	2,3,4,5,6-Pentachlorobiphenyl (PCB-116)	1786
18268-69-4	5,6-Dichlorovanillin	2988
18268-76-3	6-Chlorovanillin	2987
19044-88-3	Oryzalin	3616
19463-48-0	5-Chlorovanillin	2985
20020-02-4	1,2,3,4-Tetrachloronaphthalene	857
21087-64-9	Metribuzin	3595
21609-90-5	Leptophos	3896
21725-46-2	Cyanazine	3513
22781-23-3	Bendiocarb	3732
23103-98-2	Primicarb	3964
23135-22-0	Oxamyl	3934
23184-66-9	Butachlor	3493
23564-05-8	Thiophanate-methyl	4095
23950-58-5	Pronamide.	3634
24478-72-6	1,2,3,4-Tetrachlorodibenzofuran	2193
24691-80-3	Fenfuram.	4064

25074-67-3	3-Chlorodibenzofuran	2175
25155-15-1	1-Isopropyl-4-methylbenzene	516
25569-80-6	2,3-Dichlorobiphenyl (PCB-6)	1514
26259-45-0	<i>sec</i> -Bumeton	3491
26399-36-0	Profluralin	3626
26644-46-2	Triforine	4107
26761-40-0	Di-isodecyl phthalate	3129
27193-28-8	4-Octylphenol	2861
27314-13-2	Norflurazon	3614
27554-26-3	Di-isooctyl phthalate	3116
28076-73-5	2,2',4,4'-Tetrachloro-DPE (PCDE-47)	2368
28249-77-6	Thiobencarb	3662
28419-69-4	2,6-Dichloro DPE (PCDE-10)	2363
28533-12-0	Di-isononyl phthalate	3127
29082-74-4	Octachlorostyrene	1379
29091-05-2	Dinitramine	3542
29446-15-9	2,3-Dichlorodibenzo- <i>p</i> -dioxin	2073
29973-13-5	Ethiofencarb	3845
30560-19-1	Acephate	3715
30746-58-8	1,2,3,4-Tetrachlorodibenzo- <i>p</i> -dioxin	2092
31508-00-6	2,3',4,4',5-Pentachlorobiphenyl (PCB-118)	1790
31604-28-1	1,3,5,8-Tetrachloronaphthalene	862
31710-30-2	Decachlorodiphenyl ether (PCDE-209)	2400
32598-10-0	2,3',4,4'-Tetrachlorobiphenyl (PCB-66)	1666
32598-11-1	2,3',4',5-Tetrachlorobiphenyl (PCB-70)	1676
32598-12-2	2,4,4',6-Tetrachlorobiphenyl (PCB-75)	1689
32598-13-3	3,3',4,4'-Tetrachlorobiphenyl (PCB-77)	1693
32598-14-4	2,3,3',4,4'-Pentachlorobiphenyl (PCB-105)	1761
32690-93-0	2,4,4',5-Tetrachlorobiphenyl (PCB-74)	1686
32774-16-6	3,3',4,4',5,5'-Hexachlorobiphenyl (PCB-169)	1909
32809-16-8	Procymidone	4088
33146-45-1	2,6-Dichlorobiphenyl (PCB-10)	1525
33213-65-9	Endosulfan II, β -endosulfan	3835
33025-41-1	2,3,4,4'-Tetrachlorobiphenyl (PCB-60)	1651
33091-17-7	2,2',3,3',4,4',6,6'-Octachlorobiphenyl (PCB-197)	1969
33245-39-5	Fluchloralin	3564
33284-50-3	2,4-Dichlorobiphenyl (PCB-7)	1516
33284-52-5	3,3',5,5'-Tetrachlorobiphenyl (PCB-80)	1702
33284-53-6	2,3,4,5-Tetrachlorobiphenyl (PCB-61)	1654
33284-54-7	2,3,5,6-Tetrachlorobiphenyl (PCB-65)	1664
33423-92-6	1,3,6,8-Tetrachlorodibenzo- <i>p</i> -dioxin	2102
33629-47-9	Butralin	3495
33820-53-0	Isopropalin	3575
33857-26-0	2,7-Dichlorodibenzo- <i>p</i> -dioxin	2076
33857-28-2	2,3,7-Trichlorodibenzo- <i>p</i> -dioxin	2089
33979-03-2	2,2',4,4',6,6'-Hexachlorobiphenyl (PCB-155)	1879
34123-59-6	Isoproturon	3577
34816-53-0	1,2,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	2100
34883-39-1	2,5-Dichlorobiphenyl (PCB-9)	1522
34883-41-5	3,5-Dichlorobiphenyl (PCB-14)	1535
34883-43-7	2,4'-Dichlorobiphenyl (PCB-8)	1519
35065-27-1	2,2',4,4',5,5'-Hexachlorobiphenyl (PCB-153)	1870
35065-28-2	2,2',3,4,4',5'-Hexachlorobiphenyl (PCB-138)	1835
35065-29-3	2,2',3,4,4',5,5'-Heptachlorobiphenyl (PCB-180)	1931
35065-30-6	2,2',3,3',4,4',5-Heptachlorobiphenyl (PCB-170)	1911

35367-38-5	Diflubenzuron	3827
35554-44-0	Imazalil	4075
35693-92-6	2,4,6-Trichlorobiphenyl (PCB-30)	1578
35693-99-3	2,2',5,5'-Tetrachlorobiphenyl (PCB-52)	1629
35694-04-3	2,2',3,3',5,5'-Hexachlorobiphenyl (PCB-133)	1824
35694-06-5	2,2',3,4,4',5-Hexachlorobiphenyl (PCB-137)	1833
35694-08-7	2,2',3,3',4,4',5,5'-Octachlorobiphenyl (PCB-194)	1962
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo- <i>p</i> -dioxin	2141
36559-22-5	2,2',3,4'-Tetrachlorobiphenyl (PCB-42)	1606
37680-65-2	2,2',5-Trichlorobiphenyl (PCB-18)	1547
37680-66-3	2,2',4-Trichlorobiphenyl (PCB-17)	1545
37680-68-5	2,3',5'-Trichlorobiphenyl (PCB-34)	1589
37680-69-6	3,3',4-Trichlorobiphenyl (PCB-35)	1591
37680-72-3	2,2',4,5,5'-Pentachlorobiphenyl (PCB-101)	1748
38379-99-6	2,2',3,5',6-Pentachlorobiphenyl (PCB-95)	1733
38380-01-7	2,2',4,4',5-Pentachlorobiphenyl (PCB-99)	1743
38380-02-8	2,2',3,4,5'-Pentachlorobiphenyl (PCB-87)	1716
38380-03-9	2,3,3',4',6-Pentachlorobiphenyl (PCB-110)	1773
38380-04-0	2,2',3,4',5',6-Hexachlorobiphenyl (PCB-149)	1861
38380-05-1	2,2',3,3',4,6'-Hexachlorobiphenyl (PCB-132)	1822
38380-07-3	2,2',3,3',4,4'-Hexachlorobiphenyl (PCB-128)	1813
38380-08-4	2,3,3',4,4',5-Hexachlorobiphenyl (PCB-156)	1883
38411-22-2	2,2',3,3',6,6'-Hexachlorobiphenyl (PCB-136)	1830
38411-25-5	2,2',3,3',4,5,6'-Heptachlorobiphenyl (PCB-174)	1919
38444-73-4	2,2',6-Trichlorobiphenyl (PCB-19)	1551
38444-76-7	2,3',6-Trichlorobiphenyl (PCB-27)	1568
38444-77-8	2,4',6'-Trichlorobiphenyl (PCB-32)	1584
38444-78-9	2,2',3-Trichlorobiphenyl (PCB-16)	1542
38444-81-4	2,3',5-Trichlorobiphenyl (PCB-26)	1566
38444-84-7	2,3,3'-Trichlorobiphenyl (PCB-20)	1553
38444-85-8	2,3,4'-Trichlorobiphenyl (PCB-22)	1557
38444-86-9	2,3',4'-Trichlorobiphenyl (PCB-33)	1586
38444-87-0	3,3',5-Trichlorobiphenyl (PCB-36)	1593
38444-88-1	3,4',5-Trichlorobiphenyl (PCB-39)	1599
38444-90-5	3,4,4'-Trichlorobiphenyl (PCB-37)	1595
38444-93-8	2,2',3,3'-Tetrachlorobiphenyl (PCB-40)	1601
38964-22-6	2,8-Dichlorodibenzo- <i>p</i> -dioxin	2080
39001-02-0	Octachlorodibenzofuran	2242
39227-26-8	1,2,3,4,7,8-Hexachlorodibenzo- <i>p</i> -dioxin	2128
39227-53-7	1-Chlorodibenzo- <i>p</i> -dioxin	2067
39227-54-8	2-Chlorodibenzo- <i>p</i> -dioxin	2070
39227-58-2	1,2,4-Trichlorodibenzo- <i>p</i> -dioxin	2083
39227-61-7	1,2,3,4,7-Pentachlorodibenzo- <i>p</i> -dioxin	2119
39485-83-1	2,2',4,4',6-Pentachlorobiphenyl (PCB-100)	1746
39515-41-8	Fenpropathrin	3855
39635-31-9	2,3,3',4,4',5,5'-Heptachlorobiphenyl (PCB-189)	1952
39635-32-0	2,3,3',5,5'-Pentachlorobiphenyl (PCB-111)	1776
39635-33-1	3,3',4,5,5'-Pentachlorobiphenyl (PCB-127)	1811
39635-34-2	2,3,3',4',5,5'-Hexachlorobiphenyl (PCB-162)	1895
39635-35-3	2,3,3',4,5,5'-Hexachlorobiphenyl (PCB-159)	1889
40186-70-7	2,2',3,3',4,5',6-Heptachlorobiphenyl (PCB-175)	1921
40186-71-8	2,2',3,3',4,5',6,6'-Octachlorobiphenyl (PCB-201)	1977
40186-72-9	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl (PCB-206)	1989
40321-76-4	1,2,3,7,8-Pentachlorodibenzo- <i>p</i> -dioxin	2123
40487-42-1	Pendimethalin	3620

41318-75-6	2,4,4'-Tribromodiphenyl ether (PBDE-28)	2414
41411-61-4	2,2',3,4,5,6-Hexachlorobiphenyl (PCB-142)	1847
41411-62-5	2,3,3',4,5,6-Hexachlorobiphenyl (PCB-160).	1891
41411-63-6	2,3,4,4',5,6-Hexachlorobiphenyl (PCB-166).	1903
41411-64-7	2,3,3',4,4',5,6-Heptachlorobiphenyl (PCB-190)	1954
41464-40-8	2,2',4,5'-Tetrachlorobiphenyl (PCB-49).	1622
41464-39-5	2,2',3,5'-Tetrachlorobiphenyl (PCB-44).	1610
41464-41-9	2,2',5,6'-Tetrachlorobiphenyl (PCB-53).	1636
41464-42-0	2,4',5,5'-Tetrachlorobiphenyl (PCB-72).	1682
41464-43-1	2,3,3',4'-Tetrachlorobiphenyl (PCB-56).	1647
41464-46-4	2,3',4',6-Tetrachlorobiphenyl (PCB-71).	1680
41464-47-5	2,2',3,6'-Tetrachlorobiphenyl (PCB-46).	1615
41464-48-6	3,3',4,5'-Tetrachlorobiphenyl (PCB-79).	1700
41464-49-7	2,3,3',5'-Tetrachlorobiphenyl (PCB-58).	1647
41464-51-1	2,2',3,4',5'-Pentachlorobiphenyl (PCB-97)	1738
41483-43-6	Bupirimate	4035
42576-02-3	Bifenox	3484
42740-50-1	2,2',3,3',4,4',5,6'-Octachlorobiphenyl (PCB-196)	1967
43121-43-3	Triadimefon	4103
50471-44-8	Vinclozolin	4108
50585-46-1	1,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	2107
51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	2205
51218-45-2	Metolachlor.	3591
51230-49-0	2-Chlorodibenzofuran.	2173
51338-27-3	Diclofop-methyl	3539
51630-58-1	Fenvalerate	3862
51892-26-3	2,4-Dichloro DPE (PCDE-8)	2362
51908-16-8	2,2',3,4',5,5'-Hexachlorobiphenyl (PCB-146)	1855
51930-04-2	2,6-Dibromodiphenyl ether (PBDE-10).	2407
52315-07-8	Cypermethrin	3772
52645-53-1	Permethrin	3953
52663-58-8	2,3,4',6-Tetrachlorobiphenyl (PCB-64)	1662
52663-59-9	2,2',3,4-Tetrachlorobiphenyl(PCB-41).	1604
52663-60-2	2,2',3,3',6-Pentachlorobiphenyl (PCB-84)	1710
52663-61-3	2,2',3,5,5'-Pentachlorobiphenyl (PCB-92)	1727
52663-62-4	2,2',3,3',4-Pentachlorobiphenyl (PCB-82)	1706
52663-63-5	2,2',3,5,5',6-Heptachlorobiphenyl (PCB-151)	1865
52663-64-6	2,2',3,3',5,6,6'-Heptachlorobiphenyl (PCB-179)	1929
52663-65-7	2,2',3,3',4,6,6'-Heptachlorobiphenyl (PCB-176)	1923
52663-66-8	2,2',3,3',4,5'-Hexachlorobiphenyl (PCB-130)	1818
52663-67-9	2,2',3,3',5,5',6-Heptachlorobiphenyl (PCB-178)	1927
52663-68-0	2,2',3,4',5,5',6-Heptachlorobiphenyl (PCB-187)	1947
52663-69-1	2,2',3,4,4',5',6-Heptachlorobiphenyl (PCB-183)	1939
52663-70-4	2,2',3,3',4,5',6'-Heptachlorobiphenyl (PCB-177).	1925
52663-71-5	2,2',3,3',4,4',6-Heptachlorobiphenyl (PCB-171)	1913
52663-72-6	2,3',4,4',5,5'-Hexachlorobiphenyl (PCB-167)	1905
52663-73-7	2,2',3,3',4,5,6,6'-Octachlorobiphenyl (PCB-200)	1975
52663-74-8	2,2',3,3',4,5,5'-Heptachlorobiphenyl (PCB-172)	1915
52663-75-9	2,2',3,3',4,5,5',6'-Octachlorobiphenyl (PCB-199)	1973
52663-76-0	2,2',3,4,4',5,5',6-Octachlorobiphenyl (PCB-203)	1983
52663-77-1	2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl (PCB-208)	1993
52663-78-2	2,2',3,3',4,4',5,6-Octachlorobiphenyl (PCB-195)	1965
52663-79-3	2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl (PCB-207)	1991
52704-70-8	2,2',3,3',5,6-Hexachlorobiphenyl (PCB-134).	1826
52712-04-6	2,2',3,4,5,5'-Hexachlorobiphenyl (PCB-141).	1844

52712-05-7	2,2',3,4,5,5',6-Heptachlorobiphenyl (PCB-185)	1943
52744-13-5	2,2',3,3',5,6'-Hexachlorobiphenyl (PCB-135)	1828
52918-63-5	Deltamethrin	3798
53469-21-9	Aroclor 1242	2021
53555-64-9	1,3,5,7-Tetrachloronaphthalene	860
53555-65-0	1,2,3,5,7-Pentachloronaphthalene	865
53555-66-1	3,4,5-Trichlorobiphenyl(PCB-38)	1597
54135-80-7	2,3,4-Trichloroanisole	2339
54230-23-7	2,3,4,6-Tetrachlorobiphenyl(PCB-62)	1658
54589-71-8	2,4,8-Trichlorodibenzofuran	2190
55215-17-3	2,2',3,4,6-Pentachlorobiphenyl (PCB-88)	1719
55215-18-4	2,2',3,3',4,5-Hexachlorobiphenyl (PCB-129).	1816
55283-68-6	Ethalfuralin	3558
55285-14-8	Carbosulfan	3748
55312-69-1	2,2',3,4,5-Pentachlorobiphenyl (PCB-86)	1714
55335-06-3	Triclopyr	3668
55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzo- <i>p</i> -dioxin	2239
55702-45-9	2,3,6-Trichlorobiphenyl (PCB-24)	1561
55702-46-0	2,3,4-Trichlorobiphenyl (PCB-21)	1555
55712-37-3	2,3',4-Trichlorobiphenyl (PCB-25)	1564
55720-37-1	1,3,7-Trichloronaphthalene	855
55720-44-0	2,3,5-Trichlorobiphenyl (PCB-23)	1577
55864-04-5	<i>p</i> -Isopropylphenyl diphenyl phosphate (<i>p</i> -IPDPD).	3143
56030-56-9	2,2',3,4,4',6-Hexachlorobiphenyl (PCB-139).	1840
56348-72-2	3,3',4,4'-Tetrachloro-DPE (PCDE-77)	2371
56558-16-8	2,2',4,6,6'-Pentachlorobiphenyl (PCB-104)	1759
56558-17-9	2,3',4,4',6-Pentachlorobiphenyl (PCB-119)	1794
56558-18-0	2,3',4,5',6-Pentachlorobiphenyl (PCB-121)	1798
57018-04-9	Tolclofos-methyl	4099
57057-83-7	3,4,5-Trichloroguaiacol	2977
57117-31-4	2,3,4,7,8-Pentachlorodibenzofuran	2215
57117-32-5	2,3,8-Trichlorodibenzofuran	2186
57117-35-8	1,3,7,8-Tetrachlorodibenzofuran	2201
57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	2211
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	2223
57465-28-8	3,3',4,4',5-Pentachlorobiphenyl (PCB-126)	1808
57837-19-1	Metalaxyl	4080
58194-04-7	2,2',4,6'-Tetrachlorobiphenyl (PCB-51).	1627
58802-08-7	1,2,4,7,8-Pentachlorodibenzo- <i>p</i> -dioxin	2126
58802-14-5	2,4,6-Trichlorodibenzofuran	2188
58802-20-3	1,2,7,8-Tetrachlorodibenzofuran	2197
58863-15-3	1,2,3,4,5,6,8-Heptachloronaphthalene	872
59291-64-4	2,2',3,4,4',6'-Hexachlorobiphenyl (PCB-140)	1842
59669-26-0	Thiodicarb.	3973
59756-60-4	Fluridone	3569
60123-64-0	2,2',4,4',5-Petachloro-DPE (PCDE-99)	2374
60145-20-2	2,2',3,3',5-Pentachloro-DPE (PCB-83)	1708
60145-21-3	2,2',4,5',6-Pentachlorobiphenyl (PCB-103)	1757
60145-22-4	2,2',4,4',5,6'-Hexachlorobiphenyl (PCB-154).	1877
60145-23-5	2,2',3,4,4',5,6'-Heptachlorobiphenyl (PCB-182)	1937
60168-88-9	Fenarimol	4062
60207-90-1	Propiconazole	4091
60233-24-1	2,3',4,6-Tetrachlorobiphenyl (PCB-69)	1674
60233-25-2	2,2',3,4',6'-Pentachlorobiphenyl (PCB-98)	1741
60348-60-9	2,2',4,4',5-Pentabromodiphenyl ether (BDE-99)	2433

60851-34-5	1,2,4,6,7,8-Hexachlorodibenzofuran	2232
61328-45-8	2,4,4',5-Tetrachloro-DPE (PCDE-74)	2370
61328-46-9	2,3',4,4'-Tetrachloro-DPE (PCDE-66)	2369
61798-70-7	2,2',3,3',4,6-Hexachlorobiphenyl (PCB-131)	1820
62470-53-5	1,3,7,9-Tetrachlorodibenzo- <i>p</i> -dioxin	2109
62796-65-8	2,2',4,6-Tetrachlorobiphenyl (PCB-50)	1625
62927-67-4	1,2,3,4,5,7-Hexachloronaphthalene	867
64126-86-9	2,3-Dichlorodibenzofuran	2177
64257-84-7	Fenpropathrin (racemate)	3855
64532-94-1	Isopropylphenyl diphenyl phosphate (<i>o</i> -IPPDP)	3143
64532-97-4	Nonylphenyl diphenyl phosphate (<i>p</i> -NPDPP)	3147
64650-17-4	1,3,7,9-Tetrachlorodibenzofuran	2203
64902-72-3	Chlorsulfuron	3507
65075-00-5	2,4',5-Trichloro-DPE (PCDE-31)	2367
65510-44-3	2,3',4,4',5'-Pentachlorobiphenyl (PCB-123)	1802
65510-45-4	2,2',3,4,4'-Pentachlorobiphenyl (PCB-85)	1712
66246-88-6	Penconazole	4086
67028-18-6	1,2,3,7-Tetrachlorodibenzo- <i>p</i> -dioxin	2096
67462-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	2234
68085-85-8	Cyhalothrin	3769
68194-05-8	2,2',3,4',6-Pentachlorobiphenyl (PCB-91)	1725
68194-06-9	2,2',4,5,6'-Pentachlorobiphenyl (PCB-102)	1755
68194-07-0	2,2',3,4',5-Pentachlorobiphenyl (PCB-90)	1723
68194-08-1	2,2',3,4',6,6'-Hexachlorobiphenyl (PCB-150)	1863
68194-09-2	2,2',3,5,6,6'-Hexachlorobiphenyl (PCB-152)	1868
68194-10-5	2,3,3',5',6-Pentachlorobiphenyl (PCB-113)	1780
68194-11-6	2,3,4',5,6-Pentachlorobiphenyl (PCB-117)	1788
68194-12-7	2,3',4,5,5'-Pentachlorobiphenyl (PCB-120)	1796
68194-13-8	2,2',3,4',5,6-Hexachlorobiphenyl (PCB-147)	1857
68194-14-9	2,2',3,4,5',6-Hexachlorobiphenyl (PCB-144)	1851
68194-15-0	2,2',3,4,5,6'-Hexachlorobiphenyl (PCB-143)	1849
68194-16-1	2,2',3,3',4,5,6-Heptachlorobiphenyl (PCB-173)	1917
68194-17-2	2,2',3,3',4,5,5',6-Octachlorobiphenyl (PCB-198)	1971
68515-47-9	Di-tridecyl phthalate	3133
68515-48-0	Di-isononyl phthalate	3127
68515-50-4	Di- <i>n</i> -hexyl phthalate	3108
68631-49-2	2,2',4,4',5,5'-Hexabromodiphenyl ether (PBDE-153)	2443
68694-11-1	Triflumizole	4105
68698-59-5	1,2,4,6,8,9-Hexachlorodibenzofuran	2230
69500-28-3	Cresyl diphenyl phosphate (<i>m</i> -CDP)	3141
69515-46-4	Isopropylphenyl diphenyl phosphate (<i>m</i> -IPPDP)	3143
69698-58-4	1,2,3,4,7,8,9-Heptachlorodibenzofuran	2237
69698-60-8	1,2,3,4,6,8-Hexachlorodibenzofuran	2218
69782-90-7	2,3,3',4,4',5'-Hexachlorobiphenyl (PCB-157)	1885
69782-91-8	2,3,3',4',5,5',6-Heptachlorobiphenyl (PCB-193)	1960
70124-77-5	Flucythrinate	3865
70362-41-3	2,3,3',4,5'-Pentachlorobiphenyl (PCB-108)	1769
70362-45-7	2,2',3,6-Tetrachlorobiphenyl (PCB-45)	1613
70362-46-8	2,2',3,5-Tetrachlorobiphenyl (PCB-43)	1608
70362-47-9	2,2',4,5-Tetrachlorobiphenyl (PCB-48)	1620
70362-48-0	2,3',4',5'-Tetrachlorobiphenyl (PCB-76)	1691
70362-49-1	3,3',4,5-Tetrachlorobiphenyl (PCB-78)	1698
70362-50-4	3,4,4',5-Tetrachlorobiphenyl (PCB-81)	1704
70424-67-8	2,3,3',5-Tetrachlorobiphenyl (PCB-57)	1645
70424-68-9	2,3,3',4',5-Pentachlorobiphenyl (PCB-107)	1767

70424-69-0	2,3,3',4,5-Pentachlorobiphenyl (PCB-106)	1765
70424-70-3	2,3',4',5,5'-Pentachlorobiphenyl (PCB-124)	1804
70585-38-5	Bitertanol	4033
70658-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	2220
71585-36-9	2,2',3,4,4',5-Hexachloro-DPE (PCDE-137)	2382
71585-37-0	2,2',3,4,4'-Petachloro-DPE (PCDE-85)	2373
71585-38-1	2,2',3,4,4',5'-Hexachloro-DPE (PCDE-138)	2384
71585-39-2	2,3,3',4,4'-Petachloro-DPE (PCDE-128)	2381
71626-11-4	Benalaxyl	4029
71859-30-8	2,2',4,4',5,5'-Hexachloro-DPE (PCDE-153)	2386
71998-72-6	1,3,6,8-Tetrachlorodibenzofuran	2199
72918-21-9	1,2,3,7,8,9-Hexachlorodibenzofuran	2226
73575-52-7	2,3',4,5'-Tetrachlorobiphenyl (PCB-68)	1672
73575-53-8	2,3',4,5-Tetrachlorobiphenyl (PCB-67)	1670
73575-54-9	2,2',3,6,6'-Pentachlorobiphenyl (PCB-96)	1736
73575-55-0	2,2',3,5,6'-Pentachlorobiphenyl (PCB-94)	1731
73575-56-1	2,2',3,5,6-Pentachlorobiphenyl (PCB-93)	1729
73575-57-2	2,2',3,4,6'-Pentachlorobiphenyl (PCB-89)	1721
73992-98-6	2,7-Dichlorodibenzofuran	2179
74338-23-1	2,3',5',6-Tetrachlorobiphenyl (PCB-73)	1684
74338-24-2	2,3,3',4-Tetrachlorobiphenyl (PCB-55)	1641
74472-33-6	2,3,3',6-Tetrachlorobiphenyl (PCB-59)	1649
74472-34-7	2,3,4',5-Tetrachlorobiphenyl (PCB-63)	1660
74472-35-8	2,3,3',4,6-Pentachlorobiphenyl (PCB-109)	1771
74472-36-9	2,3,3',5,6-Pentachlorobiphenyl (PCB-112)	1778
74472-37-0	2,3,4,4',5-Pentachlorobiphenyl (PCB-114)	1782
74472-38-1	2,3,4,4',5-Pentachlorobiphenyl (PCB-115)	1784
74472-39-2	2,3',4',5',6-Pentachlorobiphenyl (PCB-125)	1806
74472-40-5	2,2',3,4,6,6'-Hexachlorobiphenyl (PCB-145)	1853
74472-41-6	2,2',3,4',5,6'-Hexachlorobiphenyl (PCB-148)	1859
74472-42-7	2,3,3',4,4',6-Hexachlorobiphenyl (PCB-158)	1887
74472-43-8	2,3,3',4,5',6-Hexachlorobiphenyl (PCB-161)	1893
74472-44-9	2,3,3',4',5,6-Hexachlorobiphenyl (PCB-163)	1897
74472-45-0	2,3,3',4',5',6-Hexachlorobiphenyl (PCB-164)	1899
74472-46-1	2,3,3',5,5',6-Hexachlorobiphenyl (PCB-165)	1901
74472-47-2	2,2',3,4,4',5,6-Heptachlorobiphenyl (PCB-181)	1935
74472-48-3	2,2',3,4,4',6,6'-Heptachlorobiphenyl (PCB-184)	1941
74472-49-4	2,2',3,4,5,6,6'-Heptachlorobiphenyl (PCB-186)	1945
74472-50-7	2,3,3',4,4',5',6-Heptachlorobiphenyl (PCB-191)	1956
74472-51-8	2,3,3',4,5,5',6-Heptachlorobiphenyl (PCB-192)	1958
74472-52-9	2,2',3,4,4',5,6,6'-Octachlorobiphenyl (PCB-204)	1985
74472-53-0	2,3,3',4,4',5,5',6-Octachlorobiphenyl (PCB-205)	1987
74487-85-7	2,2',3,4',5,6,6'-Heptachlorobiphenyl (PCB-188)	1950
76330-06-8	2,6-Dichlorosyringaldehyde	2994
76341-69-0	2-Chlorosyringaldehyde	2993
76842-07-4	2,3,3',4',5'-Pentachlorobiphenyl (PCB-122)	1800
79127-80-3	Fenoxycarb	3854
83242-22-2	<i>m</i> -tert-Butylphenyl diphenyl phosphate (<i>m</i> -TBPDP)	3139
83242-23-3	<i>o</i> -tert-Butylphenyl diphenyl phosphate (<i>o</i> -TBPDP)	3139
83694-71-7	3,4'-Dibromodiphenyl ether (PBDE-13)	2409
83704-22-7	1,2,3,7-Tetrachlorodibenzofuran	2195
83704-48-7	1,2,3,4,7-Pentachlorodibenzofuran	2209
83704-51-2	1,2,4,7,8-Pentachlorodibenzofuran	2213
83992-69-2	2,2',3,4,4',5,5'-Heptachloro-DPE (PCDE-180)	2392
83992-73-8	2,2',3,3',4,4',5,5',6-Nonachloro-DPE (PCDE-206)	2399

84602-55-1	Nonylphenyl diphenyl phosphate (<i>m</i> -NPDPP).....	3147
84602-56-2	4-Cumylphenyl diphenyl phosphate (CPDPP).....	3145
85918-31-6	2,3,3',4,4'-Pentachloro-DPE (PCDE-105).....	2379
85918-38-3	2,2',3,3',4,4',5,6'-Octachloro-DPE (PCDE-196).....	2397
88467-63-4	2,2',3,4,4',5,6'-Heptachloro-DPE (PCDE-182).....	2394
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93703-48-1	3,3',4,4'-Tetrabromodiphenyl ether (BDE-77).....	2428
94339-59-0	3,3',4,4',5-Pentachloro-DPE (PCDE-126).....	2380
94570-83-9	3,6-Dichlorodibenzofuran.....	2184
104294-16-8	2,2',4,4',6-Pentachloro-DPE (PCDE-100).....	2376
106220-81-9	2,2',4,4',5,6'-Hexachloro-DPE (PCDE-154).....	2388
106220-82-0	2,2',3,3',4,6-Hexachloro-DPE (PCDE-140).....	2385
106220-84-2	2,2',3,4,4',6,6'-Heptachloro-DPE (PCDE-184).....	2395
117948-62-6	2,2',3,3',4,4',6,6'-Octachloro-DPE (PCDE-197).....	2398
131138-20-0	2,3',4,4',5,5'-Hexachloro-DPE (PCDE-167).....	2390
131138-21-1	2,3,3',4,4'-Pentachloro-DPE (PCDE-101).....	2378
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182346-21-0	2,2',3,4,4'-Pentabromodiphenyl ether (PBDE-85).....	2431
182677-30-1	2,2',3,4,4',5-Hexabromodiphenyl ether (PBDE-138).....	2442
189084-59-1	3,4-Dibromodiphenyl ether (PBDE-12).....	2408
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